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HYDRODYNAMIC MODEL WAVEFUNCTIONS IN INTRINSIC COORDINATES AND THEIR APPLICATION TO THE STRUCTURE OF EVEN-EVEN NUCLEI

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Based on a Ph.D. thesis submitted to Iowa State University

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Hydrodynamic model wavefunctions in intrinsic coordinates and their
application to the structure of even-even nuclei

by

Frank James Margetan

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TABLE OF CONTENTS

Abstract	Page
I. INTRODUCTION	vii
II. THE BOHR EIGENFUNCTIONS AND THEIR PROPERTIES	1
A. Review of the Bohr Model	10
B. Construction of the Bohr Eigenfunctions	11
C. Properties of the Bohr Eigenfunctions	19
III. EXPANSION TECHNIQUES	24
A. Notational Conventions	41
B. Matrix Form of the Schroedinger Equation	42
C. The Influence of the Choice of Basis	46
D. E2 Transition Rates and Quadrupole Moments	51
IV. TEST CALCULATIONS USING THE GNEUSS-GREINER HAMILTONIAN	59
A. Preliminary Calculations	75
B. Convergence Calculations for Representative Isotopes	78
C. $\tilde{s}$ -curvature and Error Estimation	87
D. Application of the Error Estimation Methods	104
E. Estimating $\tilde{s}_g$ Without Diagonalizing	113
V. QUADRATIC POTENTIAL MODEL: GENERAL PROPERTIES	121
A. Computational Details	130
B. An Interpretive Framework	135
C. The Identification of Vibrational States [$J = 0$]	144
D. Rotational Band Development	153
E. Characteristics of the Ground State Band	170
	206

	Page
VI. QUADRATIC POTENTIAL MODEL: APPLICATIONS	238
A. ^{106}Pd	246
B. ^{166}Er , ^{182}W , ^{122}Te	260
C. 186 , 188 , 190 , ^{192}Os	270
VII. APPENDIX A: SYMMETRIES IN THE $(\beta, \gamma, \theta_i)$ REPRESENTATION	292
A. Collective Coordinates	292
B. A Symmetry of $\psi_{N\ell\nu\text{JM}}^S(\alpha)$	296
C. Symmetries of $\psi_{N\ell\nu\text{JM}}^S(\beta, \gamma, \theta_i)$	297
D. Symmetries of the γ Probability Density	307
E. Effects of Reflecting $V(\beta, \gamma)$ About $\gamma = 30^\circ$	309
VIII. APPENDIX B: NORMALIZATION OF THE $\psi_{N\ell\nu\text{JM}}(\beta, \gamma, \theta_i)$	318
A. Normalization of $f_{N\ell}(\beta)$	320
B. Normalization of $\phi_{\ell\nu\text{JM}}(\gamma, \theta_i)$	321
C. Computational Methods	326
IX. APPENDIX C: CALCULATIONAL TECHNIQUES IN THE SOLUTION OF $H\phi = E\phi$	335
A. Radial and Angular Matrix Elements	339
B. Transformations Between Expansion Bases	345
C. Preliminary Testing of Computational Techniques	351
D. Splitting of H_B Energies	367
X. APPENDIX D: COMPUTATIONAL TECHNIQUES IN THE CALCULATION OF QUADRUPOLE MOMENTS AND E2 TRANSITION RATES	375
A. Reduced Matrix Elements of Ω^{LAB} Operators	375
B. E2 Selection Rules	380
C. Computational Methods	386
D. Testing of the GAMME and BE2PRO Codes	388

	Page
XI. APPENDIX E: MISCELLANEOUS TABLES	403
XII. APPENDIX F. ANGULAR MOMENTUM CONVENTIONS	436
A. The Active Viewpoint	437
B. Angular Momentum Operators	452
C. Rotation Matrices	459
D. Spherical Harmonics	467
E. Clebsch-Gordon Coefficients	471
F. Irreducible Tensor Operators	477
XIII. BIBLIOGRAPHY	481
XIV. ACKNOWLEDGMENTS	486

Hydrodynamic model wavefunctions in intrinsic coordinates and their application to the structure of even-even nuclei

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A closed expression is presented for intrinsic-coordinate $(\beta, \gamma, \theta_i)$ eigenfunctions of the hydrodynamic, quadrupole-vibration Hamiltonian of A. Bohr. These functions are used as an expansion basis for the treatment of more general collective Hamiltonians. Two classes of such Hamiltonians are considered. In each the potential energy term of the Bohr Hamiltonian, $\frac{1}{2}C\beta^2$, has been replaced with a more general function of the shape coordinates, $V(\beta, \gamma)$. The potential of Gneuss and Greiner (1) is used to demonstrate the soundness of the calculational techniques, and to illustrate convergence properties of calculated energies. Potentials possessing a single minimum on $0 \leq \gamma \leq 60^\circ$ are considered through the study of a quadratic-potential [QP] Hamiltonian having

$$V(\beta, \gamma) = \frac{1}{2}C_\beta(\beta - \beta_0)^2 + C_\gamma(\gamma - \gamma_0)^2.$$

The smooth development from spherical to asymmetrically deformed nuclear shapes is investigated by systematically varying the parameters β_0 and C_γ . Model energies and E2 transition rates are traced during this process. The QP model is then applied to ^{106}Pd , ^{166}Er , ^{182}W , ^{122}Te , and $^{186, 188, 190, 192}\text{Os}$. Low-energy γ vibrations appear to play a prominent role in the latter five nuclei, and the QP model offers a better accounting of experimental spectra than does the model of Davydov and Chaban (2).

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1. G. Gneuss and W. Greiner, Nucl. Phys. A171, 449 (1971).
2. A. S. Davydov and A. A. Chaban, Nucl. Phys. 20, 499 (1960).

I. INTRODUCTION

Since the discovery of the atomic nucleus and the subsequent identification of the neutron and proton as its primary constituents, a longstanding goal has been that of deducing nuclear properties from those of these constituents. Unfortunately a typical nucleus, being composed of many nucleons, possesses several hundred degrees of freedom that may be specified in a variety of ways. It is the hope of the theorist that a proper method of specification will leave him with only a handful of coordinates that need be actively considered. In independent-particle models such a partitioning of the degrees of freedom may arise naturally as mutual interactions force the majority of nucleons to group themselves into closed shells. For the purposes of low energy structure calculations, such an "inert" core of nucleons may be either neglected entirely or specified by only a few coordinates that represent its general features. Nucleons outside of the core, on the other hand, must be followed in more detail. Such calculations become increasingly unruly as we stray farther from the closed shell nuclei and the number of active particles rises. In such circumstances it may be more instructive to focus ones attention upon the gross properties of the nuclear "fluid", and to choose the active degrees of freedom accordingly.

The discovery of nuclear fission in 1939 (1) and its subsequent interpretation (2) in terms of the surface and Coulomb energies of a deformed, charged liquid droplet, indicated that individual nucleons were capable of taking part in large scale cooperative phenomena. As

experimental techniques were refined, evidence for low-energy collective behavior began to accumulate¹, particularly in nuclei far removed from shell closures. Anomalously large quadrupole moments and electric quadrupole transition rates were observed. The low-energy spectra of many nuclei were found to contain sequences of levels resembling the rotational and vibrational bands known to occur in the excitations of molecules. Such discoveries emphasized the importance of taking the nuclear collective degrees of freedom into direct account.

A. Bohr (4) recognized that collective coordinates, used to specify the shape and orientation of the nuclear surface, could be treated as dynamical variables. In particular he studied the lowest order (quadrupole) surface vibrations of a liquid droplet about a spherical equilibrium shape, introducing the intrinsic coordinates $(\beta, \gamma, \theta_i)$ as a means to specify an arbitrary quadrupole surface. The three Euler angles, θ_i , serve to orient a set of body-fixed (BF) principal axes within the nuclear droplet, while β and γ describe the appearance of the surface to a BF observer. β is a measure of the overall deformation from sphericity, and the angle γ describes the rotational asymmetry about the BF z-axis. (The nature of quadrupole deformation, and the meanings of the coordinates β and γ , are illustrated by the figures of Appendix A.) Assuming the irrotational flowing of an incompressible nuclear fluid, Bohr developed a quadrupole vibration Hamiltonian and obtained its operator form in the intrinsic coordinate representation:

¹See for example Chapter 1 of the text by Eisenberg and Greiner (3) for an accounting of the empirical data.

$$H_B = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + \frac{1}{2}C\beta^2 \quad (1.1)$$

The two terms on the right hand side of Equation (1.1) represent respectively the kinetic and potential energies of the droplet. The latter possesses a minimum for a spherical ($\beta = 0$) shape. B and C are constants which depend upon the nature of the fluid.

H_B possesses a highly degenerate energy spectrum, and its underlying assumptions are evidently too restrictive to adequately account for observed low-energy nuclear excitations. However it has served as a starting point for a variety of collective models which seek to describe the positive parity states of even-even nuclei¹. Marty (7, 8) and later Davydov and Filippov (9) investigated the case of a triaxially deformed rotor in which β and γ are treated as fixed parameters. The model enjoyed considerable success in accounting for low-energy spectra of nuclei having $150 \lesssim A \lesssim 190$ or $A \gtrsim 220$. However systematic deviations from theory lead Davydov and Chaban (10) to partially relax the rigidity constraint, allowing vibrations in the β coordinate in addition to the rotations. Again γ was considered to be fixed, and the potential energy function in H_B was replaced by

$$\frac{1}{2}C(\beta - \beta_0)^2$$

to allow a non-spherical equilibrium shape. In a series of papers culminating with (11), A. Faessler et al. treated both β and γ as dynamical

¹The text (5) and article (6) by Davidson review these developments.

variables, and investigated the Bohr-like Hamiltonian having

$$\frac{1}{2}C_{\beta}(\beta - \beta_0)^2 + \frac{1}{2}C_{\gamma}(\gamma)^2$$

as its potential energy term. These authors showed that a triaxially deformed core (i.e., one in which the equilibrium value of γ is not zero) was not essential in achieving a good fit to the experimental data.

My own involvement in collective physics was triggered by difficulties in the theoretical interpretation of certain excited states of ^{106}Pd . Gamma-ray coincidence and angular correlation measurements enabled Hsue, Hsu, Wohn, Western and Williams (12) to deduce the experimental spectrum shown in Figure 1.1. These authors employed two models in an effort to interpret the spectrum: the anharmonic vibrational model of Brink, de Toledo Piza, and Kerman (13); and the Davydov-Chaban model (10) referred to earlier. The use of the first was motivated by the appearance of a nearly degenerate $0^+2^+4^+$ triplet at approximately twice the energy of the first 2^+ level. Such is often the signature of a quadrupole vibrator; H_B possesses such a spectrum with an exactly degenerate triplet. In the model of Brink et al., small anharmonic terms are added to H_B to remove the degeneracies. A typical spectrum of the Davydov-Chaban Hamiltonian, on the other hand, may be viewed as a series of rotational bands, each based upon a "breathing mode" or β -vibrational excitation of the deformed nuclear droplet. The purely vibrational states have angular momentum $J = 0$, and are labeled by the integers $n = 1, 2, 3, \dots$. Associated with each is an asymmetric rotor

Figure 1.1. Low-energy, positive-parity states in ^{106}Pd [from Reference 12]

spectrum having $(J+2)/2$ (J even) or $(J-1)/2$ (J odd) states for each value of angular momentum. States of like spin and β -vibrational character are enumerated by $N = 1, 2, 3, \dots$ in order of increasing energy. The Davydov-Chaban Hamiltonian contains four adjustable parameters: B and C pertain to the density and elastic properties of the nuclear fluid, as in H_B ; β_0 and $\gamma = \gamma_0$ describe the equilibrium deformation. Three combinations of these parameters may be determined by fitting the model to experimental energies and/or ratios of E2 transition rates. These are

$$\gamma_0 \quad ; \quad \hbar\omega = \hbar \left[\frac{C}{B} \right]^{\frac{1}{2}} \quad ; \quad \text{and} \quad \mu = \frac{1}{\beta_0} \left[\frac{\hbar^2}{BC} \right]^{\frac{1}{2}} \quad (1.2)$$

$\hbar\omega$ is an overall energy scale factor, while μ is a measure of the stiffness of the β -vibrator against centrifugal stretching. In the limit $\mu \rightarrow 0$, the rotations and vibrations of the Davydov-Chaban model are completely decoupled. The fourth parameter, β_0 itself, may be determined from absolute E2 transition rates.

The authors of (12) concluded that the available experimental evidence strongly supported a rotor-vibrator interpretation as opposed to that of the anharmonic spherical vibrator model. However it was not possible to account for entire low-energy spectrum of ^{106}Pd with a single application of the Davydov-Chaban model. Rather, three similar Davydov-Chaban spectra (S_1 , S_2 , and S_3 in Figure 1.1) were identified, based upon $J = 0$ levels at 0, 1134, and 1706 KeV. Dr. S. A. Williams suggested that the latter two levels may be associated with vibrations of the asymmetry coordinate γ about its equilibrium value, a degree of freedom

that is neglected in the Davydov-Chaban treatment. A careful treatment of the quadratic potential Hamiltonian

$$H_{QP} = -\frac{\hbar^2}{2B} T(\beta, \gamma, \theta_i) + \frac{1}{2}C_\beta(\beta - \beta_0)^2 + \frac{1}{2}C_\gamma(\gamma - \gamma_0)^2 \quad (1.3)$$

was clearly warranted.

Davydov (14) had considered such a Hamiltonian earlier, but had made use of several approximations in separating variables and solving the resulting differential equations. Subsequent investigations by S. Williams, W. Western, A. Gregerson and myself indicated that these approximations might have a major impact upon the solutions in the case of ^{106}Pd , and a more reliable technique was sought. One reasonable approach involved the diagonalization of H_{QP} in a large basis of H_B eigenfunctions,

$$H_B \psi_\alpha(\beta, \gamma, \theta_i) = E_\alpha \psi_\alpha(\beta, \gamma, \theta_i) \quad (1.4)$$

Unfortunately, a closed expression for the ψ_α in an angular momentum basis was not available; although several contributions had been made in that direction (15-19). However Dr. Williams noted that the underlying group-theoretical problem which prevented the attainment of such an expression had been solved by N. Kemmer, D. Pursey, and himself some years earlier (20, 21). This realization lead to a closed formula for the $\psi_\alpha(\beta, \gamma, \theta_i)$ as reported in (22) by T. Corrigan, F. Margetan, and S. Williams. A path was then opened for the study of the spectra and eigenfunctions of H_{QP} ; furthermore, calculational errors could be judged from the effects of shrinking or enlarging the expansion basis. The results of such a study are contained within this thesis.

In the following chapter the quadrupole surface vibration model of A. Bohr is reviewed, and properties of the ψ_α are discussed. The mathematical details of the expansion technique used in treating generalized versions of H_B are the subjects of Chapter III. In the course of testing the accompanying computational methods, it was discovered that several other authors (23-28) had previously employed expansion techniques to obtain the eigenfunctions of Bohr-like Hamiltonians. Though the details of their treatments differed from my own, these works provided a fertile testing ground for the refinement of my procedures. Initial test calculations are described in Appendix C, and Chapter IV is devoted to my attempts to duplicate the calculations of Habs et al. (29, 30) which employ a form of the collective Hamiltonian of Gneuss and Greiner (26). Insight is gained into the importance of the choice of expansion basis in a realistic setting, and methods of selecting an optimal basis are discussed. A procedure for estimating the sizes of calculational errors is also presented in Chapter IV.

Having concluded with these preliminary topics, the quadratic potential Hamiltonian is considered in Chapter V. The development of rotational bands is traced as H_{QP} is systematically evolved from H_B , and β and γ -vibrational states are identified. The dependence of the low energy spectrum upon the parameters of H_{QP} is investigated, and trends in electric quadrupole transition rates are described. In the final chapter, the quadratic potential model is applied to several even-even nuclei with particular attention being paid to ^{106}Pd . It is shown that

no choice of the Hamiltonian constants can result in a theoretical spectrum which resembles that of Figure 1.1 and has a γ -vibrational band head near 1134 KeV. The applicability of the model to both deformed and near-spherical nuclei is indicated by a brief examination of the spectra of ^{122}Te , ^{166}Er and ^{182}W . The osmium isotopes ^{186}Os , ^{188}Os , ^{190}Os and ^{192}Os are treated in detail.

An effort has been made to specify all model calculations in a manner that permits their precise duplication by future investigators. Many of the computational details, tables, and derivations of secondary importance have been relegated to the appendices, so as to keep the main text relatively uncluttered. As several of the chapters are quite lengthy, I have adopted the policy of beginning each chapter with a brief survey of its contents. This has also been done for the longer appendices. The angular momentum conventions employed throughout this thesis for Euler angles, rotation matrices, tensor operators, Clebsch-Gordon coefficients, spherical harmonics, and the form of the Wigner-Eckart theorem are those of Rose (31). Several of the more important formulae from that reference have been collected into the final appendix.

II. THE BOHR EIGENFUNCTIONS AND THEIR PROPERTIES

In this chapter the quadrupole surface vibration model, introduced by Aage Bohr in 1952 (4), is summarized and the intrinsic coordinate eigenfunctions of the model Hamiltonian are presented and discussed. In the initial section, the assumptions leading to the Bohr Hamiltonian are briefly reviewed, and the quantized Hamiltonian is displayed in several representations, including that of the intrinsic coordinates $(\beta, \gamma, \theta_i)$. [The Bohr model has been extensively reviewed in the literature, and the summary presented here has drawn heavily on the treatments contained in (3) and (5). The reader is referred to these texts and to the original paper (4) for proofs of the assertions given in Section A.] Section B describes the procedure used to obtain a closed expression for the eigenfunctions $\psi(\beta, \gamma, \theta_i)$. The mathematical details have been published elsewhere (22) and will not be repeated here. [References (32-37) are excellent sources for the group-theoretical concepts assumed in (22) and in Section B of this chapter.] The expression for the general eigenfunction, $\psi_{N\&\nu JM}(\beta, \gamma, \theta_i)$, is examined in the final section. Ranges of the quantum numbers, normalization, symmetries and parity are all considered. Shape-coordinate probability distributions are defined and displayed graphically for selected low-energy states. Their role in first-order perturbative calculations is the final topic of Section C.

A. Review of the Bohr Model

Ignoring structural details, we begin by visualizing the atomic nucleus as a homogeneous liquid droplet. Its classical configuration will be assumed to be completely determined by a specification of the nuclear surface. The latter may be conveniently given by expanding the surface in spherical harmonics, $Y_{\lambda\mu}$, and using the accompanying expansion coefficients, $\alpha_{\lambda\mu}$, as measures of the deviations from sphericity. In terms of spherical polar coordinates (R, θ, ϕ) measured with respect to a set of right-handed cartesian laboratory (LAB) axes, we write

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}^*(\theta, \phi) \right] \quad ; \quad \begin{array}{l} \lambda = 0, 1, 2, \dots \\ \mu = -\lambda, -\lambda+1, \dots, \lambda \end{array}$$

It is understood that R represents the radial distance to the surface along a ray specified by (θ, ϕ) . Changes in the coordinates α_{00} and $\alpha_{1\mu}$ can be shown to correspond to changes in the nuclear volume and center of mass (CM) respectively. If we position the LAB origin at the CM of a constant volume droplet, then quadrupole coordinates ($\lambda = 2$) become the lowest ones of interest. Confining our attention to these degrees of freedom, we may suppress the λ index and write

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\mu=-2}^2 \alpha_{\mu} Y_{2\mu}^*(\theta, \phi) \right] \quad . \quad (2.1)$$

The Bohr coordinates $(\beta, \gamma, \theta_i)$ may be introduced by describing the nuclear surface as it appears to an observer in a principal-axis, body-fixed (BF) frame. Again we write

$$R(\theta', \phi') = R_0 \left[1 + \sum_{\mu=-2}^2 a_{\mu} Y_{2\mu}^*(\theta', \phi') \right] , \quad (2.2)$$

where (θ', ϕ') are measured from the right-handed BF axes. The two sets of surface coordinates are related through the $J = 2$ rotation matrix

$$a_{\nu} = \sum_{\mu} D_{\mu\nu}^2(\theta_i) \alpha_{\mu} . \quad (2.3)$$

In Equation (2.3) $\theta_i = (\theta_1, \theta_2, \theta_3)$ are the LAB Euler angles parameterizing the active rotation

$$R(\theta_i): \text{ LAB} \rightarrow \text{BF}$$

which takes the LAB axes into coincidence with the BF ones. The reality of the nuclear surface is assured by demanding

$$\alpha_{\mu}^* = (-1)^{\mu} \alpha_{-\mu} ; \quad a_{\mu}^* = (-1)^{\mu} a_{-\mu} . \quad (2.4)$$

The nuclear surface is thus seen to be specified by five real numbers and hence possesses five independent degrees of freedom. We may require that the BF axes be principal axes for the droplet by insisting that the surface coordinates in Equation (2.2) satisfy

$$\begin{aligned} a_1 &= a_{-1} = 0 , \\ a_2 &= a_{-2} \text{ (real)} , \\ a_0 &\text{ (real)} . \end{aligned} \quad (2.5)$$

A quadrupole surface, as viewed from a principal axis frame, is completely specified by only two real numbers, a_0 and a_2 . Equivalently we may use

the deformation and asymmetry parameters, β and γ , defined by

$$\begin{aligned} a_0 &= \beta \cos \gamma, & 0 \leq \beta < \infty, \\ a_2 &= \frac{\beta}{\sqrt{2}} \sin \gamma, & 0 \leq \gamma \leq 2\pi. \end{aligned} \quad (2.6)$$

The radial-like coordinate $\beta = \sum_{\mu} \alpha_{\mu}^* \alpha_{\mu}$ is a measure of the overall deformation, while γ specifies the asymmetry of the surface about the BF z-axis. The $\beta = 0$ surface is a sphere, independent of the value of γ ; for $\gamma = 0$, the surface is axially symmetric about z_{BF} for all values of β . β , γ and the three Euler angles comprise the five intrinsic or Bohr coordinates.

For small oscillations about a spherical equilibrium shape, the classical Hamiltonian is expected to be of the form

$$H = T + V = \frac{1}{2} \sum_{\mu} B_{\mu} |\dot{\alpha}_{\mu}|^2 + \frac{1}{2} \sum_{\mu} C_{\mu} |\alpha_{\mu}|^2; \quad \dot{\alpha}_{\mu} = \frac{d\alpha_{\mu}}{dt}. \quad (2.7)$$

The constants B_{μ} and C_{μ} will depend upon the details of the model employed. In the case of the Bohr model, a nuclear fluid of constant mass and charge density is assumed to undergo irrotational flow: the velocity field, $\underline{v}(\underline{r})$, of nuclear matter within the droplet obeys

$$\begin{aligned} \nabla \times \underline{v} &= 0, \\ \nabla \cdot \underline{v} &= 0, \end{aligned}$$

and may be expressed as the gradient of a scalar function satisfying Laplace's equation. This equation may be solved subject to the boundary condition that the normal component of $\underline{v}$ vanishes at the nuclear surface.

The kinetic energy may then be found in terms of the α_μ and their associated generalized velocities, $\dot{\alpha}_\mu$. The potential energy is assumed to arise from electrostatic repulsion and surface tension effects. When the classical Hamiltonian is so calculated we find, to lowest order in the coordinates and velocities,

$$H_B = \frac{B}{2} \sum_{\mu} (-1)^{\mu} \dot{\alpha}_{\mu} \dot{\alpha}_{-\mu} + \frac{C}{2} \sum_{\mu} (-1)^{\mu} \alpha_{\mu} \alpha_{-\mu}, \quad (2.8)$$

or equivalently

$$H_B = \frac{1}{2B} \sum_{\mu} (-1)^{\mu} \Pi^{\mu} \Pi^{-\mu} + \frac{C}{2} \sum_{\mu} (-1)^{\mu} \alpha_{\mu} \alpha_{-\mu}, \quad (2.9)$$

where the generalized momenta $\Pi^{\mu} = \frac{\partial T}{\partial \dot{\alpha}_{\mu}}$ have been used. The two model constants B and C depend upon the size, mass, charge and surface tension of the droplet. They have units of [Energy · Time²] and [Energy] respectively.

The classical system may be quantized by replacing the generalized coordinates and momenta with operators satisfying the usual commutation relations. Some care must be taken as the α_{μ} are not real coordinates and their operator counterparts are non-Hermitian. Figure 2.1 contains the commutation relations which result for this α - Π operator representation, and illustrates the manner in which we may transform to three other useful representations. In the intrinsic coordinate representation the Hamiltonian assumes the form

$$H_B = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + \frac{C}{2} \beta^2 \quad (2.10)$$

Figure 2.1. Appearance of H_B in several representations. The operators α_{μ} , Π_{μ} , b_{μ}^{+} and b_{μ} are non-Hermitian. If $\dagger$ denotes Hermitian conjugation, then $(\alpha_{\mu})^{\dagger} = (-1)^{\mu} \alpha_{-\mu}$, $(\Pi^{\mu})^{\dagger} = (-1)^{\mu} \Pi^{-\mu}$, and $(b_{\mu}^{+})^{\dagger} = (-1)^{\mu} b_{-\mu}$.

where T is the differential operator

$$T(\beta, \gamma, \theta_i) = \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} - \frac{1}{4\beta^2} \sum_{k=1}^3 \frac{L_k^2}{\sin^2[\gamma - \frac{2\pi}{3}k]} . \quad (2.11)$$

The L_k appearing in Equation (2.11) are the (dimensionless) body frame components of the angular momentum operator¹ and are realized as functions of the θ_i and their partial derivatives. Their specific form will not be required here. The intrinsic coordinate eigenfunctions $\psi^{BC}(\beta, \gamma, \theta_i)$ are solutions to the Schroedinger equation

$$H_B \psi^{BC}(\beta, \gamma, \theta_i) = E \psi^{BC}(\beta, \gamma, \theta_i) . \quad (2.12)$$

As we shall see shortly, five lower labels N, ℓ, v, J and M will be required to distinguish the states of good angular momentum. The upper labels, B and C , are the values of the physical parameters appearing in H_B . The interpretation given such an eigenfunction (representing a nuclear state) is:

$$|\psi^{BC}(\beta, \gamma, \theta_i)|^2 d\Omega(\beta, \gamma, \theta_i) \propto \begin{array}{l} \text{probability that a measure-} \\ \text{ment made of the nuclear} \\ \text{surface finds } \beta, \gamma, \text{ and the} \\ \theta_i \text{ to be in the ranges} \\ [\beta, \beta+d\beta], [\gamma, \gamma+d\gamma], \\ [\theta_i, \theta_i+d\theta_i] \text{ respectively} \\ (i = 1, 2, 3). \end{array} \quad (2.13)$$

The appropriate volume element in Equation (2.13) is found to be

$$d\Omega(\beta, \gamma, \theta_i) = \beta^4 |\sin 3\gamma| \frac{\sin \theta_2}{8\pi^2} d\beta d\gamma d\theta_1 d\theta_2 d\theta_3 , \quad (2.14)$$

¹ LAB components are denoted by $(J_1, J_2, J_3) = (J_x, J_y, J_z)$; hence $J^2 = L^2$.

and collective coordinates range over the region

$$\begin{aligned} \Omega(\beta, \gamma, \theta_i): \quad & 0 \leq \beta < \infty \\ & 0 \leq \gamma \leq 2\pi \\ & 0 \leq \theta_1 \leq 2\pi \\ & 0 \leq \theta_2 \leq \pi \\ & 0 \leq \theta_3 \leq 2\pi \end{aligned} \quad (2.15)$$

The operator $T(\beta, \gamma, \theta_i)$ has the useful property that under scaling transformations of the β variable, the functional form of the operator is preserved to within a factor. In particular, if $\beta' = s\beta$ (s a constant), then reexpressing T in terms of the new variable gives

$$T(\beta, \gamma, \theta_i) = s^2 T(\beta', \gamma, \theta_i) \quad (2.16)$$

The result is helpful when passing from liquid-drop problems with units to those without, and vice versa. By an appropriate choice of s we may transform the Schroedinger Equation (2.12) into a standard reduced (SR) form in which the two physical constants no longer appear. Solutions of the SR problem are associated with solutions of the original equation. The connection is depicted in Figure 2.2. The symbol ψ will be used exclusively to denote eigenfunctions of the Bohr Hamiltonian. When lower but no upper labels appear, the eigenfunctions are assumed to be those of the standard reduced form, H_B^I :

$$H_B^I(\beta', \gamma, \theta_i) = -\frac{1}{2}T(\beta', \gamma, \theta_i) + \frac{1}{2}(\beta')^2 \quad (2.17)$$

FORM WITH UNITS

$$H_B \psi^{BC}(\beta, \gamma, \theta_i) = E \psi^{BC}(\beta, \gamma, \theta_i)$$

$$H_B = -\frac{\hbar^2}{2B} T(\beta, \gamma, \theta_i) + \frac{C}{2} \beta^2$$

Coordinates range over

$\Omega(\beta, \gamma, \theta_i)$ of Equation (2.15).

Normalized eigenfunctions obey

$$1 = \int_{\Omega(\beta, \gamma, \theta_i)} |\psi^{BC}(\beta, \gamma, \theta_i)|^2 d\Omega(\beta, \gamma, \theta_i) \dots [C].$$

Change variables to

$$\beta' = s\beta,$$

and divide the
Schroedinger equation
by $\hbar\omega$:

$$s = \left[\frac{BC}{\hbar^2} \right]^{1/2}; \quad \omega = \sqrt{\frac{C}{B}}.$$

STANDARD REDUCED FORM

$$H'_B \psi(\beta', \gamma, \theta_i) = E' \psi(\beta', \gamma, \theta_i)$$

$$H'_B = -\frac{1}{2} T(\beta', \gamma, \theta_i) + \frac{1}{2} \beta'^2$$

Coordinates range over

$\Omega(\beta', \gamma, \theta_i)$ of Equation (2.15)

with β' written in place of β .

Normalized eigenfunctions obey

$$1 = \int_{\Omega(\beta', \gamma, \theta_i)} |\psi(\beta', \gamma, \theta_i)|^2 d\Omega(\beta', \gamma, \theta_i) \dots [C'].$$

Solutions are connected by:

$$H_B = \hbar\omega H'_B,$$

$$E = \hbar\omega E',$$

$$\psi^{BC}(\beta, \gamma, \theta_i) = s^{5/2} \psi(s\beta, \gamma, \theta_i).$$

$$\psi^{BC} \text{ obeys } [C] \text{ if } \psi \text{ obeys } [C'].$$

Figure 2.2. Connection between original and SR forms of the Bohr liquid-drop problem

B. Construction of the Bohr Eigenfunctions

The Bohr Hamiltonian H_B commutes with J^2 and J_z , the square of the total angular momentum operator and the z-component respectively. It is therefore possible to construct eigenstates of H_B which are simultaneously eigenstates of J^2 and J_z . We will now briefly take up the problem of labeling and constructing all such normalizable states. Furthermore we desire their form in the Bohr coordinate representation.

Initially we work in the creation/destruction operator representation defined in Figure 2.1. From the commutation relations of H_B^I with the b^+ and b , we deduce that eigenstates of H_B^I may be built by applying a succession of creation operators upon an angular momentum zero vacuum state:

$$b_{\mu_1}^+ b_{\mu_2}^+ \dots b_{\mu_N}^+ |0\rangle \quad (\text{N phonon state}) \quad (2.18a)$$

The vacuum state $|0\rangle$ is defined by its property of being rendered zero by the action of any destruction operator:

$$b_{\mu} |0\rangle = 0 \quad \mu = 2, 1, \dots, -2 \quad (2.18b)$$

From the known transformation properties of the α_{μ} under rotations, we may deduce those of b , b^+ and of the states (2.18a). For example $b_{\mu}^+ |0\rangle$ may be shown to be an eigenstate of J^2 and J_z , with eigenvalues $2(2+1)\hbar^2$ and $\mu\hbar$ respectively. Any one of the b_{μ}^+ is then said to create a phonon of angular momentum two. The state (2.18a) consists of N such phonons.

Each of the twenty-five operators $A_{\mu\nu} = b_{\mu}^+ b_{\nu}$ commutes with H_B^I .

Together they generate the continuous group $U(5)$, the maximal symmetry group of the Bohr Hamiltonian. Thus the degenerate eigenfunctions of H_B^I will form a basis for an irreducible representation (IR) of $U(5)$. Because of the symmetry of expression (2.18a) under the interchange of subscripts, only the so-called symmetric representations of $U(5)$ will be involved. These may be labeled by the single quantum number N which counts the number of creation operators acting upon $|0\rangle$. Equivalently N is the eigenvalue of the $U(5)$ Casimir operator

$$C_{U(5)}^I = \sum_{\mu} (-1)^{\mu} b_{\mu}^{+} b_{-\mu} = H_B^I - \frac{5}{2} \quad (2.19)$$

Eigenstates belonging to the $[N]$ symmetric IR of $U(5)$ require four additional labels to distinguish them. $U(5)$ contains two chains of nested subgroups

$$\begin{aligned} U(5) &\supset R(5) \supset \text{Physical } R(3) && \text{(Physical Chain)} \\ U(5) &\supset R(5) \supset R(4) \sim SU(2) \times SU(2) && \text{(Natural Chain)} \end{aligned} \quad (2.20)$$

either of which may be used to provide a labeling scheme. To do this we choose to span $[N]$ with states which are simultaneous eigenfunctions of a mutually commuting set of operators constructed from the $A_{\mu\nu}$. This set, S , consists of

- (1) the Casimir operators (C_G^i , $i = 1, 2, \dots$) of each subgroup (G) in the chain, and
- (2) the largest set of mutually commuting generators $\{H_1, H_2, \dots\}$ of the right-most subgroup in the chain.

The states may then be labeled by the eigenvalues of these operators. This method works well for the natural chain and supplies a complete set of labels for enumerating the states of $[N]$. The operators comprising S may be built, and simultaneous eigenstates of the form (2.18a) may be identified. Unfortunately, such states are not eigenstates of J^2 which is proportional to the single independent Casimir operator of the physical $R(3)$ subgroup.

When the physical chain is used in the labeling method, S may be taken to be

$$S: \{C_{U(5)}^1, C_{R(5)}^1, J^2 \propto C_{R(3)}^1, J_z \propto H_1\}.$$

The eigenvalues of S are in one-to-one correspondence with the integers N , λ , J , and M respectively. They do not uniquely specify a state belonging to the $[N]$ IR of $U(5)$, as two or more distinct states may possess the same four eigenvalues. An inherent difficulty arises: when the states that span a single symmetric IR of $R(5)$ are grouped into sets which transform among one another under spatial rotations, two or more sets may be found which transform in the same way (i.e., according to the same IR of $R(3)$). An additional label ν is required to distinguish such sets. One could attempt to enlarge S with a fifth operator whose eigenvalue would supply the missing label. A different approach is taken in (22). There, basis functions for the physical chain, $|N\lambda\nu JM\rangle$, are projected from selected "intrinsic" states, $|N\lambda\nu\rangle$, belonging to the natural chain basis:

$$|N\ell v JM\rangle = \int d\Omega D_{M, \ell-3v}^{J*}(\Omega) R(\Omega) |N\ell v\rangle \quad (2.21)$$

$R(\Omega)$ is an active rotation operator, and the integration is over all rotations (Ω) . For fixed ℓ , the integer v runs over the range

$$v = 0, 1, 2, \dots, [\ell/3]_{G1}$$

where $[x]_{G1}$ designates the greatest integer $\leq x$. The intrinsic states may be identified by their eigenvalues to be

$$|N\ell v\rangle = \{[b^+ b^+]_{00}\}^{\frac{N-\ell}{2}} (b_{-2}^+)^v (b_1^+)^{\ell-v} |0\rangle \quad (2.22)$$

in the creation/destruction operator representation, where the notation

$$[b^+ b^+]_{JM} = \sum_{\mu\nu} C(22J; \mu\nu M) b_{\mu}^+ b_{\nu}^+ \quad (2.23)$$

has been employed. The projected states of Equation (2.21) are shown to properly span the $[N]$ IR of $U(5)$; hence, the integral label v completely resolves the $R(5) \supset R(3)$ multiplicity difficulty.

Our original problem of spanning the space of degenerate eigenstates of H_B with states of good angular momentum is now solved in principle. It remains only to translate Equations (2.18b), (2.21), and (2.22) into the intrinsic coordinate representation. The vacuum state eigenfunction becomes

$$\langle \beta', \gamma, \theta_i | 0 \rangle = e^{-\frac{1}{2} \sum_{\mu} \alpha_{\mu}^* \alpha_{\mu}} = e^{-\frac{1}{2} \beta'^2} \quad (2.24)$$

and the normalized eigenfunctions of the standard reduced problem are

found to possess the factored form

$$\psi_{N\ell\nu JM}(\beta', \gamma, \theta_i) = f_{N\ell}(\beta') \phi_{\ell\nu JM}(\gamma, \theta_i) \quad (2.25)$$

The radial and angular terms are given respectively by

$$f_{N\ell}(\beta') = \eta_{N\ell} \beta'^{\ell} e^{-\frac{1}{2}\beta'^2} {}_1F_1(-n; \alpha; \beta'^2) \quad (2.26)$$

$$n = \frac{N-\ell}{2}, \quad \alpha = \ell + \frac{5}{2};$$

and

$$\phi_{\ell\nu JM}(\gamma, \theta_i) = \eta_{\ell\nu J} \sum_{\substack{K \geq 0 \\ \text{even}}}^J g_{\ell\nu JK}(\gamma) \frac{D_{M,K}^{J*}(\theta_i) + (-1)^J D_{M,-K}^{J*}(\theta_i)}{(1 + \delta_{K,0})}, \quad (2.27)$$

$$g_{\ell\nu JK}(\gamma) = (\cos \gamma)^{\ell} \sum_{\sigma=0}^{\sigma_{\max}} A_{\sigma}(\ell\nu JK) (\tan \gamma)^{2\sigma + \frac{1}{2}K} \quad (2.28)$$

A closed form expression for the coefficients $A_{\sigma}(\ell\nu JK)$, derived in Reference (22), is given by Equations (B.15) and (B.16). $\eta_{N\ell}$ and $\eta_{\ell\nu J}$ are normalization coefficients which are chosen to insure that Equation (C') of Figure 2.2 is satisfied. As discussed in Appendix B, the radial and angular factors of $\psi_{N\ell\nu JM}$ may be separately normalized. If $\eta_{\ell\nu J}$ is absorbed by the A-coefficient in Equation (2.28), the angular factor can be written

$$\phi_{\ell\nu JM}(\gamma, \theta_i) = \sum_{\substack{K \geq 0 \\ \text{even}}}^J g_{\ell\nu JK}^{\eta}(\gamma) \frac{D_{M,K}^{J*}(\theta_i) + (-1)^J D_{M,-K}^{J*}(\theta_i)}{(1 + \delta_{K,0})} \quad (2.29)$$

$$g_{\ell\nu JK}^{\eta}(\gamma) = (\cos \gamma)^{\ell} \sum_{\sigma=0}^{\sigma_{\max}} A_{\sigma}^{\eta}(\ell\nu JK) (\tan \gamma)^{2\sigma+\frac{1}{2}K} \quad (2.30)$$

The calculation of the normalized A-coefficients, A^{η} , and the upper limit on the summation over σ are described in Appendix B.

C. Properties of the Bohr Eigenfunctions

The ranges of the quantum numbers N , ℓ , ν , J , and M follow from the group-theoretical meaning given them in the derivation of Reference (22). N , the number of phonon excitations above the ground state, labels the $U(5)$ symmetric IR to which ψ belongs:

$$N = 0, 1, 2, \dots \quad (2.31)$$

For $N = 0$ the IR is one-dimensional and the corresponding Bohr eigenfunction is just the properly normalized vacuum state of Equation (2.24). Because of the similarity between H_B^1 and the $U(5)$ Casimir operator [Equation (2.19)], distinct states with the same N quantum number are degenerate in energy. In particular we have

$$\begin{aligned} H_B^1 \psi_{N\ell\nu JM}(\beta', \gamma, \theta_i) &= (N + \frac{5}{2}) \psi_{N\ell\nu JM}(\beta', \gamma, \theta_i) \\ H_B^1 &= -\frac{1}{2}T(\beta', \gamma, \theta_i) + \frac{1}{2}\beta'^2 \end{aligned} \quad (2.32)$$

If we confine our attention only to transformation properties under the operations of the $R(5)$ subgroup, the states of the $[N]$ IR of $U(5)$ may be decomposed into a direct sum of symmetric $R(5)$ multiplets according to the simple rule

$$[N]_{U(5)} = [N]_{R(5)} \oplus [N-2]_{R(5)} \oplus \dots \oplus \begin{matrix} [0]_{R(5)} \\ [1]_{R(5)} \end{matrix} \quad \text{or} \quad .$$

Hence for fixed N , the ℓ quantum number, which labels the $R(5)$ content of ψ , may range over

$$\ell = N, N-2, \dots, 0 \text{ or } 1 \quad . \quad (2.33)$$

When we restrict our attention to transformation properties under physical rotations, further decomposition is complicated by the $R(5) \supset R(3)$ multiplicity problem. As stated in (22), the rule for the angular momentum content of the $[\ell]_{R(5)}$ IR is as follows.

For each value of ℓ , the empirical quantum number ranges over

$$v = 0, 1, 2, \dots, [\ell/3]_{G_1} \quad . \quad (2.34)$$

For each (ℓ, v) pair, the allowed values of angular momentum are

$$J = 2k, 2k-2, 2k-3, \dots, k \quad ; \quad k = \ell - 3v \quad . \quad (2.35)$$

For each value of J , the projection M may be anyone of

$$M = -J, -J+1, \dots, J \quad . \quad (2.36)$$

The energy spectrum of H_B^1 may be quickly deduced from Equations (2.31)-(2.36). Figure 2.3 illustrates the low energy portion of the highly degenerate spectrum. Notice that $J = 2k-1$ does not occur in Equation (2.35), and subsequently there are no states of angular momentum 1. $J = 0$ states may only occur for $k = 0$, i.e., for

$$(\ell, v) = (0, 0), (3, 1), (6, 2), \dots \quad .$$

LOW ENERGY SPECTRUM OF H_B' .
 N runs vertically.
 J is labeled directly above each level.

Figure 2.3. Quantum numbers ($N \setminus v \setminus J$) and absolute energies for low-lying eigenstates of H_B' .

The v label is then never required to distinguish states having the same values of N , ℓ , and $J = 0$. This is also the case for $J = 2, 3, 4, 5$, and 7 ; however, it is not true in general. For example $(6, 0)$ and $(6, 1)$ each give rise to $J = 6$. The possible angular momenta occurring for each value of ℓ may be deduced from Equations (2.34) and (2.35). For $\ell \leq 10$, they are listed in Table 2.1. When the superscript p is attached to J , that value of J occurs p times in the angular momentum decomposition of the $[\ell]$ symmetric IR of $R(5)$. The label v is then required to resolve the multiplicity. The complexity of the decomposition and the degree of multiplicity grow with increasing ℓ . For $\ell < 6$, the label v is seen to be redundant.

The total number of states of the form $\psi_{N\ell v J, M=J}$ for which the principal quantum number obeys $N \leq N_{\max}$ is given in Table 2.2 for several values of J and $N_{\max}$. The normalized A-coefficients of Equation (2.30) have been calculated only for the states described in Table 2.3. For a given value of J , all states having $N \leq N_{\max}(J)$ have been determined. These states comprise the maximal expansion basis that may be employed in the calculations of the later chapters.

Of the five quantum numbers which label ψ , only v is not associated with the eigenvalue of an Hermitian operator. The normalized eigenfunctions must therefore possess the orthogonality property:

$$\int_{\Omega} d\Omega \psi_{N\ell v J M}^* \psi_{N'\ell'v'J'M'} = \delta_{NN'} \delta_{\ell\ell'} \delta_{JJ'} \delta_{MM'} \langle \ell v J M | \ell v' J M \rangle \quad ; \quad (2.37)$$

with

Table 2.1. Angular momentum decomposition of $R(5)$ symmetric IR.

λ	J-decomposition of $[\lambda]_{R(5)}$ J^p indicates that J occurs p times <p>($p = 1$ is not written)</p>
0	0
1	2
2	2, 4
3	0, 3, 4, 6
4	2, 4, 5, 6, 8
5	2, 4, 5, 6, 7, 8, 10
6	0, 3, 4, 6^2 , 7, 8, 9, 10, 12
7	2, 4, 5, 6, 7, 8^2 , 9, 10, 11, 12, 14
8	2, 4, 5, 6, 7, 8^2 , 9, 10^2 , 11, 12, 13, 14, 16
9	0, 3, 4, 6^2 , 7, 8, 9^2 , 10^2 , 11, 12^2 , 13, 14, 15, 16, 18
10	2, 4, 5, 6, 7, 8^2 , 9, 10^2 , 11^2 , 12^2 , 13, 14^2 , 15, 16, 17, 18, 20

Table 2.2. The number of states $\psi_{N\ell vJJ}$ for which $N \leq N_{\max}$

J	$N_{\max}$	10	15	20	25	30
0		14	27	44	65	91
2		22	45	77	117	165
3		8	19	33	52	75
4		25	56	100	156	225
5		12	30	57	92	135
6		24	61	114	184	271
7		12	36	72	121	182
8		21	60	121	202	304
9		10	37	80	140	217
10		16	56	121	211	326
11		7	34	82	151	240
12		11	49	116	212	338
13		4	29	79	154	254
14		7	40	107	207	340
15		2	23	72	151	259
16		4	31	95	196	335
17		1	16	63	143	256
18		2	23	81	181	323
19		0	11	52	131	247
20		1	16	67	163	305

Table 2.3. Particulars for the maximum usable expansion basis (grouped by angular momentum J)

J	$N_{\max}(J)$	Number of $\psi_{N\ell v J J}$ with $N \leq N_{\max}(J)$	Number of $A_{\sigma}^{\eta}(\ell v J K)$ $\ell \leq \ell_{\max}; K \geq 0$	Number of distinct $\langle \ell v J J \ell v' J J \rangle$ ($v < v'$)
0	30	91	91	0
2	27	135	261	0
3	30	75	85	0
4	25	156	504	0
5	27	108	240	0
6	25	184	854	7
7	25	121	457	0
8	25	202	1266	13
9	25	140	766	6
10	25	211	1719	18
11	15	34	319	4
12	25	212	2191	27
13	15	29	393	5
14	25	207	2660	34
15	15	23	431	6
16	25	196	3098	39
17	15	16	360	3
18	25	181	3480	45
19	15	11	313	2
20	25	163	3778	48

$$\langle \ell \nu J M | \ell \nu J M \rangle = 1$$

The general overlap bracket $\langle \ell \nu J M | \ell \nu' J M \rangle$ is independent of M , and its accurate calculation for $\nu \neq \nu'$ is described in Appendix B. The number of distinct overlap brackets between maximal basis states of a given spin is listed in Table 2.3. An abbreviated listing of their values can be found in Table B.5. The overlaps will be required in Chapter III when an orthonormal set of eigenfunctions is constructed from the

$$\psi_{N \ell \nu J M}$$

All of the Bohr eigenfunctions are associated with positive parity nuclear states. Under a simultaneous inversion through the origin of the positions of all nucleons, the wavefunction $\psi_{N \ell \nu J M}$ is left unaltered. This statement of course requires that a connection be made between the collective coordinates and those of the individual nucleons. For instance, if the collective and microscopic expressions for the nuclear quadrupole moment are equated (38), one finds to lowest order

$$\alpha_\mu \propto \sum_{i=1}^A r_i^2 Y_{2\mu}(\theta_i, \phi_i) \quad (2.38)$$

Here (r_i, θ_i, ϕ_i) are the spherical polar coordinates of the i^{th} nucleon, and A is the number of nucleons. The surface coordinates α may then be seen to be unaffected by the parity operation;

$$\pi: (r_i, \theta_i, \phi_i) \rightarrow (r_i, \pi - \theta_i, \phi_i + \pi)$$

As the eigenfunctions ψ are single valued in the α coordinates, they too will be unaffected by π . The positive parity of the ψ is simply a

manifestation of the inversion symmetry of the general quadrupole surface [Equation (2.1)].

The α coordinates are in one-to-one correspondence with the distinct quadrupole surfaces; however, this is not the case for the Bohr coordinates $(\beta, \gamma, \theta_1)$. There exist 24 possible choices for the body-fixed, principal-axis system, and hence any given quadrupole surface may be properly described by any one of 24 sets $(\beta, \gamma, \theta_1)$. As a result, the Bohr-coordinate eigenfunctions possess a number of symmetries which may be deduced from

$$\psi_{N\ell\nu JM}(\alpha) = \psi_{N\ell\nu JM}(\alpha) \quad ; \quad \psi_{N\ell\nu JM}(-\alpha) = (-1)^\ell \psi_{N\ell\nu JM}(\alpha) \quad (2.39)$$

The first relationship is trivial, and the second follows from Equation (2.22) and the form of the creation operators in the α -representation [Figure 2.1]. In Appendix A, four independent symmetries are found. They may be written in terms of the g^η functions of Equation (2.30) as

$$\begin{aligned} R_1: \quad g_{\ell\nu JK}^\eta(\gamma) &= (-1)^J g_{\ell\nu J-K}^\eta(\gamma) \\ R_2: \quad &= e^{iK\pi/2} g_{\ell\nu JK}^\eta(-\gamma) \\ R_3: \quad &= \sum_{K'} g_{\ell\nu JK'}^\eta\left(\gamma - \frac{2\pi}{3}\right) D_{KK'}^{J*}\left(0, \frac{\pi}{2}, \frac{\pi}{2}\right) \\ R_4: \quad &= (-1)^\ell g_{\ell\nu JK}^\eta(\gamma + \pi) \end{aligned} \quad (2.40)$$

The first symmetry permits the angular portion of ψ to be written in either of two equivalent forms: that of Equation (2.29), or

$$\phi_{\ell\nu JM}(\gamma, \theta_i) = \sum_{K=-J}^J g_{\ell\nu JK}^{\eta}(\gamma) D_{MK}^{J*}(\theta_i) \quad (2.41)$$

The second symmetry applied twice restricts K to even values in Equations (2.29) and (2.41).

The γ -coordinate probability density $P(\gamma)$ of a normalized state function $\phi(\beta', \gamma, \theta_i)$ is defined by

$$P(\gamma)d\gamma = \int_{\beta'}^{\infty} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} \phi^* \phi \, d\Omega(\beta', \gamma, \theta_i) \quad (2.42)$$

$P(\gamma)d\gamma$ is then the probability that a measurement of the nuclear surface will find γ to be in the range $[\gamma, \gamma + d\gamma]$. For the $\psi_{N\ell\nu JM}$, $P(\gamma)$ depends only on the ℓ , ν , and J quantum numbers. As a consequence of the symmetries expressed by Equations (2.40), $P(\gamma)$ is shown in Appendix A to satisfy

$$P(\gamma) = P(-\gamma) = P(\gamma - \frac{2\pi}{3}) = P(\gamma + \pi) \quad (2.43)$$

for any Bohr eigenfunction. $P(\gamma)$ thus possesses reflection symmetries about $\gamma = 0, 30^\circ, 60^\circ, \dots$, and has translational symmetries under shifts of $60^\circ, 120^\circ, 180^\circ, \dots$. If $P(\gamma)$ is specified on $0 \leq \gamma \leq \pi/6$, it is then determined elsewhere by Equation (2.43). In Figures 2.4-2.6, $P(\gamma)$ is displayed for selected low energy states. The drawings have been grouped by angular momentum, and were prepared by evaluating $P(\gamma)$ at one hundred equally spaced values of γ on $[0, \pi/6]$. $P_{\ell\nu J}(\gamma)$ of the same J and ν are often similar in appearance. In fact for the states of

Figure 2.4. γ -probability densities of selected $J = 0, 2, 3$ Bohr eigenfunctions

Figure 2.5. γ -probability densities of selected $J = 4, 5$ Bohr eigenfunctions

Figure 2.6. γ -probability densities of selected $J = 6, 7$ Bohr eigenfunctions

angular momentum 2 and 5, we have the identity

$$\begin{aligned}
 & J = 2; \ell = 1, 4, 7, 10, \dots \\
 P_{\ell, \nu, J}(\gamma) &= P_{\ell+1, \nu, J}(\gamma) \quad \text{or} \quad (2.44) \\
 & J = 5; \ell = 4, 7, 10, \dots
 \end{aligned}$$

Furthermore, for the $J = 0, 2, 4$ states of the $N = 2$ triplet in Figure 2.3, we may use

$$\begin{aligned}
 g_{0000}^n &= \frac{1}{2} \\
 g_{202K}^n &= \begin{cases} \sqrt{\frac{5}{4}} (\cos^2 \gamma - \sin^2 \gamma) & , \quad K = 0 \\ -\sqrt{\frac{5}{2}} \sin \gamma \cos \gamma & , \quad K = 2 \end{cases} ,
 \end{aligned}$$

and

$$g_{204K}^n = \begin{cases} \frac{3}{2} \cos^2 \gamma + \frac{1}{4} \sin^2 \gamma & , \quad K = 0 \\ \sqrt{\frac{15}{8}} \sin \gamma \cos \gamma & , \quad K = 2 \\ \sqrt{\frac{35}{32}} \sin^2 \gamma & , \quad K = 4 \end{cases} ,$$

to show that $P_{\ell \nu J}(\gamma)$ is identical for all:

$$P_{000}(\gamma) = P_{202}(\gamma) = P_{204}(\gamma) = \frac{1}{4} |\sin 3\gamma| \quad (2.45)$$

If a perturbation $V(\gamma)$ is slowly added to H_B^I , the energy of the

perturbed state growing from $\psi_{N\ell vJM}$ is given to first order¹ by

$$\begin{aligned} E_V^{(1)} &= (N + \frac{5}{2}) + \int_{\Omega} d\Omega \psi_{N\ell vJM}^* V(\gamma) \psi_{N\ell vJM} \\ &= (N + \frac{5}{2}) + \int_0^{2\pi} d\gamma P_{\ell vJ}(\gamma) V(\gamma) \end{aligned} \quad (2.46)$$

By virtue of Equation (2.45), the $N = 2$ triplet states are, in first order, neither split nor shifted in energy with respect to the new ground state.

In a manner similar to that used for $P(\gamma)$, a radial coordinate density $P(\beta')$ may be defined by

$$P(\beta') d\beta' = \int_0^{2\pi} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} \phi^* \phi d\Omega(\beta', \gamma, \theta, \varphi) \quad (2.47)$$

As a consequence of the factored form of Equation (2.25), we have

$$P(\beta') = P_{N\ell}(\beta') = [\beta'^2 f_{N\ell}(\beta')]^2 \quad (2.48)$$

for any Bohr eigenfunction, $\psi_{N\ell vJM}$. The function in brackets is displayed in Figure 2.7 for selected low-energy states. The drawings have been grouped according to the value of

¹Here it is assumed that the perturbed eigenfunction approaches $\psi_{N\ell vJM}$ as $V(\gamma) \rightarrow 0$. This will not generally be the case if there are two or more distinct Bohr eigenfunctions which differ only in their ℓ or v values. Such states will be strongly mixed by $V(\gamma)$ and degenerate perturbation theory [see Chapter 16 of (39)] must be applied. However any function $V(\beta', \gamma)$ is an angular momentum scalar, and consequently cannot connect states of different (J, M) .

Figure 2.7. Square root of radial probability distribution for selected low-energy Bohr eigenfunctions

$$\frac{N - \ell}{2} = \text{number of zeroes of } P_{N\ell}(\beta') \text{ on } 0 < \beta' < \infty \quad (2.49)$$

In preparing the drawings, $\beta'^2 f_{N\ell}(\beta')$ was evaluated at one hundred equally spaced values of β' on $[0, 7]$. We can see that even for the ground state there is only a negligible probability of finding the nuclear surface to be spherical ($\beta' = 0$). Because of the zero-point vibrations, the mean value of β' is given by

$$\langle \beta' \rangle = \int_0^\infty \beta' P_{00}(\beta') d\beta' = \frac{8}{3\sqrt{\pi}} \int_0^\infty (\beta')^5 e^{-\beta'^2} d\beta' = \frac{8}{3\sqrt{\pi}} \approx 1.50$$

If a perturbation $V(\beta')$ is added to H_B' , the radial counterpart of Equation (2.46) is

$$E_V^{(1)} = (N + \frac{5}{2}) + \int_0^\infty d\beta' P_{N\ell}(\beta') V(\beta') \quad (2.50)$$

If we consider the $N = 2$ triplet to first order, we notice that the $J = 2, 4$ states each possess $\ell = 2$; they will remain degenerate but will in general be split away from the $J = 0, \ell = 0$ state. Any function which depends solely on the radial coordinate will commute with the generators of the $R(5)$ subgroup in the physical chain (2.20). Consequently

$$H = H_B' + V(\beta') \quad (2.51)$$

possesses $R(5)$ symmetry, and ℓ remains a good quantum number for describing degenerate multiplets of H . Two eigenstates of H which arise from $\psi_{N\ell\nu JM}$ and $\psi_{N\ell\nu' J'M'}$ respectively, will remain degenerate to all orders of perturbation theory.

III. EXPANSION TECHNIQUES

We now begin an investigation of the mathematical details necessary for treating the more general problem

$$H\phi(\beta, \gamma, \theta_i) = E\phi(\beta, \gamma, \theta_i) \quad (3.1a)$$

$$H = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \quad (3.1b)$$

Here the potential energy term of the Bohr Hamiltonian, $\frac{1}{2}C\beta^2$, has been replaced with a more general function of the shape coordinates. For any choice of the constants B and C in Equation (2.10), the eigenfunctions of H_B form a complete set in terms of which we may expand the normalizable solutions of any similar problem having the same degrees of freedom and boundary conditions. When such an expansion is made, the Schroedinger Equation (3.1a) may be cast into the form of a matrix eigenvalue problem. Computer solution of the resulting equation is more economical if the matrix whose eigenvalues are desired is both real and symmetric. This will be the case for Equation (3.1a) if the expansion basis is orthonormal. In Section B of this chapter we take up the problem of forming an orthonormal basis of H_B eigenfunctions from the original $\psi_{N\ell v J M}$ basis of Chapter II, and we examine the matrix form of the Schroedinger equation in each basis.

The method of solution by expansion requires the calculation of matrix elements of H between states of the expansion basis. Different selections of the two physical constants in H_B lead to different sets of expansion functions and hence affect the calculations. In principle

this presents no difficulties when the entire expansion basis is used; calculated eigenvalues and eigenfunctions of H should be independent of the choice of basis since each basis is a complete set. However for practical purposes, ϕ will be expanded in a finite (truncated) basis and the independence of basis is no longer guaranteed. In Section C the choice of expansion basis is shown to effect the calculated matrix elements through a single parameter s . The meaning of s is discussed and methods for selecting the optimal basis of a given size are described. These methods will be examined in a practical setting in Chapter IV.

The final section contains a summary of the calculation of electric quadrupole transition rates between the eigenstates of Equation (3.1a). Details of the derivation and programming methods can be found in Appendix D. First-order transition rates between Bohr eigenstates having $N \leq 5$ are presented and discussed.

A. Notational Conventions

A "Bohr-like" problem will be defined to be one having the form

$$H_B(\beta, \gamma, \theta_i) \psi_\alpha^s(\beta, \gamma, \theta_i) = E_\alpha \psi_\alpha^s(\beta, \gamma, \theta_i) \quad (3.2a)$$

$$H_B(\beta, \gamma, \theta_i) = A_1[-\frac{1}{2}T(\beta, \gamma, \theta_i)] + A_2[\frac{1}{2}\beta^2] \quad (3.2b)$$

Here A_1 and A_2 are constants; they may be dimensionless or have units of energy. The coordinate β may represent either the original deformation parameter appearing in Equations (2.6), or a rescaled version such as the β' of Figure 2.2. The lower labels on ψ serve to distinguish the

various eigenstates. Greek letters $\alpha, \beta, \dots$ will be used to denote the set of labels employed in Chapter II:

$$\alpha = (N_\alpha, \ell_\alpha, v_\alpha, J_\alpha, M_\alpha) \quad (3.3)$$

The ψ^s will be assumed to be normalized over the region $\Omega(\beta, \gamma, \theta_i)$ of Equation (2.15) with respect to the volume element $d\Omega(\beta, \gamma, \theta_i)$ of Equation (2.14). The ψ_α^s are then normalized but they are not orthogonal on the v label. Roman letters $i, j, \dots$ will denote the labels for an orthonormal set of solutions to Equations (3.2),

$$i = (N_i, \ell_i, t_i, J_i, M_i) \quad (3.4)$$

Presumably each of the ψ_i^s will be some linear combination

$$\psi_i^s = \sum_{v_\alpha} U_{i\alpha} \psi_\alpha^s \quad ; \quad \left\{ \begin{array}{l} N_\alpha = N_i \\ \ell_\alpha = \ell_i \\ J_\alpha = J_i \\ M_\alpha = M_i \end{array} \right. \quad \dots$$

A method for determining the constants $U_{i\alpha}$ will be presented in Section B.

The upper label on the ψ^s will again indicate the form of H_B for which ψ^s is an eigenfunction. Rather than listing the two physical parameters of H_B as was done in Chapter II, the single label s will be employed. s relates the solutions of Equations (3.2) to those of the standard reduced Bohr problem ($A_1 = A_2 = 1$). In the manner of Figure 2.2, we may write the former as

$$\psi_{\alpha}^s(\beta, \gamma, \theta_i) = s^{5/2} \psi_{\alpha}(s\beta, \gamma, \theta_i) \quad ; \quad s = \left[\frac{A_2}{A_1} \right]^{1/4} \quad (3.5)$$

$$E_{\alpha} = \sqrt{A_1 A_2} (N_{\alpha} + 5/2) \quad (3.6)$$

As before, the SR solutions, $\psi_{\alpha}(\beta, \gamma, \theta_i)$, will bear no upper label.

Matrix elements of an arbitrary operator $\mathcal{O}(\beta, \gamma, \theta_i)$ between normalized Bohr eigenfunctions will be written as

$$\begin{aligned} \langle \psi_{\alpha}^s | \mathcal{O}(\beta, \gamma, \theta_i) | \psi_{\beta}^s \rangle &\equiv \int_{\Omega(\beta, \gamma, \theta_i)} d\Omega(\beta, \gamma, \theta_i) \psi_{\alpha}^{s*}(\beta, \gamma, \theta_i) \\ &\times \mathcal{O}(\beta, \gamma, \theta_i) \psi_{\beta}^s(\beta, \gamma, \theta_i) \quad (3.7) \end{aligned}$$

When SR eigenfunctions are involved only the subscripts will appear, as in

$$\langle i | \mathcal{O}(\beta, \gamma, \theta_i) | j \rangle \equiv \langle \psi_i | \mathcal{O}(\beta, \gamma, \theta_i) | \psi_j \rangle \quad (3.8)$$

Finally we agree that if $\mathcal{O}$ is the unit operator it will be suppressed.

For example,

$$\langle \psi_i^s | 1 | \psi_j^s \rangle = \langle \psi_i^s | \psi_j^s \rangle = \delta_{ij} \quad .$$

A "generalized" Bohr problem will be defined as one having the form

$$H(\beta, \gamma, \theta_i) \phi(\beta, \gamma, \theta_i) = E \phi(\beta, \gamma, \theta_i) \quad (3.9a)$$

$$H = A[-\frac{1}{2}T(\beta, \gamma, \theta_i)] + V(\beta, \gamma) \quad (3.9b)$$

where A is constant. The potential energy function $V(\beta, \gamma)$ is expected to possess the symmetries of a quadrupole surface as discussed in

Appendix A. $V(\beta, \gamma)$ may be arbitrarily defined on the region $0 \leq \beta < \infty$, $0 \leq \gamma \leq \pi/3$; the symmetries will then determine it elsewhere. The eigenfunctions ϕ will be assumed to be normalized in the same manner as the ψ of Equations (3.2).

Equation (3.1a) is in the form of a generalized Bohr problem where $A = \hbar^2/B$ and V have units of energy. Because of the scaling property [Equation (2.16)] of the kinetic energy operator, a linear change in the β variable in Equations (3.9) will again result in a problem of the same form. In particular, let $\bar{B}$ and $\bar{C}$ be two arbitrary constants having units of $[\text{energy} \cdot \text{time}^2]$ and energy respectively. We can cast Equation (3.1a) into dimensionless form by making the change of variable

$$\beta' = \bar{s}\beta, \quad \bar{s} = \left[\frac{\bar{B} \bar{C}}{\hbar^2} \right]^{1/4}, \quad (3.10)$$

and then dividing by the energy factor $\hbar[\bar{C}/\bar{B}]^{1/2}$. This results in the "reduced" form

$$\begin{aligned} \bar{H}(\beta', \gamma, \theta_i) \bar{\phi}(\beta', \gamma, \theta_i) &= \bar{E} \bar{\phi}(\beta', \gamma, \theta_i), \\ \bar{H}(\beta', \gamma, \theta_i) &= \frac{\bar{B}}{B} [-\frac{1}{2}T(\beta', \gamma, \theta_i)] + \frac{1}{\hbar} \left[\frac{\bar{B}}{\bar{C}} \right]^{1/2} V\left(\frac{\beta'}{\bar{s}}, \gamma\right). \end{aligned} \quad (3.11)$$

The solutions of the original problem (3.1) are related to those of the reduced version by

$$E = \hbar \left[\frac{\bar{C}}{\bar{B}} \right]^{1/2} \bar{E} \quad (3.12)$$

$$\phi(\beta, \gamma, \theta_i) = \bar{s}^{5/2} \bar{\phi}(\bar{s}\beta, \gamma, \theta_i) \quad (3.13)$$

The raised bar, $\bar{}$, will be used to denote the energies and eigenfunctions of the reduced (dimensionless) form of a generalized Bohr problem. It is also used when writing $\bar{B}$, $\bar{C}$, and $\bar{s}$ which specify the transformation connecting the original and reduced forms.

The collection of energy eigenvalues, $\{E_i\}$, each having an associated state label i , comprises the energy spectrum of a Hamiltonian. The members of the reduced energy spectrum are obtained from

$$E_j^{\text{RED}} = \frac{E_j - E_{\text{GS}}}{E_{2_1} - E_{\text{GS}}} \quad (3.14)$$

where E_{GS} and E_{2_1} are the energies of the ground state and the first excited $J = 2$ state respectively. From Equation (3.12) it is clear that H and $\bar{H}$ will have the same reduced energy spectrum. Let us suppose that H depends upon n adjustable parameters. By a judicious choice of $\bar{B}$ and $\bar{C}$, $\bar{H}$ can be made to depend on only $(n - 2)$ combinations of these parameters. The search for the distinct reduced energy spectra that H may possess is then considerably simplified by investigating the spectra of $\bar{H}$. Notice that the general Bohr-like problem [Equations (3.2)] depends upon the two constants A_1 and A_2 ; however its reduced spectrum may be seen from Equation (3.6) to be independent of either constant.

B. Matrix Form of the Schroedinger Equation

In the Bohr coordinate representation, the operators for the laboratory components of angular momentum $[J_i]$ involve only the Euler angles and their partial derivatives; hence they will commute with an arbitrary function of β and γ . In as much as the three operators also

commute with H_B , we conclude that they will commute with the Hamiltonian operator for a generalized Bohr problem. This follows because the latter may be written as the sum of two terms,

$$H = H_B + [V(\beta, \gamma) - \frac{1}{2}C\beta^2] ,$$

each of which commutes with the J_i . We may seek solutions to the generalized Bohr problem [Equations (3.9)] which are also eigenstates of the total angular momentum operator and its z projection, with eigenvalues $J(J+1)\hbar^2$ and $M\hbar$ respectively. We write

$$H\phi_{JMq} = E_q \phi_{JMq} , \quad (3.15)$$

where J and M label the angular momentum eigenvalues, and q represents the remaining labels. For the purposes of this section, it will be convenient to suppress the arguments $(\beta, \gamma, \theta_i)$ when they occur.

Let us expand ϕ_{JMq} in terms of the closed-form solutions to some Bohr-like Schroedinger equation:

$$\phi_{JMq} = \sum_{\alpha} b_{\alpha}^q \psi_{\alpha}^s ; \quad \alpha = (N_{\alpha}, l_{\alpha}, v_{\alpha}, J_{\alpha} = J, M_{\alpha} = M) . \quad (3.16)$$

[It follows from the Wigner-Eckart theorem [Equation (F.79)] that only those ψ_{α}^s having $J_{\alpha} = J$ and $M_{\alpha} = M$ can have a non-zero overlap with ϕ_{JMq} . Hence only these need occur in the sum of Equation (3.16).] Substituting Equation (3.16) into Equation (3.15), multiplying the result by ψ_{β}^{s*} , and integrating over the space of the coordinates gives

$$\sum_{\alpha} \langle \psi_{\beta}^s | H | \psi_{\alpha}^s \rangle b_{\alpha}^q = E_q \sum_{\alpha} \langle \psi_{\beta}^s | \psi_{\alpha}^s \rangle b_{\alpha}^q , \quad (3.17)$$

or as a matrix equation¹

$$[H'] \tilde{b}^q = E_q [N] \tilde{b}^q \quad (3.18)$$

Here elements of the matrices have been defined by

$$[H']_{\beta\alpha} = \langle \psi_\beta^S | H | \psi_\alpha^S \rangle = \int_\Omega d\Omega \psi_\beta^{S*} H \psi_\alpha^S, \quad \text{and} \quad (3.19)$$

$$[N]_{\beta\alpha} = \langle \psi_\beta^S | \psi_\alpha^S \rangle = \int_\Omega d\Omega \psi_\beta^{S*} \psi_\alpha^S. \quad (3.20)$$

The prime on H is to remind us that the matrix elements of the Hamiltonian are computed in a (generally) non-orthogonal basis. The inverse of the matrix [N] exists, and Equation (3.18) may be rewritten in the form of an eigenvalue equation:

$$\left[[N]^{-1} [H'] \right] \tilde{b}^q = E_q \tilde{b}^q \quad (3.21)$$

[H'] is an Hermitean matrix. In Appendix C its matrix elements are calculated to be real. Hence [H'] is real and symmetric:

$[H'] = [H']^T = [H']^*$. The same may be said of the matrix [N], but not of the product $[N]^{-1} [H']$.

Rather than solving Equation (3.21) we may transform to an orthonormal basis $\{\psi_i^S\}$, $i = (N_i, \ell_i, t_i, J_i, M_i)$. The Schroedinger equation will then be replaced by an eigenvalue equation for a real symmetric

¹In this section, brackets [] will be used to denote a matrix; superscripts T, -1, and * will denote the transposed, inverse, and complex conjugate matrices respectively.

matrix. The original and orthonormal bases will be connected by some linear transformation

$$\psi_i^S = \sum_{\beta} U_{i\beta} \psi_{\beta}^S \quad (3.22)$$

The orthonormality of the ψ_i^S , $\langle \psi_i^S | \psi_j^S \rangle = \delta_{ij}$, imposes the condition

$$[1] = [U]^* [N] [U]^t \quad (3.23)$$

The matrix $[U]$ may be found from $[N]$ by the following procedure.

$[N]$ is a real, symmetric matrix. Its diagonal elements are all unity; some of its non-zero off-diagonal elements for selected values of J are listed in Table B.5. $[N]$ is also positive definite in the sense that

$$\sum_{i,j} v_i [N]_{ij} v_j > 0 \text{ for all real } v \neq 0$$

There will exist¹ a real, orthogonal matrix $[P]$ which diagonalizes $[N]$:

$$[P]^{-1} [N] [P] = [P]^t [N] [P] = \begin{bmatrix} n_1 & 0 & 0 & \dots \\ 0 & n_2 & 0 & \dots \\ 0 & 0 & n_3 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix} \quad (3.24)$$

The eigenvalues n_i will be real and positive. If we define a real diagonal matrix by

¹See for example Chapter 7 of Reference (40).

$$\left[\frac{1}{\sqrt{N}} \right] \equiv \begin{bmatrix} (n_1)^{-\frac{1}{2}} & 0 & 0 & \cdot \\ 0 & (n_2)^{-\frac{1}{2}} & 0 & \cdot \\ 0 & 0 & (n_3)^{-\frac{1}{2}} & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} \quad (3.25)$$

then the real matrix

$$[U] = \left[\frac{1}{\sqrt{N}} \right] [P]^t \quad (3.26)$$

can be easily shown to satisfy Equation (3.23).

If we use the set of orthonormal states as an expansion basis

$$\phi_{JMq} = \sum_i a_i^q \psi_i^s \quad i = (N_i, \ell_i, t_i, J_i = J, M_i = M) \quad (3.27)$$

and repeat the procedure that led to Equation (3.18), we find

$$[H]_{\tilde{q}} a^q = E_{\tilde{q}} a^q \quad ; \quad [H]_{ij} = \langle \psi_i^s | H | \psi_j^s \rangle \quad (3.28)$$

which may be compared with Equation (3.21). From Equation (3.22) it follows that the relationship between the two sets of expansion coefficients is

$$b_{\alpha} = \sum_i U_{i\alpha} a_i \quad \text{or} \quad \underline{b} = [U]^t \underline{a} \quad , \quad (3.29)$$

and the Hamiltonian matrices are related by

$$[H] = [U][H'] [U]^t \quad . \quad (3.30)$$

From the last equation and the previously mentioned properties of $[H']$

and $[U]$, $[H]$ may be shown to be real and symmetric.

If the set of expansion functions is truncated, and the matrix elements of H between orthonormal states are calculated, the eigenvalues and eigenvectors of Equation (3.28) may be found through standard computational techniques. In my work, the Argonne National Laboratory EISPACK (41) routines for matrix manipulation and diagonalization were used. Appendix C describes how standard reduced matrix elements of

$$V_1 = \beta^p f(\gamma) \quad , \quad p = 0, 1, 2, \dots \quad ; \quad (3.31a)$$

and

$$V_2 = e^{-a\beta^2} \beta^p f(\gamma) \quad , \quad a \geq 0 \quad (3.31b)$$

between orthonormal Bohr eigenfunctions may be calculated. $f(\gamma)$ must obey the symmetries of the quadrupole surface, but is otherwise quite arbitrary. Conventions for enumerating the expansion functions and for storing the matrix elements on magnetic tape are set forth in Appendix C.

The potential energy functions, $V(\beta, \gamma)$, employed in this thesis are predominantly linear combinations of terms of the form V_1 . Terms of the form V_2 were added in one instance during the preliminary test calculations described in Appendix C. In the next section we shall see that the matrix $[H]$ for such Hamiltonians may be assembled from $\langle i|V_1|j\rangle$ and $\langle i|V_2|j\rangle$.

C. The Influence of the Choice of Basis

A single parameter s relates the eigenfunctions of any Bohr-like Hamiltonian to those of the standard reduced problem. Only matrix

elements of these functions are required in Equation (3.28); hence the choice of the basis Hamiltonian [H_B of Equation (3.2b)] can effect the outcome of the calculations only through $s = [A_2/A_1]^{\frac{1}{4}}$. When the eigenfunctions of

$$H = A[-\frac{1}{2}T(\beta, \gamma, \theta_i)] + V(\beta, \gamma)$$

are to be found by expanding in solutions of

$$H_B = A_1[-\frac{1}{2}T(\beta, \gamma, \theta_i)] + A_2[\frac{1}{2}\beta^2] \quad ,$$

there is no loss of generality if we restrict $A_1 = A$. In this case H and H_B differ only in their potential energy terms, and the basis parameter s may be varied by changing A_2 . Figure 3.1a compares a typical potential energy term of H with those of H_B for three choices of s . For the optimal value of s , we expect that

$$V_{Bohr} = A_2[\frac{1}{2}\beta^2] = s^4 A[\frac{1}{2}\beta^2]$$

should approximate $V(\beta, \gamma)$ as well as is possible over that portion of the potential well that is strongly sensed by the eigenfunctions of H . For a finite basis calculation, the optimal value of s may be empirically defined as that value of s for which small changes in s leave the output energies and eigenfunctions unaltered. For example if we repeatedly solve Equation (3.15) using a succession of different expansion bases, we could plot the calculated energy of some state ϕ versus the basis parameter as shown in Figure 3.1b. The optimal value of s , s^{best} , would then lie in the center of the flat region (if it exists). This issue will be investigated at length in Chapter IV.

Figure 3.1. Dependence of $V_{Bohr} = s^4 A[\frac{1}{2}\beta^2]$ and calculated energy $[E$ in $H\phi = E\phi; H = \Lambda(-\frac{1}{2}T(\beta, \gamma, \theta_1)) + V(\beta, \gamma)]$ upon the basis parameter, s , in a typical application

The manner in which the choice of s enters the calculations may be isolated by expressing the required matrix elements $[H]_{ij}$ in terms of standard reduced ones.

$$\begin{aligned}
 [H]_{ij} &= \langle \psi_i^s | H | \psi_j^s \rangle \\
 &= \int_{\Omega} d\Omega(\beta, \gamma, \theta_i) \psi_i^{s*}(\beta, \gamma, \theta_i) \left[\frac{-A}{2} T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \right] \psi_j^s(\beta, \gamma, \theta_i) \\
 &= s^5 \int_{\Omega} d\Omega(\beta, \gamma, \theta_i) \psi_i^*(s\beta, \gamma, \theta_i) \left[\frac{-A}{2} T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \right] \\
 &\quad \times \psi_j(s\beta, \gamma, \theta_i) ,
 \end{aligned}$$

where Equation (3.5) has been used to write the ψ_i^s in terms of the SR functions ψ_i . Changing the radial variable to $\beta' = s\beta$, we have:

$$d\Omega \propto \beta^4 d\beta \rightarrow d\Omega(\beta, \gamma, \theta_i) = s^{-5} d\Omega(\beta', \gamma, \theta_i) ,$$

$$\text{Equation (2.16)} \rightarrow T(\beta, \gamma, \theta_i) = s^2 T(\beta', \gamma, \theta_i) ,$$

and

$$\begin{aligned}
 [H]_{ij} &= \int_{\Omega(\beta', \gamma, \theta_i)} d\Omega(\beta', \gamma, \theta_i) \psi_i^*(\beta', \gamma, \theta_i) \left[\frac{-A s^2}{2} T(\beta', \gamma, \theta_i) \right. \\
 &\quad \left. + V\left(\frac{\beta'}{s}, \gamma\right) \right] \psi_j(\beta', \gamma, \theta_i) .
 \end{aligned}$$

Finally we use

$$-\frac{1}{2} T(\beta', \gamma, \theta_i) \psi_j(\beta', \gamma, \theta_i) = (N_j + \frac{5}{2} - \frac{1}{2} \beta'^2) \psi_j(\beta', \gamma, \theta_i)$$

to obtain the result

$$[H]_{ij} = A s^2 (N_j + \frac{5}{2}) \delta_{ij} + \langle i | V(\frac{\beta}{s}, \gamma) - \frac{A s^2 \beta^2}{2} | j \rangle \quad (3.32)$$

In the usual case, the potential energy function has the form

$$V(\beta, \gamma) = \sum_{p=0}^m c_p \beta^p f_p(\gamma) \quad (3.33)$$

where some of the constants c_p may be zero. In order that bound solutions may exist, the coefficient of the highest power of β is assumed to satisfy

$$c_m f_m(\gamma) > 0 \text{ for all } 0 \leq \gamma \leq 2\pi$$

For the above potential, Equation (3.32) becomes

$$[H]_{ij} = A s^2 (N_j + \frac{5}{2}) \delta_{ij} - A s^2 \langle i | \frac{1}{2} \beta^2 | j \rangle + \sum_{p=0}^m c_p s^{-p} \langle i | \beta^p f_p(\gamma) | j \rangle \quad (3.34)$$

The expression for the diagonal elements may be simplified by making use of the virial theorem (42) [or Equation D.31] to write

$$\langle i | -\frac{1}{2} T | i \rangle = \langle i | \frac{1}{2} \beta^2 | i \rangle = \frac{1}{2} (N_i + \frac{5}{2})$$

Using this result we have

$$[H]_{ii} = \frac{A}{2} (N_i + \frac{5}{2}) s^2 + \sum_{p=0}^m c_p \langle i | \beta^p f_p(\gamma) | i \rangle s^{-p}, \quad (3.35)$$

and the asymptotic properties

$$[H]_{ii} \xrightarrow{s \rightarrow 0^+} \{c_m \langle i | \beta^m f_m(\gamma) | i \rangle\} s^{-m}, \quad (3.36a)$$

$$[H]_{ii} \xrightarrow{s \rightarrow \infty} \left\{ \frac{A}{2} (N_i + \frac{5}{2}) \right\} s^2 \quad (3.36b)$$

The two quantities in braces $\{\}$ are necessarily positive. Regarded as a function of s , $[H]_{ii}$ will have at least one minimum on $0 < s < \infty$. The same may be said of the trace of $[H]$:

$$\text{tr}[H] = \sum_{\substack{\text{all basis} \\ \text{states, } i}} [H]_{ii} = \text{sum of the eigenvalues of the finite matrix } [H] \quad (3.37)$$

Equation (3.35) affords us an opportunity for estimating s^{best} . We wish to know the optimal value of s for use in a finite basis expansion of the few lowest energy ($E_1, E_2, \dots, E_k$) eigenstates of H . Empirically we could proceed by calculating the curve of Figure 3.1b for each of these states. The center of the region where the E_j^i - vrs - s curves are mutually flat could be taken to be s^{best} . (Here E_j^i refers to the calculated value of the exact eigenvalue E_j .) Because of the asymptotic properties of the diagonal elements, the curves might be expected to rise away from the flat region for both large and small values of s . If this is indeed the case, s^{best} should lie not too distant from the lowest minimum of the sum of the k curves:

$$\left. \frac{d}{ds} \left[\sum_{j=1}^k E_j^i \right] \right|_{s = s^{\text{best}}} = 0 \quad (3.38)$$

Because the eigenvalues of $[H]$ are very complicated functions of s , Equation (3.38) is difficult to use. The E_j^i - vrs - s curves must be

obtained by repeated diagonalization. On the other hand

$$\left. \frac{d}{ds} \left[\sum_{k \text{ lowest energy basis states}} [H]_{ii} \right] \right|_{s = s^{\text{best}}} = 0 \quad (3.39)$$

requires only that we find the roots of a polynomial in s . Furthermore, as k is increased to the size of the expansion basis, Equations (3.38) and (3.39) become identical by virtue of Equation (3.37). The two criteria will be compared for realistic calculations in Chapter IV.

I will close this section with a few comments on style in the solution of the generalized Bohr problem [Equations (3.1)] which opened this chapter. For any such problem two approaches are open to us:

- 1) we may diagonalize H directly in an expansion basis $\{\psi_i^s\}$; or
- 2) we may transform to a reduced problem, diagonalize $\tilde{H}$ in a basis $\{\tilde{\psi}_i^s\}$, and then reconstruct the energies and eigenfunctions of the original Hamiltonian.

The two methods are summarized and compared in Figure 3.2. For every choice of s in the first approach, there is a corresponding value of $\tilde{s}$ which will lead to an identical solution of Equation (3.1a). The second approach appears roundabout, but as was noted in section B of this chapter, it is useful in limiting the search for possible reduced spectra when a class of Hamiltonians is being investigated. The second approach will be used exclusively in the ensuing chapters.

To be solved
(for fixed J,M):

$$\left\{ \begin{array}{l} H \phi_{JMq}(\beta, \gamma, \theta_i) = E_q \phi_{JMq}(\beta, \gamma, \theta_i) \\ H = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \end{array} \right\}$$

DIRECT METHOD

Select an orthonormal, truncated expansion basis by choosing s at will. Write

$$\phi_{JMq} = \sum_i^{i_{\max}} a_i^q \psi_i^s, \quad i = (N_i, l_i, t_i, J, M).$$

E_q and a_i^q are the eigenvalues and associated eigenvectors of the matrix problem

$$[H] a_i^q = E_q a_i^q,$$

where

$$[H]_{ij} = \langle \psi_i^s | H | \psi_j^s \rangle.$$

$[H]_{ij}$ may be written in terms of standard reduced matrix elements:

$$[H]_{ij} = \frac{\hbar^2 s^2}{B} \left[\left(N_j + \frac{5}{2} \right) \delta_{ij} - \frac{1}{2} \langle i | \beta^2 | j \rangle + \frac{B}{\hbar^2 s^2} \langle i | V\left(\frac{\beta}{s}, \gamma\right) | j \rangle \right].$$

If $s = \bar{s}$ it follows that

$$[H]_{ij} = \hbar \sqrt{\frac{\bar{C}}{B}} [\bar{H}]_{ij}.$$

Thus if the same size expansion basis $[i_{\max}]$ is used, the two methods will result in identical solutions to the original problem.

VIA REDUCED PROBLEM

Choose $\bar{B}$ [energy·time²] and $\bar{C}$ [energy] at will. Make the change of variable

$$\beta' = \left[\frac{\bar{B} \bar{C}}{\hbar^2} \right]^{\frac{1}{2}} \beta = \bar{s} \beta,$$

and divide by $\hbar \sqrt{\bar{C}/\bar{B}} = \hbar \bar{\omega}$

This results in a dimensionless problem

$$\bar{H} \bar{\phi}_{JMq}(\beta', \gamma, \theta_i) = \bar{E}_q \bar{\phi}_{JMq}(\beta', \gamma, \theta_i)$$

$$\bar{H} = -\frac{\bar{B}}{\bar{B}} \left[\frac{1}{2} T(\beta', \gamma, \theta_i) \right] + \frac{1}{\hbar} \sqrt{\frac{\bar{B}}{\bar{C}}} V\left(\frac{\beta'}{\bar{s}}, \gamma\right).$$

The solutions of the original problem are related to the normalized solutions of this reduced problem by

$$E_q = \hbar \sqrt{\frac{\bar{C}}{\bar{B}}} \bar{E}_q$$

$$\phi_{JMq}(\beta, \gamma, \theta_i) = \bar{s}^{5/2} \bar{\phi}_{JMq}(\bar{s}\beta, \gamma, \theta_i).$$

The reduced problem is solved by choosing $\bar{s}$ and expanding in an orthonormal, truncated basis:

$$\bar{\phi}_{JMq} = \sum_i^{i_{\max}} \bar{a}_i^q \bar{\psi}_i^{\bar{s}}.$$

$\bar{E}_q$ and $\bar{a}_i^q$ are the eigenvalues and eigenvectors of the matrix problem

$$[\bar{H}] \bar{a}_i^q = \bar{E}_q \bar{a}_i^q$$

where

$$[\bar{H}]_{ij} = \langle \bar{\psi}_i^{\bar{s}} | \bar{H} | \bar{\psi}_j^{\bar{s}} \rangle.$$

$[\bar{H}]_{ij}$ may be written in terms of standard reduced matrix elements:

$$[\bar{H}]_{ij} = \frac{\bar{B}}{\bar{B}} \bar{s}^2 \left[\left(N_j + \frac{5}{2} \right) \delta_{ij} - \frac{1}{2} \langle i | \beta^2 | j \rangle + \frac{B}{\hbar^2 \bar{s}^2} \langle i | V\left(\frac{\beta}{\bar{s}}, \gamma\right) | j \rangle \right].$$

Figure 3.2. Direct and indirect methods of solving a generalized Bohr problem

D. E2 Transition Rates and Quadrupole Moments

The probability per unit time that a nucleus in an initial state ϕ_i will undergo a transition into a final state ϕ_f will be denoted T_{fi} ¹.

If the transition is effected by the emission of a photon of energy $\hbar\omega_p$, angular momentum L , projection μ , and parity $(-1)^L$, then T_{fi} is related to the matrix element of the electric multipole operator $E_{L\mu}$ by (3):

$$T_{fi} = \frac{8\pi(L+1)}{L[(2L+1)!!]^2} \frac{1}{\hbar} \left(\frac{\omega_p}{c} \right)^{2L+1} |\langle \phi_f | E_{L\mu}^* | \phi_i \rangle|^2 \quad (3.40)$$

As we are dealing with quadrupole surface vibrations, we expect that transitions between the positive parity states may be rapid when induced by the quadrupole operators $E_{2\mu}$. The spectroscopic quadrupole moment of the degenerate multiplet $(\phi_{JM}; M = 0, \pm 1, \dots, \pm J)$ will also be of interest, and is defined (3) as

$$Q = \left[\frac{16}{5} \pi \right]^{\frac{1}{2}} \langle \phi_{J,M=J} | E_{20} | \phi_{JJ} \rangle \quad (3.41)$$

Neglecting spin degrees of freedom, the electric multipole operators for a system of nucleons are (3)

$$E_{L\mu} = e \sum_{k=1}^Z (r_k)^L Y_{L\mu}(\theta_k, \phi_k) \quad (3.42)$$

¹The subscripts f and i will be understood to represent the angular momentum quantum numbers J and M , as well as any remaining labels q that may be required to further distinguish the states. For the purposes of this section, $J_i M_i$ will often be written in place of i , with q not being explicitly carried.

The neutrons do not contribute and (r_K, θ_K, ϕ_K) are the spherical polar coordinates of the K^{th} proton. The corresponding collective operator may be deduced in an adiabatic approximation (3) to be

$$E_{L\mu} = \int_{\text{nuclear volume}} \rho(r) r^L Y_{L\mu}(\theta, \phi) dV \quad (3.43)$$

where $\rho(r)$ is the charge density within the nuclear surface. If the charge density is assumed to have the uniform value ρ_e within the surface specified by

$$R = R_0 [1 + \sum_{\mu} \alpha_{\mu} Y_{2\mu}^*(\theta, \phi)] \quad , \quad (3.44)$$

then $E_{2\mu}$ may be easily expressed in terms of the collective coordinates

α_{μ} :

$$E_{2\mu} = \rho_e \int_S \left[\int_0^R r^2 (r^2 dr) \right] Y_{2\mu}(\theta, \phi) dS$$

$$dS = \sin \theta d\theta d\phi$$

$$S: \quad \begin{aligned} 0 &\leq \theta \leq \pi \\ 0 &\leq \phi \leq 2\pi \end{aligned}$$

$$= \frac{\rho_e R_0^5}{5} \int_S \left[1 + \sum_{\nu} \alpha_{\nu} Y_{2\nu}^* \right]^5 Y_{2\mu} dS$$

$$= \frac{\rho_e R_0^5}{5} \left\{ \int_S Y_{2\mu} dS + 5 \sum_{\nu} \alpha_{\nu} \int_S Y_{2\nu}^* Y_{2\mu} dS + 10 \sum_{\nu \epsilon} \alpha_{\nu} \alpha_{\epsilon} \right. \\ \left. \times \int_S Y_{2\epsilon}^* Y_{2\nu}^* Y_{2\mu} dS + \dots \right\}$$

$$\begin{aligned}
&= \frac{\rho_e R_o^5}{5} \left\{ 0 + 5\alpha_\mu + 10 \left[\frac{5}{4\pi} \right]^{\frac{1}{2}} C(222; 000) \right. \\
&\quad \left. \times \sum_{\nu \epsilon} C(222; \nu \epsilon \mu) \alpha_\nu \alpha_\epsilon + \dots \right\} \\
&= D_1 \alpha_\mu + D_2 [\alpha\alpha]_{2\mu} \quad , \tag{3.45}
\end{aligned}$$

through second order with

$$D_1 = \frac{3ZeR_o^2}{4\pi} = \rho_e R_o^5 ; \quad D_2 = -D_1 \left[\frac{10}{\sqrt{70} \pi} \right] \quad . \tag{3.46}$$

The second order term has been written in the notation of Equation (2.23).

In developing higher-order expressions, care must be taken to first modify Equation (3.44) which conserves volume only to first order in the α_μ . From the known transformation properties of the α_μ under rotations, $E_{2\mu}$ in Equation (3.45) may be seen to be properly labeled as the μ^{th} component of an irreducible tensor of angular momentum 2.

The expression for T_{fi} depends strongly on the energy difference between the initial and final states. Ignoring this, we concentrate on the state dependence. Furthermore we disregard information concerning the orientations of the initial and final states by averaging over the initial state projections, and summing over those of the final state and outgoing photon. In doing so we define the reduced transition rate

$$B(E2: J_i \rightarrow J_f) = \frac{1}{(2J_i + 1)} \sum_{M_i, M_f, \mu} |\langle \phi_{J_f M_f} | E_{2\mu}^* | \phi_{J_i M_i} \rangle|^2. \tag{3.47}$$

Equation (3.47) may be rewritten by making use of the Wigner-Eckart theorem [Equation F.79], the orthogonality of the Clebsch-Gordon coefficients [Equation (F.46a)] and $E_{2\mu}^* = (-1)^\mu E_{2, -\mu}$ [Equations (2.4) and

(3.45)]. The last relation permits us to replace $E_{2\mu}^*$ by $E_{2\mu}$ in Equation (3.47).

$$\begin{aligned}
 B(E2: J_i \rightarrow J_f) &= \frac{1}{2J_i + 1} \sum_{M_i M_f \mu} |C(J_i 2J_f; M_i \mu M_f) \langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle|^2 \\
 &= \frac{|\langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle|^2}{(2J_i + 1)} \sum_{M_f} \left\{ \sum_{M_i \mu} [C(J_i 2J_f; M_i \mu M_f)]^2 \right\} \\
 &= \frac{(2J_f + 1)}{(2J_i + 1)} |\langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle|^2. \quad (3.48)
 \end{aligned}$$

The spectroscopic quadrupole moment may also be expressed in terms of the same reduced matrix element:

$$\begin{aligned}
 Q &= \sqrt{\frac{16\pi}{5}} C(J2J; J0J) \langle \phi_J || E_2 || \phi_J \rangle \\
 &= \sqrt{\frac{16\pi}{5}} \left[\frac{(2J)(2J-1)}{(2J+2)(2J+3)} \right]^{\frac{1}{2}} \langle \phi_J || E_2 || \phi_J \rangle. \quad (3.49)
 \end{aligned}$$

As illustrated in Figure 3.2, the eigenfunctions ϕ_{JM_q} of a generalized Bohr Hamiltonian are found, in practice, by solving an associated reduced problem. Matrix elements of any operator, for example

$$M_{fi} = \langle \phi_{J_f M_f} | E_{2\mu} | \phi_{J_i M_i} \rangle \quad (3.50)$$

$$= \int_{\Omega} d\Omega(\beta, \gamma, \theta_i) \phi_{J_f M_f}(\beta, \gamma, \theta_i) E_{2\mu}(\beta, \gamma, \theta_i) \phi_{J_i M_i}(\beta, \gamma, \theta_i), \quad (3.51)$$

should be independent of the method of solution. That is they should be

independent of the choice of the reduced problem $(\bar{B}, \bar{C})$ and of the expansion basis used in solving the reduced problem $(\tilde{s})$. Using the change of variables $\beta' = \bar{s}\beta = [\bar{B} \bar{C}/\hbar^2]^{\frac{1}{4}} \beta$, M_{fi} may be written in terms of the corresponding eigenfunctions of the reduced Hamiltonian, $\bar{\phi}_f$ and $\bar{\phi}_i$:

$$M_{fi} = \int_{\Omega(\beta', \gamma, \theta_i)} d\Omega(\beta', \gamma, \theta_i) \bar{\phi}_{J_f M_f}(\beta', \gamma, \theta_i) E_{2\mu}(\frac{\beta'}{\bar{s}}, \gamma, \theta_i) \bar{\phi}_{J_i M_i}(\beta', \gamma, \theta_i) \quad (3.52)$$

$$= \langle \bar{\phi}_{J_f M_f} | E_{2\mu}(\frac{\beta}{\bar{s}}, \gamma, \theta_i) | \bar{\phi}_{J_i M_i} \rangle \quad (3.53)$$

The prime on the (dummy) integration variable has been dropped in Equation (3.53). The radial dependence of $E_{2\mu}$ may be found by expressing Equation (3.45) in terms of Bohr coordinates. For the moment it is sufficient to recognize that $\alpha_\mu \propto \beta$ and hence we have

$$E_{2\mu}(\frac{\beta}{\bar{s}}, \gamma, \theta_i) = \frac{1}{\bar{s}} D_1 \alpha_\mu + \frac{1}{\bar{s}^2} D_2 [\alpha\alpha]_{2\mu} \quad (3.54)$$

We may now write

$$M_{fi} = \sum_{k=1}^2 \frac{D_k}{\bar{s}^k} \langle \bar{\phi}_{J_f M_f} | \Omega_{k,\mu}^{LAB} | \bar{\phi}_{J_i M_i} \rangle \quad (3.55)$$

with the definitions

$$\Omega_{1,\mu}^{LAB}(\beta, \gamma, \theta_i) = \alpha_\mu(\beta, \gamma, \theta_i) \quad ; \quad \Omega_{2,\mu}^{LAB} = [\alpha\alpha]_{2\mu} \quad (3.56)$$

Notice that in $\Omega_{k,\mu}^{LAB}$, the label k refers not to the angular momentum classification ($J = 2$ is understood) but rather to the fact that k factors of α are involved. The upper label LAB emphasizes that the

components μ are pseudo-spherical projections upon laboratory axes.

Equation (3.55) has a counterpart for reduced matrix elements,

$$\langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle = \sum_{k=1}^2 \frac{D_k}{\bar{s}^k} \langle \bar{\phi}_{J_f} || \Omega_k^{LAB} || \bar{\phi}_{J_i} \rangle \quad (3.57)$$

Matrix elements appearing on the right hand sides of Equations (3.55) and (3.57) depend implicitly upon $\bar{B}$ and $\bar{C}$ as the latter determine the form of the reduced Hamiltonian and hence affect its eigensolutions, $\bar{\phi}$.

However these matrix elements are fully determined by the reduced problem and their values should be independent of the choice of the expansion basis parameter $\tilde{s}$. This will be strictly true, of course, only when a complete (non-truncated) basis is employed.

As described in Appendix C, the computer code THEORY returns the original (non-orthonormal) basis expansion coefficients, b , of the $\bar{\phi}$:

$$\bar{\phi}_{J_f M_f} = \sum_{\alpha_f} b_{\alpha_f} \psi_{\alpha_f}^{\tilde{s}} \quad (3.58)$$

The numerical values of the b_{α_f} depend upon the choice of $\tilde{s}$. Reduced matrix elements may be conveniently evaluated by using Equation (3.58) to write

$$\langle \bar{\phi}_{J_f} || \Omega_k^{LAB} || \bar{\phi}_{J_i} \rangle = \sum_{\alpha_i \alpha_f} b_{\alpha_f}^* b_{\alpha_i} \langle \psi_{\alpha_f}^{\tilde{s}} || \Omega_k^{LAB} || \psi_{\alpha_i}^{\tilde{s}} \rangle \quad (3.59)$$

As shown in Appendix D, the explicit dependence upon $\tilde{s}$ may be isolated by rewriting the right hand side of the above equation in terms of standard reduced ($\tilde{s} = 1$) integrals. This results in

$$\begin{aligned}
\langle \bar{\phi}_{J_f} || \Omega_k^{LAB} || \bar{\phi}_{J_i} \rangle &= \left(\frac{1}{s} \right)^k \sum_{\alpha_i \alpha_f} b_{\alpha_f}^* b_{\alpha_i} \langle N_f l_f | \beta^k | N_i l_i \rangle \\
&\times \langle l_f v_f J_f || \frac{\Omega_k^{LAB}}{\beta^k} || l_i v_i J_i \rangle \quad . \quad (3.60)
\end{aligned}$$

The radial factor is defined to be

$$\langle N_f l_f | \beta^k | N_i l_i \rangle = \int_0^\infty f_{N_f l_f}(\beta) \beta^k f_{N_i l_i}(\beta) \beta^4 d\beta \quad . \quad (3.61)$$

Expressions for the remaining angular term may be found in Appendix D, where the manner of their accurate computation is described.

Recapitulating, energies, B(E2) transition rates and quadrupole moments are obtained by the following procedure:

- 1) $\bar{B}$ and $\bar{C}$ are chosen, and the original Schroedinger equation is transformed to a reduced problem with Hamiltonian $\bar{H}$.
- 2) The reduced problem is solved by expanding in the ψ^S . Energies and expansion coefficients (b) are returned for the eigenstates of $\bar{H}$ by the THEORY program.
- 3) Equation (3.60) is used to find reduced matrix elements of Ω_k^{LAB} between eigenstates ϕ of $\bar{H}$. [Angular matrix elements are precomputed as described in Appendix D. Radial factors may be rapidly found by using Equations (D.30)-(D.32).]
- 4) Reduced matrix elements between eigenstates of the original Hamiltonian are found with the aid of Equation (3.57).
- 5) Q and B(E2: $J_i \rightarrow J_f$) are calculated using Equations (3.49) and (3.48) respectively.

The calculation of quadrupole moments and transition rates is greatly speeded by the recognition that a number of selection rules exist which severely limit the contributing terms on the right-hand side

of Equation (3.59). As discussed in Section B of Appendix D, we have for the first and second order operators respectively:

$$\langle \tilde{\psi}_{N\ell\nu JM}^S | \Omega_{1\mu}^{LAB} | \tilde{\psi}_{N'\ell'\nu' J'M'}^S \rangle = 0 \text{ unless } \begin{cases} N = N' \pm 1 \\ \ell = \ell' \pm 1 \\ J' + 2 \geq J \geq |J' - 2| \\ M = M' + \mu \end{cases} \quad (3.62)$$

and

$$\langle \tilde{\psi}_{N\ell\nu JM}^S | \Omega_{2\mu}^{LAB} | \tilde{\psi}_{N'\ell'\nu' J'M'}^S \rangle = 0 \text{ unless } \begin{cases} N = N', N' \pm 2 \\ \ell = \ell', \ell' \pm 2 \\ J' + 2 \geq J \geq |J' - 2| \\ M = M' + \mu \end{cases} \quad (3.63)$$

The calculations required for the employment of Equation (3.60) may be further limited by restricting its use to cases for which $J_i \geq J_f$. For transitions in which this is not the case, $B(E2: J_f \rightarrow J_i)$ may be computed and a reversal formula employed. By virtue of Equation (3.42), the $E_{2\mu}$ operators obey

$$(E_{2\mu})^\dagger = (-1)^\mu E_{2,-\mu} \quad (3.64)$$

where $\dagger$ denotes Hermitean conjugation. For the collective form of the operators, Equation (3.40), this property may be seen to follow from

$$(\alpha_\mu)^\dagger = (\alpha_\mu)^* = (-1)^\mu \alpha_{-\mu} \quad (3.65)$$

As a consequence of Equation (3.64) we have

$$\langle \phi_{J_f M_f} | E_{2\mu} | \phi_{J_i M_i} \rangle = (-1)^{\mu} \langle \phi_{J_i M_i} | E_{2, -\mu} | \phi_{J_f M_f} \rangle^* \quad (3.66)$$

Applying the Wigner-Eckart theorem, and making use of symmetry properties of the Clebsch-Gordon coefficients, we deduce the reversal formula

$$\langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle = (-1)^{J_i - J_f} \left[\frac{2J_i + 1}{2J_f + 1} \right]^{\frac{1}{2}} \langle \phi_{J_i} || E_2 || \phi_{J_f} \rangle^* \quad (3.67)$$

This equation will, of course, hold if E_2 is replaced by either of the Ω_k^{LAB} .

In Section A of this chapter we saw that the reduced energy spectrum was the same for both H and $\bar{H}$. As a result, the investigation of possible reduced spectra possessed by a class of Hamiltonians could be speeded by an appropriate choice of a common reduced form. A similar situation exists for the ratios of $B(E2)$ transition rates if we confine ourselves to the first order term in the expression for $E_{2\mu}$. Then

$$\begin{aligned} \frac{B(E2: J_i^1 \rightarrow J_f^1)}{B(E2: J_i \rightarrow J_f)} &= \frac{\left(\frac{2J_f^1 + 1}{2J_i^1 + 1} \right) |\langle \phi_{J_f^1} || E_2 || \phi_{J_i^1} \rangle|^2}{\left(\frac{2J_f + 1}{2J_i + 1} \right) |\langle \phi_{J_f} || E_2 || \phi_{J_i} \rangle|^2} \\ &= \frac{\left(\frac{2J_f^1 + 1}{2J_i^1 + 1} \right) \left(\frac{D_1}{\bar{s}} \right)^2 |\langle \bar{\phi}_{J_f^1} || \Omega_1^{\text{LAB}} || \bar{\phi}_{J_i^1} \rangle|^2}{\left(\frac{2J_f + 1}{2J_i + 1} \right) \left(\frac{D_1}{\bar{s}} \right)^2 |\langle \bar{\phi}_{J_f} || \Omega_1^{\text{LAB}} || \bar{\phi}_{J_i} \rangle|^2} \quad (3.68) \end{aligned}$$

The dependence on $\bar{s}$ as well as that on the charge and radius of the droplet are seen to cancel. The ratio then depends solely on the

eigenfunctions of the reduced Hamiltonian.

I will close this chapter with a presentation of $B(E2)$'s for transitions between selected eigenstates of the Bohr Hamiltonian. They will prove useful for comparisons with later studies of generalized problems. Only the first order term of E_{2u} has been employed, and the selection rules of Equation (3.62) may be invoked. Restricting the principal quantum number to $N \leq 5$, 74 E2 transitions are allowed, and their reduced transition rates are presented in units of $[D_1/\bar{s}]^2$. The bulk of the results is contained in Figure 3.3. Anticipating the discussion of Chapter V, the levels have been grouped into wedge-shaped bands sitting atop $J = 0$ states. Individual levels have been labeled by the abbreviated notation J_i where i increases with increasing energy. The associated N , ℓ , and ν quantum numbers may be read from the figure.

Each $B(E2)$ is a product of a radial and an angular factor. The $m\beta$ band may be obtained by adding $2m$ units of N quantum number to every state of the ground state (GS) band. As a result, corresponding transitions within each band (i.e., $2_1 \rightarrow 0_1$, $2_3 \rightarrow 0_2$, $2_6 \rightarrow 0_4$, etc.) differ only in their radial factors. By arranging for these factors to cancel, we can obtain a large number of identities which connect transitions rates within the GS band to their counterparts among the β bands. For example

$$\frac{B(E2: 6_1 \rightarrow 4_1)}{B(E2: 3_1 \rightarrow 2_2)} = \frac{B(E2: 6_3 \rightarrow 4_3)}{B(E2: 3_2 \rightarrow 2_4)} = 1.4$$

The situation is more complicated for the γ bands which are obtained by

Figure 3.3. Selected B(E2) rates for transitions which connect Bohr eigenstates $[N \leq 5]$ belonging to the same band

Figure 3.4. Ground state band transitions not shown in Figure 3.3

Table 3.1. Comparison of $B(E2)$'s for in-band and interband transitions

$4_i \rightarrow 2_f$					$2_i \rightarrow 0_f$				
i	f	band _i	band _f	$B(E2: 4_i \rightarrow 2_f)$	i	f	band _i	band _f	$B(E2: 2_i \rightarrow 0_f)$
1	1	G ^a	G	1.00000	1	1	G	G	.50000
2	2	G	G	.78571					
3	3	β	β	1.28571	3	2	β	β	.70000
5	4	β	β	.96032	5	3	γ	γ	.73333
6	5	γ	γ	1.26623	6	4	2 β	2 β	.90000
<hr/>									
1	3	G	β	.28571	1	2	G	β	.20000
2	4	G	β	.17460	2	3	G	γ	.30000
2	5	G	γ	.19444	3	4	β	2 β	.40000
4	7	G	γ	.35714	4	3	β	γ	.06667
3	6	β	2 β	.57143	4	5	β	$\gamma+\beta$	.36667
5	5	β	γ	.03535	5	5	γ	$\gamma+\beta$	.13333

^aQuantum numbers and band assignments for a given Bohr state [such as 4_1] may be determined from Figure 3.3. G denotes the ground state band.

Table 3.2. Remaining transition rates for $N \leq 5$ states

J_i	J_f	band _i	band _f	$B(E2: J_i \rightarrow J_f)$	J_i	J_f	band _i	band _f	$B(E2: J_i \rightarrow J_f)$
2_3	2_2	B	G	.28571	6_3	4_4	B	G	.00271
3_1	2_4	G	B	.23810	6_3	5_1	B	G	.07273
4_3	3_1	B	G	.07407	6_3	6_2	B	G	.11570
4_4	3_2	G	B	.19259	8_1	6_3	G	B	.36364
4_2	4_3	G	B	.15873	3_1	2_5	G	γ	.65476
4_5	4_4	B	G	.16713	4_6	4_4	γ	G	.20401
5_1	3_2	G	B	.19091	5_1	4_6	G	γ	.67686
5_1	4_5	G	B	.08678	6_2	4_6	G	γ	.14018
6_1	4_3	G	B	.33333	3_2	2_5	B	γ	.11905
6_2	4_5	G	B	.24793	2_6	2_4	2B	B	.57143

adding multiples of $(N, \ell) = (3, 3)$ to the GS band. Nonetheless the sets of $B(E2)$'s for in-band transitions have a similar structure, with the magnitudes of the transition rates growing as we progress to higher bands. This results from the growth of the radial term:

$$|\langle N, \ell | \beta | N', \ell+1 \rangle|^2 = \frac{N + \ell + 5}{2} \delta_{N', N+1} + \frac{N - \ell}{2} \delta_{N', N-1} \quad (3.69)$$

For the in-band transitions shown in Figures 3.3 and 3.4,

$$\Delta \ell = \ell_f - \ell_i$$

and

$$\Delta N = N_f - N_i$$

have the same sign, and the first term in Equation (3.69) contributes. For the majority of the allowed transitions between bands, the opposite situation exists. $\Delta \ell$ and ΔN have opposite signs, the rightmost term in Equation (3.69) contributes, and the radial factor is consequently smaller on the average. This is the case in Tables 3.1 and 3.2 for the transitions of the types $GS \leftrightarrow \beta$, $\beta \leftrightarrow 2\beta$, and $\gamma + \beta \leftrightarrow \gamma$.

Care must be taken when comparing $B(E2)$ transition rates because of the angular momentum factors involved. In Table 3.1, all $4 \rightarrow 2$ and $2 \rightarrow 0$ transitions ($N \leq 5$) allowed in first order are listed, and in-band transitions may be directly compared with interband ones of the same initial and final angular momenta. $B(E2)$'s for transitions between states belonging to a single band are seen to be larger on the average by factors of 3.9 and 2.9 respectively for the two spin types.

Modulation by the radial factor is of course only part of the story as can be seen in Figure 3.4. $B(E2)$'s for the eight transitions in the topmost row range in value from .02 to 1, but all possess the same radial factor. The angular factor evidently discriminates against allowed in-band transitions between two levels that have a large lateral separation in the figure. In Chapter V we shall return to this point in connection with K-bands in deformed nuclei.

IV. TEST CALCULATIONS USING THE GNEUSS-GREINER HAMILTONIAN

Having concluded the mathematical preliminaries, we stand ready to explore the consequences of employing various collective potential energy functions in the generalized Bohr problem, Equation (3.1a). Once $V(\beta, \gamma)$ has been selected, such calculations may be carried out with the battery of computer programs described in Appendices C and D. As these codes are quite lengthy, a systematic testing policy was followed to establish their trustworthiness. The initial phase, including efforts to duplicate calculations reported by Rabotnov and Seregin (28), and Kumar and Baranger (43, 44), is summarized in Appendix C. An excellent opportunity for further testing was afforded by the model calculations which sprang from the work of G. Gneuss and W. Greiner (23-26). The present chapter reports my attempts to duplicate a collection of these calculations and to examine, in a realistic setting, the limitations of moderate basis calculations and their sensitivity to variations in $\tilde{s}$.

The Gneuss-Greiner (GG) technique is identical to my own in spirit. Each involves the diagonalization of a collective Hamiltonian in a basis of Bohr eigenfunctions. Each method calculates matrix elements between states [of good J] belonging to the physical chain of Equation (2.20); however, the calculational details differ vastly. In my own work, matrix elements are found within the intrinsic coordinate representation. The closed expressions of Chapter II are used for the ψ_α , and integrations which arise are analytically or numerically performed. Gneuss and Greiner, on the other hand, work exclusively in the creation/destruction

(C/D) operator representation, and write all dynamical quantities in terms of b^+ and b .

The form of the collective Hamiltonian of interest in this chapter is that employed by Habs et al. (29, 30):

$$H_{GG} = B_2 [\ddot{\alpha}\ddot{\alpha}]_0 + C_2 [\alpha\alpha]_0 + C_3 \left[[\alpha\alpha]_{2\alpha} \right]_0 + C_4 \{ [\alpha\alpha]_0 \}^2 + C_5 [\alpha\alpha]_0 \\ \times \left[[\alpha\alpha]_{2\alpha} \right]_0 + C_6 \left\{ \left[[\alpha\alpha]_{2\alpha} \right]_0 \right\}^2 + D_6 \{ [\alpha\alpha]_0 \}^3 \quad (4.1)$$

H_{GG} is clearly rotationally invariant, having been constructed from angular momentum scalars. The kinetic energy term may be rewritten in terms of the generalized momenta $\Pi^\mu \equiv \frac{\partial H_{GG}}{\partial \dot{\alpha}_\mu} = 2B_2 (-1)^\mu \alpha_{-\mu} / \sqrt{5}$,

$$B_2 [\ddot{\alpha}\ddot{\alpha}]_0 = B_2 \frac{1}{\sqrt{5}} \sum_\mu (-1)^\mu \dot{\alpha}_\mu \dot{\alpha}_{-\mu} \\ = \frac{\sqrt{5}}{4B_2} \sum_\mu (-1)^\mu \Pi^\mu \Pi^{-\mu} \\ = \frac{5}{4B_2} [\Pi\Pi]_0 \quad (4.2)$$

H_{GG} may consequently be written in terms of b^+ and b by the use of Figure 2.1. In the $(\beta, \gamma, \theta_i)$ representation, H_{GG} assumes the form

$$H_{GG} = \frac{\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V_{GG}(\beta, \gamma) \quad (4.3)$$

$$V_{GG}(\beta, \gamma) = \frac{C_2}{\sqrt{5}} \beta^2 - C_3 \sqrt{\frac{2}{35}} \beta^3 \cos 3\gamma + \frac{C_4}{5} \beta^4 - C_5 \sqrt{\frac{2}{175}} \beta^5 \cos 3\gamma \\ + C_6 \frac{2}{35} \beta^6 \cos^2 3\gamma + D_6 \frac{1}{5\sqrt{5}} \beta^6 \quad (4.4)$$

$$B = \frac{2B_2}{\sqrt{5}} \quad (4.5)$$

In the C/D representation, the calculation of matrix elements of H_{GG} may be reduced to the calculation of reduced matrix elements of b^+ between states of the physical chain. Such matrix elements are easily obtained between states of the natural chain, and Hecht (45) has done this. To make use of his values it is necessary to find the transformation coefficients which relate member states of the natural and physical chains. In the GG method this is accomplished by numerically solving a homogeneous system of linear equations. The equations are given by Hecht (45) and typically involve several hundred simultaneous unknowns for large values (~ 25) of the ℓ quantum number. Matrix elements of H_{GG} are eventually found in a truncated basis of eigenstates of

$$H_B = B_{2s} [\ddot{\alpha}\ddot{\alpha}]_0 + C_{2s} [\alpha\alpha]_0 \quad (4.6)$$

which appears as

$$H_B = \frac{-\hbar^2}{2 \left[\frac{2B_{2s}}{\sqrt{5}} \right]} T(\beta, \gamma, \theta_i) + \frac{1}{2} \left[\frac{2C_{2s}}{\sqrt{5}} \right] \beta^2 \quad (4.7)$$

in the intrinsic representation. In my notation, the eigenfunctions of Equation (4.7) are $\psi_\alpha^s(\beta, \gamma, \theta_i)$ with

$$s = \left[\frac{4B_{2s} C_{2s}}{5\hbar^2} \right]^{\frac{1}{4}} \quad (4.8)$$

My technique has been used to obtain the energy spectrum of H_{GG} for 23 sets of the parameters appearing in Equation (4.4). In Section A of this chapter I compare my results with those of equivalent calculations.

which use the GG method. Of the 23 cases, five representatives were selected for further study; the effects of varying $\tilde{s}$ and $N_{\text{MAX}}(J)$ are described in Section B. An analysis of the resulting calculations leads to the introduction of $\tilde{s}$ -curvature in Section C, where empirical methods for estimating $\tilde{s}^{\text{best}}$ and errors in calculated energies are set forth. In light of these methods, all 23 cases are reconsidered in Section D. Low spin calculations are again compared with those of Habs et al., and higher spin ($J \geq 8$) results are compared with experiment. In the final section, a method of estimating $\tilde{s}^{\text{best}}$ without diagonalizing is considered.

A. Preliminary Calculations

H_{GG} depends upon seven adjustable parameters: $B_2, C_2, C_3, C_4, C_5, C_6$ and D_6 . In 1972 D. Habs et al. applied this Hamiltonian to 21 nuclei in the $50 \leq (N, Z) \leq 82$ region. In each case the seven parameters were determined by fitting the low-energy experimental spectrum together with one quadrupole moment or reduced E2 transition rate. Theoretical energies for spins $0 \leq J \leq 6$, quadrupole moments, and $B(E2)$ rates were reported in (29) and (30). The second reference is essentially an abridged version of the first. Twenty-one isotopes divided among six elements were treated in each, however ^{134}Ba and ^{142}Sm were assigned different sets of parameters in the two references. The distinct parameter sets appearing in the second reference are denoted here as BA-134P and SM-142P respectively. The values of $B_2, C_2, \dots, D_6$ are tabulated to four significant digits in each reference; however, the

first also contains a series of figures which specify the parameters more precisely. When legible, values were taken from these figures which were available on microfilm only. Table 4.1 lists the parameter values assumed in the calculations of this chapter. Even though the values $B_2, C_2, \dots, D_6$ often differ markedly for neighboring nuclei, the shape of the potential well $[V_{GG}(\beta, \gamma)]$ varies systematically over the mass region. This may be seen in Figure 2 of Reference (30).

To obtain solutions to the Schroedinger equation for H_{GG} , I first performed a reduction of the type indicated in Figure 3.2.

$$H_{GG}(\beta', \gamma, \theta_i) \bar{\phi}(\beta', \gamma, \theta_i) = \bar{E} \bar{\phi}(\beta', \gamma, \theta_i)$$

results, and in every case the transformation constants, $\bar{B}$ and $\bar{C}$, were chosen such that the reduced Hamiltonian had:

- 1) $-\frac{1}{2}T(\beta', \gamma, \theta_i)$ as the kinetic energy operator, and
- 2) $\epsilon = 10^{-3}$ as the coefficient of $(\beta')^6$.

The mass parameter and asymptotic behavior of

$$\bar{H}_{GG}(\beta', \gamma, \theta_i) = -\frac{1}{2}T(\beta', \gamma, \theta_i) + \bar{V}_{GG}(\beta', \gamma) \quad , \quad (4.9)$$

$$\bar{V}_{GG}(\beta', \gamma) = \frac{1}{\hbar} \sqrt{\frac{\bar{B}}{\bar{C}}} V_{GG}\left(\frac{\beta'}{\bar{s}}, \gamma\right) \quad . \quad (4.10)$$

$$\bar{s} = \left[\frac{\bar{B} \bar{C}}{\hbar^2} \right]^{\frac{1}{4}} \quad (4.11)$$

for large β' were thus fixed. The two constraints force the choices

$$\bar{B} = B = \frac{2B_2}{\sqrt{5}} \quad , \quad (4.12)$$

Table 4.1. Model parameters for the Gneuss-Greiner Hamiltonian
[from References (29) and (30)]

Isotope	B_2 (10^{-42} MeV-sec ²)	C_2 (MeV)	C_3 (MeV)	C_4 (MeV)
BA-128	0.3585000D 02	-0.1989600D 03	0.2806000D 02	-0.1010800D 05
BA-130	0.8155000D 02	-0.2833000D 03	0.9978400D 03	-0.3527800D 05
BA-132	0.7435600D 02	-0.4492000D 03	-0.6271699D 04	-0.3235500D 05
BA-134	0.6362500D 02	-0.4334500D 03	-0.5868000D 05	-0.1028400D 06
BA-134P	0.6141000D 02	-0.3971000D 03	-0.5334000D 05	-0.9334000D 05
BA-136	0.8262000D 02	0.7016000D 02	-0.3348000D 04	-0.1720000D 04
CE-136	0.5610500D 02	-0.3464200D 03	-0.1516700D 05	-0.5223100D 05
CE-138	0.4464900D 02	0.1097500D 03	-0.1534460D 05	-0.3372600D 05
ND-138	0.5560000D 02	-0.3137300D 03	-0.1337000D 05	-0.4481300D 05
ND-140	0.3937100D 02	0.9529300D 02	-0.1246300D 05	-0.2562300D 05
SM-142	0.4422000D 02	0.1234200D 03	-0.1834200D 05	-0.4177500D 05
SM-142P	0.5095000D 02	0.8623000D 02	-0.3636000D 04	-0.4708000D 04
TE-120	0.7025000D 02	0.1680800D 03	0.4199400D 03	-0.7881098D 04
TE-122	0.6305700D 02	0.1175000D 02	-0.1612300D 03	-0.2988100D 03
TE-124	0.6445300D 02	-0.4270700D 02	-0.7177300D 03	0.2572600D 04
TE-126	0.7167000D 02	0.1936000D 02	-0.4213900D 03	0.1656100D 04
TE-128	0.8240000D 02	-0.8547000D 02	-0.1328700D 04	0.8149797D 04
TE-130	0.8904800D 02	-0.1035900D 03	-0.2620700D 04	0.1176700D 05
XE-126	0.7683400D 02	-0.5006500D 03	-0.8853797D 04	-0.2498800D 05
XE-128	0.8172000D 02	0.4917700D 03	0.1503200D 04	-0.7396500D 05
XE-130	0.1011800D 03	0.5543800D 03	-0.1608100D 04	-0.9816100D 05
XE-132	0.1295000D 03	-0.6865900D 02	-0.6858800D 03	-0.1479000D 04
XE-134	0.1568600D 03	0.1334200D 03	-0.8906500D 04	-0.1694800D 04

	C_5 (MeV)	C_6 (MeV)	D_6 (MeV)
BA-128	-0.9671898D 04	0.1206800D 06	0.1921500D 06
BA-130	-0.1235800D 06	0.2046700D 07	0.1585500D 07
BA-132	0.4886900D 06	0.4687600D 07	0.1815000D 07
BA-134	0.5621100D 07	0.5054259D 08	0.5709100D 07
BA-134P	0.4745000D 07	0.4285000D 08	0.4740000D 07
BA-136	0.2051000D 06	0.5337000D 06	0.1908000D 06
CE-136	0.1233800D 07	0.1584900D 08	0.2089600D 07
CE-138	0.7748430D 06	0.2041020D 07	0.1143800D 07
ND-138	0.1030300D 07	0.1288200D 08	0.1698500D 07
ND-140	0.5506600D 06	0.1356800D 07	0.7603600D 06
SM-142	0.9507300D 06	0.2674600D 07	0.1411200D 07
SM-142P	0.1356000D 06	0.3241000D 06	0.1227000D 06
TE-120	-0.1083200D 05	0.1158400D 04	0.1419400D 06
TE-122	0.1155600D 05	-0.6761500D 04	0.4371900D 05
TE-124	0.4194300D 05	0.8434200D 05	0.1739800D 05
TE-126	0.2734000D 05	0.5319000D 05	0.8438699D 04
TE-128	0.1324900D 06	0.1969400D 06	0.1168100D 06
TE-130	0.2730000D 06	0.5575000D 06	0.2340000D 06
XE-126	0.5553500D 06	0.2075700D 07	0.1486600D 07
XE-128	-0.3276400D 05	0.4168300D 07	0.2073200D 07
XE-130	0.1486800D 06	0.4894300D 07	0.3561000D 07
XE-132	0.6409900D 05	0.8351100D 07	0.9756900D 05
XE-134	0.1021500D 07	0.3716000D 07	0.1084800D 07

Table 4.2. Expansion basis data used in reproducing the H_{GG} calculations of Habs et al. (29, 30)

	B_{2S} (10^{-42} MeV-sec ²)	C_{2S} (MeV)	$\bar{B}$ (10^{-42} MeV-sec ²)	$\bar{C}$ (MeV)	$\bar{A}\omega$ (MeV)	$\bar{s}$	$\bar{s}$	$\bar{s}$
BA-128	100.0000	250.0000	32.0652	481.8874	2.5517	14.6579	13.7423	1.0666
BA-130	100.0000	600.0000	72.9405	917.7853	2.3348	18.2442	19.8263	0.9202
BA-132	100.0000	1000.0000	66.5060	1028.3720	2.5883	20.7294	19.9328	1.0400
BA-134	100.0000	1200.0000	56.9079	1571.6957	3.8744	21.6962	22.5589	0.9618
BA-134 ^D	100.0000	1050.0000	54.9268	1828.6878	3.7979	20.9838	21.9430	0.9563
BA-136	100.0000	100.0000	73.8976	316.3126	1.3616	11.6570	15.2406	0.7649
CE-136	100.0000	1000.0000	50.1818	1270.2838	3.3117	20.7294	19.5851	1.0584
CE-138	100.0000	300.0000	39.9353	1053.5111	3.3607	15.3415	17.6528	0.8691
ND-138	100.0000	1200.0000	49.7302	1150.4436	3.1659	21.6962	19.0628	1.1381
ND-140	100.0000	230.0000	35.2145	914.7267	3.3547	14.3555	16.5127	0.8694
SM-142	100.0000	300.0000	39.5516	1175.8580	3.5889	15.3415	18.1007	0.8476
SM-142 ^D	100.0000	100.0000	45.5711	323.0131	1.7524	11.6570	13.5766	0.8586
TE-120	100.0000	400.0000	62.8335	295.8668	1.4283	16.4855	14.3925	1.1454
TE-122	100.0000	200.0000	56.3999	173.3159	1.1539	13.8626	12.2559	1.1311
TE-124	100.0000	40.0000	57.6485	108.1429	0.9015	9.2705	10.9525	0.8464
TE-126	100.0000	20.0000	64.1036	71.4231	0.6948	7.7955	10.1390	0.7689
TE-128	100.0000	70.0000	73.7008	247.8257	1.2070	10.6626	14.3291	0.7441
TE-130	100.0000	500.0000	79.6470	337.4161	1.3548	17.4313	15.7815	1.1045
XE-126	100.0000	900.0000	68.7224	915.5673	2.4025	20.1905	19.5215	1.0343
XE-128	100.0000	750.0000	73.0926	1048.3985	2.4929	19.2909	20.5076	0.9407
XE-130	100.0000	1100.0000	90.4581	1234.8341	2.4314	21.2293	22.5360	0.9420
XE-132	100.0000	4000.0000	115.8283	180.6721	0.8221	29.3159	14.8249	1.9775
XE-134	100.0000	500.0000	140.2998	547.3797	1.3001	17.4313	20.5188	0.8495

and

$$\bar{c} = \left[\frac{D_6 \hbar^2}{10B_2 \epsilon} \right]^{\frac{1}{2}} \quad (4.13)$$

So as to mirror the reported GG-model calculations, I employed an expansion basis approximately equivalent to that used by Habs et al. The latter authors resorted to bases of 25 phonons in the fitting process which determined the potential parameters. Slightly larger bases may have been used for their final diagonalizations. I chose to employ the largest basis available to me (Table 2.3), with $N_{MAX}(J)$ equaling 30, 27, 30, 25, 27 and 25 for $J = 0, 2, 3, 4, 5$ and 6 respectively. In diagonalizing H_{GG} , Habs et al. used eigenstates of H_B [Equation 4.6]. B_{2s} was fixed at 10^{-40} MeV-sec², and C_{2s} was stepped through a coarse grid to locate an optimal basis for each isotope. The best value of C_{2s} was taken by these authors to be that which roughly minimized the sum of the calculated absolute energies of the lowest few $J = 0$ levels. The values of B_{2s} and C_{2s} employed in the final diagonalizations were reported in (29) and (30), and they have been tabulated in Table 4.2. The corresponding values of s follow from Equation (4.8) and have also been listed.

Rather than diagonalizing H_{GG} in a basis ψ^s , we may, according to Figure 3.2, achieve an identical end result by diagonalizing $\bar{H}_{GG}$ in a basis $\psi^{\bar{s}}$ where

$$\bar{s} = \frac{s}{\bar{s}} = \left[\frac{4B_{2s}C_{2s}}{5\bar{B}\bar{c}} \right]^{\frac{1}{4}} \quad (4.14)$$

This in fact was done for the calculations performed for the present work. The value of $\tilde{s}$ used for each isotope may be found in Table 4.2, together with those of the transformation constants, $\bar{B}$ and $\bar{C}$. $\hbar\bar{\omega}$ is the scale factor relating the eigenvalues of H_{GG} and $\bar{H}_{GG}$:

$$E = (\hbar\bar{\omega})\bar{E} = \left(\hbar \sqrt{\frac{\bar{C}}{\bar{B}}} \right) \bar{E} \quad (4.15)$$

$\tilde{s}$ is approximately constant over the mass region due to the common form adopted for the reduced Hamiltonians. In the second constraint, ϵ was assigned the value 10^{-3} so as to make $\tilde{s} \sim 1$. The most notable exception occurs for Xe-132, with $\tilde{s} \approx 2.0$. This discrepancy arises from the fact that $C_6 \gg D_6$ for this parameter set. The asymptotic behavior of the potential,

$$V_{GG}(\beta, \gamma) \xrightarrow{\beta \rightarrow \infty} C_6 \frac{2}{35} \beta^6 \cos^2 3\gamma + D_6 \frac{1}{5\sqrt{5}} \beta^6, \quad (4.16)$$

is then not dominated by the D_6 term which appears as $\epsilon(\beta')^6$ in $\bar{H}_{GG}$.

In my initial energy calculations, all 23 isotopes were treated using the expansion bases described in Tables 2.3 and 4.2. The results appear in Table 4.3 where, for the most part, only those energies which have a counterpart in Reference (29) or (30) have been given. For each level, the result of the present work has been placed directly above the value quoted by Habs et al. All values are in MeV and refer to the relative energy above the ground state, with the exception of the ground state itself for which the absolute energy has been given. Overall agreement between the two sets of results is very good, indicating that

Table 4.3. Comparison of GG-model calculations. My result is listed above that of Habs et al. All energies are in MeV

J_i	0_1^+ (Abs.)	0_2^+	0_3^+	2_1^+	2_2^+	2_3^+	3_1^+	3_2^+	4_1^+	4_2^+	4_3^+	5_1^+	6_1^+	6_2^+
BA-128	-8.209	3.085	4.303	.281	.880	3.564	1.207	5.391	.770	1.639	2.348	1.959	1.405	2.623
	-8.209	3.085	4.303	.281	.879	3.563	1.207	5.390	.770	1.638	2.347	1.956	1.405	2.621
BA-130	-3.783	2.997	3.471	.356	.907	3.592	1.300	5.316	.903	1.816	2.415	2.126	1.592	2.925
	-3.783	2.997	3.469	.356	.906	3.591	1.300	5.316	.903	1.813	2.414	2.126	1.591	2.923
BA-132	-3.634	2.939	4.750	.465	1.034	3.621	1.507	5.669	1.126	2.207	2.764	2.497	1.941	3.573
	-3.634	2.939	4.748	.465	1.032	3.621	1.507	5.669	1.125	2.205	2.762	2.496	1.940	3.570
BA-134	-2.417	1.666	6.061	.645	1.175	2.652	1.469	5.495	1.448	2.522	3.212	2.606	2.321	4.016
	-2.339	1.725	6.200	.600	1.178	2.672	1.701	5.708	1.361	2.433	3.123	2.714	2.192	3.935
BA-134P	-2.487	1.710	6.057	.656	1.199	2.652	1.522	5.440	1.472	2.582	3.198	2.647	2.370	4.070
	-2.431	1.771		.607	1.164		1.622		1.369	2.431			2.190	
BA-136	1.723	1.584	2.178	.819	1.618	1.985	2.517	3.033	1.678	2.033	2.832	3.021	2.199	2.797
	1.723	1.589	2.181	.819	1.616	1.985	2.521	3.047	1.679	2.033	2.826	3.034	2.201	2.795
CE-136	-2.631	2.912	6.803	.549	1.113	3.926	1.572	6.245	1.308	2.538	3.121	2.723	2.245	4.164
	-2.620	2.927	6.852	.545	1.102	3.931	1.578	6.276	1.295	2.518	3.108	2.716	2.223	4.148
CE-138	.105	1.386	4.390	.781	1.481	2.465	2.514	4.359	1.732	2.318	3.030	3.189	2.433	3.577
	.105	1.392	4.393	.780	1.481	2.469	2.529	4.370	1.725	2.314	3.024	3.197	2.414	3.557
ND-138	-2.515	2.784	6.504	.523	1.064	3.751	1.500	5.962	1.248	2.427	2.979	2.604	2.144	3.979
	-2.504	2.798	6.553	.521	1.050	3.758	1.500	6.001	1.236	2.411	2.965	2.593	2.131	3.963
ND-140	.104	1.376	4.356	.775	1.470	2.446	2.495	4.326	1.719	2.301	3.007	3.165	2.414	3.550
	.104	1.382	4.359	.774	1.469	2.450	2.510	4.336	1.712	2.296	3.001	3.172	2.405	3.542

Table 4.3. Continued

J_i :	0_1^+ (Abs.)	0_2^+	0_3^+	2_1^+	2_2^+	2_3^+	3_1^+	3_2^+	4_1^+	4_2^+	4_3^+	5_1^+	6_1^+	6_2^+
SM-142	- .342	1.414	4.763	.768	1.499	2.389	2.417	4.528	1.747	2.373	2.992	3.130	2.490	3.620
	- .342	1.426	4.770	.768	1.498	2.398	2.442	4.545	1.741	2.367	2.986	3.144	2.481	3.609
SM-142F	1.710	1.431	2.343	.768	1.514	2.022	2.163	2.932	1.635	1.899	2.398	2.514	2.076	2.726
	1.709	1.420		.768	1.496		2.162		1.623	1.882			2.048	
TE-120	1.817	1.217	1.869	.560	1.201	2.038	1.830	3.804	1.151	1.854	2.547	2.532	1.800	2.555
	1.817	1.216	1.868	.560	1.200	2.038	1.830	3.803	1.151	1.853	2.545	2.531	1.800	2.553
TE-122	1.095	1.297	2.014	.565	1.226	2.028	1.984	3.758	1.178	1.900	2.749	2.742	1.834	2.625
	1.094	1.291	2.008	.564	1.215	2.018	1.982	3.755	1.175	1.881	2.736	2.742	1.831	2.602
TE-124	.953	1.147	1.945	.603	1.240	1.669	2.067	3.055	1.191	1.778	2.314	2.735	1.703	2.360
	.953	1.144	1.942	.602	1.234	1.663	2.066	3.053	1.190	1.773	2.302	2.734	1.830	2.601
TE-126	1.392	1.341	1.811	.669	1.361	1.745	2.139	2.945	1.345	1.849	2.182	2.834	1.909	2.209
	1.392	1.338	1.811	.668	1.354	1.740	2.138	2.954	1.343	1.840	2.170	2.833	1.852	2.136
TE-128	1.171	1.321	1.934	.743	1.459	1.795	2.663	4.224	1.433	1.877	2.574	3.604	1.879	2.517
	1.171	1.318	1.935	.743	1.452	1.789	2.663	4.229	1.429	1.867	2.562	3.603	1.828	2.502
TE-130	1.331	1.328	2.088	.839	1.468	1.917	2.919	4.233	1.520	1.963	2.829	3.901	1.894	2.791
	1.331	1.329	2.089	.838	1.468	1.917	2.919	4.235	1.520	1.963	2.824	3.901	1.894	2.791
XE-126	-5.062	2.094	4.435	.388	.891	2.642	1.352	4.413	.944	1.805	2.385	2.174	1.632	2.869
	-5.060	2.094	4.432	.388	.890	2.641	1.351	4.412	.944	1.803	2.383	2.174	1.632	2.867
XE-128	1.208	1.921	4.100	.444	.967	2.880	1.351	4.900	1.038	1.987	2.426	2.201	1.746	3.179
	1.210	1.920	4.099	.444	.965	2.879	1.351	4.902	1.038	1.985	2.425	2.200	1.746	3.177

Table 4.3. Continued

$J_i:$	0_1^+ (Abs.)	0_2^+	0_3^+	2_1^+	2_2^+	2_3^+	3_1^+	3_2^+	4_1^+	4_2^+	4_3^+	5_1^+	6_1^+	6_2^+
XE-130	1.475	1.877	3.573	.529	1.123	2.894	1.604	5.041	1.188	2.198	2.668	2.504	1.955	3.418
	1.475	1.877	3.571	.529	1.121	2.893	1.603	5.040	1.188	2.196	2.666	2.504	1.955	3.415
XE-132	1.031	1.619	3.220	.669	1.342	2.321	1.808	3.662	1.403	2.362	2.753	2.604	2.148	3.451
	1.032	1.638	3.340	.668	1.342	2.328	1.817	3.750	1.397	2.350	2.729	2.631	2.138	3.421
XE-134	1.789	1.503	2.089	.848	1.575	1.893	2.397	2.780	1.697	1.878	2.527	2.627	1.999	2.747
	1.789	1.513	2.089	.848	1.577	1.888	2.407	2.783	1.694	1.876	2.521	2.627	2.000	2.735

the MEWORK and THEORY computer codes perform properly. The same may be said of the BE2 package (see Appendix D). The largest anomalies occur for BA-134 and BA-134P, and are presumably due to differences in basis size. We shall see that even 25 phonons may not be enough to guarantee convergence in certain "realistic" situations.

B. Convergence Calculations for Representative Isotopes

The convergence properties of the expansion technique were next examined, in the hope of clarifying the minor discrepancies which appear in Table 4.3. In particular, the effects of the choices for $N_{MAX}(J)$ and $\tilde{s}$ upon the calculated energies were studied. Rather than treating all 23 isotopes, a representative sample of five was selected, and the investigation was further limited to the angular momentum values contained in $\{0, 3, 9, 10, 20\}$. This set includes the largest and smallest even and odd spins for which $N_{MAX}(J) \geq 25$ bases are readily available [Table 2.3].

In selecting the representative nuclei, preliminary calculations were needed to approximately rank all 23 isotopes on the basis of their convergence properties. The reduced form of the Schroedinger equation was used so as to treat all isotopes on an equal footing. As the potential energy function is of the form

$$\bar{V}_{GG}(\beta', \gamma) = \sum_{p=2}^6 c_p \beta'^p f_p(\gamma) \quad , \quad (4.17)$$

the results of Chapter III, Section C apply, and matrix elements of the reduced Hamiltonian may be written as

$$\begin{aligned} \langle \tilde{\psi}_i | \bar{H}_{GG} | \tilde{\psi}_j \rangle = \tilde{s}^2 \left[(N_i + \frac{5}{2}) \delta_{ij} - \langle i | \frac{1}{2} \beta^2 | j \rangle \right] \\ + \sum_{p=2}^6 c_p \tilde{s}^{-p} \langle i | \beta^p f_p(\gamma) | j \rangle \end{aligned} \quad (4.18)$$

Diagonal elements have the asymptotic properties

$$[\bar{H}_{GG}]_{ii} \xrightarrow{\tilde{s} \rightarrow 0^+} \epsilon [\langle i | \beta^6 | i \rangle + c'_6 \langle i | \beta^6 \cos^2 3\gamma | i \rangle] \tilde{s}^{-6}, \quad (4.19)$$

$$c'_6 = \frac{2\sqrt{5} c_6}{7D_6},$$

$$[\bar{H}_{GG}]_{ii} \xrightarrow{\tilde{s} \rightarrow \infty} \left[\frac{1}{2} (N_i + \frac{5}{2}) \right] \tilde{s}^2, \quad (4.20)$$

and we may expect the calculated energies, regarded as functions of $\tilde{s}$, to behave similarly in these limits. Such was indeed found to be the case for the $J = 0$ states of each of the 23 isotopes. An $N_{MAX}(0) = 30$ expansion basis was used with $\tilde{s}$ swept over sixteen equally spaced values in the range $.4 \leq \tilde{s} \leq 1.7$. For each isotope, calculated absolute energies of the five lowest states were graphed as functions of $\tilde{s}$, and curves resembling that of Figure 3.1b resulted. A healthy variety was observed in the widths of the central "flat" regions.

Such a region is of course only approximately flat, and typically possesses an absolute minimum near its center. In the vicinity of this minimum, the $\bar{E}$ - vs - $\tilde{s}$ curve is approximately parabolic:

$$\bar{E} - \bar{E}_B = K_1 (\tilde{s} - \tilde{s}_B)^2 \quad (4.21)$$

The constants $\bar{E}_B$, $\tilde{s}_B$ and K_1 may be found by fitting the parabolic form through three adjacent calculated points. The local curvature K_1 serves as an estimate of the sensitivity of $\bar{E}$ to changes in $\tilde{s}$. It was computed for the ground states of the 23 isotopes, and the isotopes were ordered accordingly. TE-122 had the lowest value of K_1 and was ranked first; BA-134 ranked twenty-third. The five isotopes selected for inclusion in the representative set, together with their rankings were

TE-122	BA-130	XE-126	SM-142	BA-134
1	9	11	18	23

The potential energy surfaces of these five isotopes exhibit a variety of shapes, as depicted in Figure 4.1.¹ Lines of constant $V_{GG}(\beta, \gamma)$ are shown on a polar coordinate system in which β is the radial variable and γ is measured counter-clockwise from the horizontal. Four of the surfaces possess non-spherical ($\beta \neq 0$) minima, with TE-122 being the lone exception. The surface for BA-134 differs most strongly from the paraboloid of the expansion basis Hamiltonian. Reflection symmetry about $\gamma = 60^\circ$ is evident in all five cases.

Following the selection of the representative isotopes, a series of calculations was performed in which both $\tilde{s}$ and $N_{MAX}(J)$ were varied. The former was swept through twenty equally spaced values in the range $.45 \leq \tilde{s} \leq 1.7$, while the latter assumed each of the values:

¹Figure 4.1 has been assembled from drawings contained in Reference (29).

Figure 4.1. Potential energy functions $V_{GG}(\beta, \gamma)$ for the representative isotopes [taken from Reference (29)]

Time required to assemble $\bar{H}_{GG}$
and find the first five
eigenvalues and eigenvectors

J:	0	3	9	10	20
$N_{MAX}(J)$:	30	30	25	25	25

Figure 4.2. Typical computation times [IBM 370/158] for maximal-basis calculations

$^{130}_{56}\text{Ba}_{74}$
 Convergence
 Studies

Figure 4.3. Dependence of calculated absolute energy on $\tilde{S}$ and $N_{\max}(J)$ for selected eigenstates (J_i^+) of H_{GG} [BA-130]

Figure 4.4. Dependence of calculated absolute energy on $\tilde{s}$ and $N_{\max}(J)$ for selected eigenstates (J_i^+) of H_{GG} [BA-134]

$^{142}_{62}\text{Sm}_{80}$
Convergence
Studies

Figure 4.5. Dependence of calculated absolute energy on $\tilde{s}$ and $N_{max}(J)$ for selected eigenstates (J_i^+) of H_{GG} [SM-142]

$^{122}_{52}\text{Te}_{70}$
Convergence
Studies

Figure 4.6. Dependence of calculated absolute energy on $\tilde{s}$ and $N_{\max}(J)$ for selected eigenstates (J_i^+) of H_{GG} [TE-122].

$^{126}_{54}\text{Xe}_{72}$
Convergence
Studies

Figure 4.7. Dependence of calculated absolute energy on $\tilde{S}$ and $N_{\text{max}}(J)$ for selected eigenstates (J_i^+) of H_{GG} [XE-126]

$$N_{\text{MAX}}(J) = \begin{cases} 15, 20, 25, 30 & [J = 0, 3] \\ 15, 20, 25 & [J = 9, 10, 20] \end{cases}$$

Absolute energies for the five lowest states of each spin were computed and stored, 340 diagonalizations being required for each isotope.

Typical computation times for maximal basis calculations are indicated in Figure 4.2.

The results of the energy level calculations are displayed graphically in Figures 4.3-4.7. The horizontal coordinate is $\tilde{s}$, and each curve represents the calculated absolute energy (MeV) found when using a fixed value of $N_{\text{MAX}}(J)$. $N_{\text{MAX}}(J)$ has been labeled for the uppermost energy level only; without exception increasing $N_{\text{MAX}}(J)$ was found to lower the resulting curve. As always, J_i denotes the i^{th} lowest energy state of angular momentum J . To avoid overcrowding and intersections, all J_i have not been shown, and some of the individual curves have been truncated past the points where they rise steeply. Convergence [in both $N_{\text{MAX}}(J)$ and $\tilde{s}$] can be seen to range from excellent in the case of TE-122, where 15 phonons usually suffice, to poor for BA-134 where 25 phonons do not. The double minimum in the potential energy surface of SM-142 results in an additional ripple upon the calculated energy curves of certain states.

The main features of Figures 4.3-4.7 may be summarized as follows:

- 1) The energy curves rise very sharply for $\tilde{s} \ll 1$ and more slowly for $\tilde{s} \gg 1$, in qualitative agreement with the expected asymptotic behavior.
- 2) In all cases, increasing the size of the basis while holding $\tilde{s}$ fixed lowered the calculated energy.

- 3) The central "flat" region broadens as the number of phonons is increased. This effect is not very pronounced in the case of BA-134.
- 4) Within a given isotope, the rate of convergence [in $N_{MAX}(J)$] is best for states of lower energy. For fixed J and $N_{MAX}(J)$, states of lower energy possess broader flat regions.
- 5) For fixed $N_{MAX}(J)$, the optimal value of $\tilde{s}$ (center of the flat region) is approximately the same for all levels within a given isotope. As $N_{MAX}(J)$ increases, the optimal $\tilde{s}$ shifts slightly to higher values.

The expansion technique used throughout this thesis possesses an inherent flaw: the expansion basis upon truncation is no longer a complete set. A given function [such as $\phi_{JMq}(\beta, \gamma, \theta_i)$ of H] can be only approximately represented as a finite linear combination of basis functions. Calculated quantities consequently differ from their exact counterparts. The coefficients a_i in the calculated solution

$$\phi = \sum_{i=1}^n a_i \psi_i^s$$

are determined by solving the set of n linear equations

$$\sum_{j=1}^n \langle \psi_i^s | H | \psi_j^s \rangle a_j = E a_i \quad [i = 1, 2, \dots, n]$$

Multiplication by a_i^* and summing over i yields

$$\sum_{i,j} a_i^* \langle \psi_i^s | H | \psi_j^s \rangle a_j = E \sum_{i=1}^n a_i^* a_i$$

Hence, the calculated energy E is seen to equal the expectation value of H in the calculated state ψ :

$$\langle \phi | H | \phi \rangle = E$$

A lower limit for E may be deduced by expanding ϕ in terms of the exact eigenfunctions ϕ_i^x of H (ordered by increasing energy: $E_i^x \leq E_{i+1}^x$). In this case

$$\phi = \sum_{i=1}^{\infty} a_i^x \phi_i^x$$

and

$$\begin{aligned} E &= \langle \phi | H | \phi \rangle \\ &= \sum_{i=1}^{\infty} |a_i^x|^2 E_i^x \\ &\geq \sum_{i=1}^{\infty} |a_i^x|^2 E_1^x = E_1^x \end{aligned} \quad (4.22)$$

Hence the calculated energy may be no smaller than the lowest exact eigenvalue of the spin in question. As $N_{\text{MAX}}(J)$ tends to infinity, the source of the inherent error is removed and calculated energies approach their exact counterparts. For the lowest-lying state of a given spin, the exact energy is approached from above. The same appears to be true for all states considered in the representative isotope calculations. However there is no guarantee that this will always be the case.

The curves in Figures 4.3-4.7 have been only coarsely determined due to the limited number of $\tilde{s}$ values used. To further investigate the flatness of the central regions, finer resolution is required. Such calculations were carried out for the $J = 0, 3$ states of Xe-126, with $\tilde{s}$

Figure 4.8. Calculated absolute GS energy for H_{GG} [XE-126]. [The vertical (energy) scale and zero are different for each curve.]

Figure 4.9. Calculated absolute energies for $J = 0$ states of H_{GG} [$XE=126$]. [The vertical zero of energy is different for each curve.]

Figure 4.10. Calculated absolute energy of the 3_1 state of ^{126}Xe [XE-126].
[The vertical (energy) scale and zero are different for each curve.]

Figure 4.11. Calculated absolute energy of the $J_i = 3_2$ state of HgG [XE-126]. [The vertical (energy) scale and zero are different for each curve.]

varied from .7 to 1.4 in increments of .01. Results are displayed in Figures 4.8-4.11 which have been assembled and scaled to illustrate several of the points previously made in summary of the convergence calculations. The flat regions have been magnified and display considerable fine structure that is not due to arithmetical inaccuracies. [In TE-122, the ground state energy varies only in the tenth decimal place as $\tilde{s}$ varies by 20%; this sets an upper limit on numerical errors.] For the 3_1^+ level of XE-126, the form of the fine structure persists as $N_{\text{MAX}}(3)$ is increased.

C. $\tilde{s}$ -curvature and Error Estimation

In light of Figures 4.3-4.7, it is clear that the result of diagonalizing H_{GG} in a 25-phonon expansion basis need not produce accurate results, particularly if $V_{\text{GG}}(\beta, \gamma)$ is strongly γ dependent. Even if the basis is large enough, a proper choice of $\tilde{s}$ is crucial and some searching on this parameter will be inevitable. Such a series of calculations, in which $N_{\text{MAX}}(J)$ is fixed and $\tilde{s}$ varied, will produce curves like those of the previous section, leaving us with the problem of selecting a best estimate for each energy eigenvalue. Two methods were used in analyzing the representative-isotope calculations. For fixed $N_{\text{MAX}}(J)$ and J_i , each method yields:

- 1) $\bar{E}_B$, a best estimate of the eigenvalue $\bar{E}$ of $\bar{H}_{\text{GG}}$;
- 2) an associated optimal value, s_B , of the basis parameter;
and
- 3) the $\tilde{s}$ -curvature, K , which measures the sensitivity of $\bar{E}_B$

to changes in $\tilde{s}$ near $\tilde{s}_B$.

As we shall see, the third quantity may be used to estimate the error in the calculated energy.

The first method is based on the premise that increasing $N_{MAX}(J)$ will lower the calculated energies. Hence, for fixed $N_{MAX}(J)$, the lowest calculated value of an energy eigenvalue would be the most accurate. Following the procedure used in Section B to select the representative isotopes, a parabola was fit to the lowest minimum of each $\bar{E} - \text{vrs} - \tilde{s}$ curve. The curves appearing in Figures 4.3-4.7 have each been determined by twenty points, $\{(\tilde{s}^i, \bar{E}^i); i = 1, 2, \dots, 20\}$. The point with lowest energy, $(\tilde{s}^M, \bar{E}^M)$, and its two immediate neighbors were used in the fitting:

$$\bar{E}^i - \bar{E}_B = K_1 (\tilde{s}^i - \tilde{s}_B)^2 \quad ; \quad i = M-1, M, M+1. \quad [\text{Method I}] \quad (4.23)$$

Local fluctuations in $\bar{E} - \text{vrs} - \tilde{s}$ curves, of the type seen in Figures 4.8-4.11, may occur for changes in $\tilde{s}$ on the order of the step size

$$\Delta \tilde{s} = (\tilde{s}^{i+1} - \tilde{s}^i)$$

The values of $\bar{E}_B$, $\tilde{s}_B$ and K_1 consequently depend to some extent upon the placement of the $\tilde{s}^i$, as illustrated in Figure 4.12. [The variability of K_1 could perhaps be moderated by foregoing the local curvature in favor of a global one, W . However this avenue was not pursued.] When a relative maximum neighbors the lowest minimum, method I was generally found to overestimate the local curvature and to shift $\tilde{s}_B$ from the visually estimated optimal value. In such cases, a second parabola was

Figure 4.12. Global and local approaches to defining the $\bar{s}$ -curvature. In the latter approach, $K = K_i$ [of Equation (4.23)] may be sensitive to the locations of calculated points

fitted through the maximum, and the values of $\tilde{s}_B$ and $|K_1|$ were averaged. $\bar{E}_B$ was not modified.

The second method for estimating energies adopts the view that $\bar{E}_B$ should be locally independent of $\tilde{s}$. $\tilde{s}_B$ is consequently chosen to lie in the center of the "locally flattest" region, i.e. that three-point region over which the $(\tilde{s}^i, \bar{E}^i)$ data are most nearly a horizontal line. For each three-point region ($j = 2, 3, 4, \dots, 19$), $\bar{E}_B$ and

$$\chi^2 = \frac{1}{3} \sum_{i=j-1}^{j+1} (\bar{E}^i - \bar{E}_B)^2$$

are determined by the condition that

$$\frac{d(\chi^2)}{d\bar{E}_B} = 0 \rightarrow \bar{E}_B = \frac{1}{3} \sum_{i=j-1}^{j+1} \bar{E}^i \quad [\text{Method II}] \quad (4.24)$$

The best energy estimate is taken from that region for which χ^2 is smallest ($j = M'$), and s_B lies at the center

$$\tilde{s}_B = \tilde{s}^{M'} \quad [\text{Method II}] \quad (4.25)$$

For the curvature

$$K_2 = \frac{\chi^2}{[\tilde{s}^{M'+1} - \tilde{s}^{M'-1}]^2} \quad [\text{Method II}] \quad (4.26)$$

is used. The denominator represents an effort to make K_2 approximately independent of the lateral distance between neighboring points.

Each of these two methods was applied to the information gathered during the representative isotope diagonalizations, and the resulting

values of E_B , $\tilde{s}_B$ and K have been listed in Tables E.1 and E.2. Absolute energies in MeV

$$E_B = [\hbar\omega]\bar{E}_B$$

have been given. Method I is guaranteed to produce a lower value for a given energy eigenvalue, but this small difference is not usually apparent in the tables. The observations of Section B which summarized the basic properties of the $\bar{E}$ - vs - $\tilde{s}$ curves are given quantitative verification by Tables E.1 and E.2. With only scattered exceptions, the following trends may be noted for each isotope.

- 1) Both $\bar{E}_B$ and K_i decrease as $N_{MAX}(J)$ increases.
- 2) For fixed J and $N_{MAX}(J)$, K_i is lower for states of lower energy; furthermore the values of $\bar{E}_B$ converge faster for such states as $N_{MAX}(J)$ increases.
- 3) For fixed $N_{MAX}(J)$, $\tilde{s}_B$ is approximately independent of spin and eigenvalue number. $\tilde{s}_B$ increases with increasing $N_{MAX}(J)$.

The first two points suggest a relationship between K_i and the rate of change of $\bar{E}_B$ with increasing N_{MAX} . Such a relationship may be exploited to estimate the magnitude of errors in calculated energies.

If we adopt the detailed notation

$\bar{E}_N(J_i)$ = calculated eigenvalue of $\bar{H}_{GG}$ for the state J_i ,
found using an N -phonon, $\tilde{s}_B$ basis;

$K_N(J_i)$ = associated $\tilde{s}$ -curvature near $\tilde{s}_B$ (determined by
either of the two methods)

then the (positive) error in the calculated eigenvalue is

$$\begin{aligned}\Delta\bar{E}_N(J_i) &= \bar{E}_N(J_i) - \bar{E}_\infty(J_i) \\ &= \bar{E}_N(J_i) - \bar{E}_{N_T}(J_i) + [\bar{E}_{N_T}(J_i) - \bar{E}_\infty(J_i)]\end{aligned}$$

The term in brackets is simply the error in the N_T -phonon calculation.

It may be neglected if $N_T \gg N$ and if the N_T -phonon calculation is well converged. The latter is expected to be true if $K_T = K_{N_T}(J_i)$ is less than some small upper value K^{TOP} . Hence

$$\Delta\bar{E}_N(J_i) \approx \bar{E}_N(J_i) - \bar{E}_{N_T}(J_i) \quad \text{if} \quad \begin{cases} N_T \gg N \\ K_T < K^{TOP} \end{cases} \quad (4.27)$$

Equation (4.27) may be used in conjunction with Tables E.1 and E.2 to estimate the error in $\bar{E}_B$ for each state included in the representative-isotope calculations. In this manner an approximate relationship between $\Delta\bar{E}_N(J)$ and $K_N(J_i)$ can be established. In practice $N_T = 30, 30, 25, 25, 25$ were used for $J = 0, 3, 9, 10, 20$ respectively, and $N_T \gg N$ was taken to mean $N_T \geq N + 5$. K^{TOP} was chosen such that Equation (4.27) was satisfied in ~100 instances. The resulting values of estimated error extended over several orders of magnitude, as did the previously calculated curvatures. Consequently the pairs $(K_N(J_i), \Delta\bar{E}_N(J_i))$ were plotted on log-log axes. The results are shown in Figures 4.13 and 4.14, where methods I and II have been used respectively. In each case the points appear to be randomly distributed about a straight line

Figure 4.13. Estimated error [Equation (4.27)] versus curvature K_1 [Equation (4.23)] compiled from H_{GG} representative isotope calculations

Figure 4.14. Estimated error [Equation (4.27)] versus curvature K_2 [Equation (4.26)] compiled from H_{GG} representative isotope calculations

$$y = b_0 + b_1 x \quad \begin{cases} y_i = \log_{10}[\Delta \bar{E}_N(J_i)] \\ x_i = \log_{10}[K_N(J_i)] \end{cases} \quad (4.28)$$

The central line in either figure represents the least squares straight line [LSSL] through the data. The neighboring lines are parallel to the LSSL and one standard deviation

$$\sigma = \left[\frac{1}{n} \sum_{j=1}^n (y - y_j)^2 \right]^{\frac{1}{2}}, \quad n = \text{number of } (x_j, y_j) \text{ pairs} \quad (4.29)$$

above and below it. For a gaussian distribution, 68% of the n points would be expected to lie within the two outer lines. The LSSL was found to be relatively independent of isotope, spin and basis size.

The energy error and $\tilde{s}$ -curvature are related by a power law

$$\Delta \bar{E}_N(J_i) = 10^{b_0} [K_N(J_i)]^{b_1} \quad (4.30)$$

for points on the LSSL. The power law parameters and standard deviations are listed in Table 4.4 for several choices of K^{TOP} .

Table 4.4. Power law parameters

	K^{TOP}	Number of points (n)	b_0	b_1	σ
Method I	10^{-3}	83	-2.103	1.036	.477
	* 5×10^{-3}	118	-2.081	1.035	.461
	10^{-2}	130	-2.054	1.043	.455
Method II	10^{-9}	85	- .1430	.511	.410
	* 10^{-8}	114	- .1116	.512	.394
	10^{-7}	139	+ .0267	.527	.393

Asterisks indicate the values of K^{TOP} employed throughout the remainder of this chapter, and used in the construction of Table 4.5. For a given curvature, the five columns list respectively the errors associated with points that are 2σ below, σ below, on, σ above, and 2σ above the LSSL. The table may be used to estimate the error in the calculated energy when only the curvature is known. For example if method I finds K_1 to be .01, the associated $\Delta\bar{E}$ has only a .16 probability of lying higher than 1σ above the LSSL. Consequently $\Delta\bar{E}$ will be less than .0002041 84% of the time. Similarly $\Delta\bar{E} < .00059$ 95 times out of 100.

D. Application of the Error Estimation Methods

The most straightforward way to test the adequacy of an N-phonon diagonalization consists of dramatically increasing the size of the basis and redoing the problem. If the additional basis functions do not

Table 4.5. Estimated energy error versus $\tilde{s}$ -curvature for methods I and II. Least squares straight lines [LSSL's] are those of Figures 4.13 and 4.14

s-curvature		Estimated error $\Delta \bar{E}$ for points that are				
K_1		2 σ below LSSL	1 σ below LSSL	on LSSL	1 σ above LSSL	2 σ above LSSL
0.10000D-04	Method I	0.0000000	0.0000000	0.0000001	0.0000002	0.0000005
0.50000D-04		0.0000000	0.0000001	0.0000003	0.0000008	0.0000025
0.10000D-03		0.0000001	0.0000002	0.0000006	0.0000017	0.0000050
0.50000D-03		0.0000004	0.0000011	0.0000032	0.0000092	0.0000266
0.10000D-02		0.0000009	0.0000023	0.0000065	0.0000188	0.0000544
0.50000D-02		0.0000041	0.0000119	0.0000344	0.0000996	0.0002880
0.10000D-01		0.0000084	0.0000244	0.0000706	0.0002041	0.0005902
0.50000D-01		0.0000447	0.0001291	0.0003734	0.0010797	0.0031221
0.10000D 00		0.0000915	0.0002646	0.0007652	0.0022125	0.0063977
0.50000D 00		0.0004841	0.0013999	0.0040478	0.0117045	0.0338443
0.10000D 01		0.0009920	0.0028685	0.0082946	0.0239843	0.0693525
0.50000D 01		0.0052479	0.0151746	0.0438786	0.1268781	0.3668777
0.10000D 02		0.0107538	0.0310953	0.0899144	0.2599942	0.7517926
K_2						
0.10000D-12	Method II	0.0000000	0.0000001	0.0000002	0.0000004	0.0000011
0.50000D-12		0.0000001	0.0000002	0.0000004	0.0000010	0.0000024
0.10000D-11		0.0000001	0.0000002	0.0000006	0.0000014	0.0000034
0.50000D-11		0.0000002	0.0000005	0.0000013	0.0000032	0.0000078
0.10000D-10		0.0000003	0.0000007	0.0000018	0.0000045	0.0000112
0.50000D-10		0.0000007	0.0000017	0.0000041	0.0000103	0.0000254
0.10000D-09		0.0000010	0.0000024	0.0000059	0.0000146	0.0000363
0.50000D-09		0.0000022	0.0000054	0.0000134	0.0000333	0.0000826
0.10000D-08		0.0000031	0.0000077	0.0000192	0.0000475	0.0001178
0.50000D-08		0.0000071	0.0000176	0.0000437	0.0001083	0.0002684
0.10000D-07		0.0000101	0.0000251	0.0000623	0.0001544	0.0003827
0.50000D-07		0.0000231	0.0000572	0.0001419	0.0003518	0.0008722
0.10000D-06		0.0000329	0.0000816	0.0002023	0.0005016	0.0012435
0.50000D-06		0.0000750	0.0001860	0.0004611	0.0011431	0.0028338
0.10000D-05		0.0001070	0.0002652	0.0006574	0.0016298	0.0040403
0.50000D-05		0.0002438	0.0006043	0.0014981	0.0037139	0.0092070
0.10000D-04		0.0003476	0.0008616	0.0021360	0.0052953	0.0131272
0.50000D-04		0.0007920	0.0019634	0.0048675	0.0120667	0.0299140
0.10000D-03		0.0011292	0.0027994	0.0069400	0.0172045	0.0426510
0.50000D-03		0.0025733	0.0063793	0.0158146	0.0392053	0.0971921
0.10000D-02		0.0036689	0.0090955	0.0225482	0.0558983	0.1385740
0.50000D-02		0.0083607	0.0207266	0.0513824	0.1273798	0.3157814

significantly contribute in the expansions of the lower energy states, convergence is indicated for these states. Unfortunately such an approach is not always practical, though some insight may be gained by observing the effect of reducing the basis size. The work of the previous section offers an alternative method of estimating the convergence of energy eigenvalues. Furthermore, the information required to compute the $\tilde{s}$ -curvature will be readily available from the $\tilde{s}_B$ search that necessarily accompanies a careful calculation.

Armed with this method, the 23 parameter sets of Table 4.1 were reconsidered. For each isotope and each of the spins $J = 0, 2, 3, 4, 5, 6$, $[\bar{H}_{GG}]$ was diagonalized in a maximal basis for five values of $\tilde{s}$. The step size satisfied $\Delta\tilde{s}/\tilde{s}_B \approx .05$ as was the case in the calculations leading to the power law, Equation (4.30). The center of the $\tilde{s}$ region surveyed for each isotope had been indicated by the original 16-point $\tilde{s}$ -sweep of the $J = 0$ states. It was further refined as the calculations for higher spins progressed. Results appear in Table E.3, with method I having been used in the computation of $\bar{E}_B$, $\tilde{s}_B$, K_1 and $\Delta\bar{E}$. Relative energies above the ground state [in MeV] have been tabulated for the excited states. They may be readily compared with the values of Habs et al., which have been placed immediately below my own. Error estimates given in Table E.3 are for points one σ above the LSSL, and hence are upper limits on the true error in $\sim 84\%$ of the cases. The estimates have been translated into MeV by using Table 4.2, and

$$\Delta E = [\hbar\omega]\Delta\bar{E} \quad (4.31)$$

Averages of the percentage energy difference

$$\left| \frac{\begin{array}{c} E(J_i) \\ \text{this work} \end{array} - \begin{array}{c} E(J_i) \\ \text{Habs et al.} \end{array}}{\begin{array}{c} E(J_i) \\ \text{Habs et al.} \end{array}} \right| \cdot 100\%$$

have been tabulated and are listed by level type and isotope in Tables 4.6 and 4.7 respectively.

Table 4.6. Mean percentage energy difference (averaged over isotopes)

Spin	Level:	1	2	3
0		0.495	0.753	0.535
2		0.915	0.570	0.250
3		1.048	0.562	
4		0.924	0.635	0.424
5		0.470		
6		1.352	0.952	

Table 4.7. Mean percentage energy difference (averaged over J_i)

BA-128	0.05	BA-130	0.04	BA-132	0.05
BA-134	4.76	BA-134P	6.26	BA-136	0.20
CE-136	0.56	CE-138	0.30	ND-138	0.57
ND-140	0.25	SM-142	0.35	SM-142P	0.55
TE-120	0.04	TE-122	0.39	TE-124	1.33
TE-126	0.63	TE-128	0.34	TE-130	0.04
XE-126	0.05	XE-128	0.05	XE-130	0.05
XE-132	1.62	XE-134	0.22		

As was the case in Section A, differences between my own values and those of Habs et al. are generally minor. Often they are on the order of the estimated errors. Convergence is particularly poor for BA-134 and BA-134P, and the considerable disagreement in calculated eigenvalues is not unexpected. For the generally well-converged tellurium isotopes, the discrepancies indicated in Table 4.7 are primarily due to differences in $J = 6$ eigenvalues. This prompted a further investigation of these states using smaller $[N_{\text{MAX}}(6) = 15, 20]$ expansion bases. For each of TE-120, TE-122, ..., TE-128, $\tilde{s}$ was swept over a range of $\sim 20\%$ and the lowest energy so obtained for a given level has been listed in Table 4.8. The energies reported by Habs et al. appear in the rows marked H; they differ markedly from my 25-phonon results in several instances. The discrepancies, particularly those for TE-124, are not connected with convergence difficulties in the present work.

For ten of the 21 nuclei considered in References (29) and (30), experimental energies for states of higher spin [$J = 8$ and/or 10] have been reported. No attempt was made by Habs et al. to extend the GG technique and allow the calculation of such states. My methods have been applied to this end and the resulting theoretical energies [assuming the model parameters of Table 4.1] are given in Tables 4.9 and 4.10. Methods I and II have been used respectively; theoretical energies have been "corrected" by subtracting off the error expected for points on the LSSL. Experimental values taken from Nuclear Data Sheets (46) appear below their theoretical counterparts. The agreement between theory and experiment is fairly good for the barium and xenon

Table 4.8. Calculated absolute energies (MeV) of $J = 6$ states. [H denotes values taken from (29) and (30)]

	$N_{\max}$	$J_i: 6_1$	6_2	6_3
TE-120 <1.08> ^a	15	3.61766	4.37237	5.12865
	20	3.61738	4.37204	5.12786
	25	3.61737	4.37202	5.12782
	H	3.617	4.370	
TE-122 <1.06>	15	2.92893	3.71997	4.62801
	20	2.92876	3.71960	4.62702
	25	2.92876	3.71958	4.62699
	H	2.925	3.696	
TE-124 <1.07>	15	2.66213	3.32635	3.97767
	20	2.65719	3.31470	3.96334
	25	2.65670	3.31335	3.96054
	H	2.783	3.554	
TE-126 <1.03>	15	3.31055	3.62809	4.22493
	20	3.30196	3.60317	4.20115
	25	3.29946	3.59656	4.19422
	H	3.244	3.528	
TE-128 <.97>	15	3.15511	3.82099	4.70693
	20	3.05796	3.69767	4.57535
	25	3.04454	3.68167	4.55256
	H	2.999	3.673	
TE-130 <.96>	15	3.31190	4.18816	5.17244
	20	3.23045	4.12670	5.08171
	25	3.22367	4.12092	5.07073
	H	3.225	4.122	

^aCentral value $\langle \tilde{s} \rangle$. For each isotope, $J = 6$ energies of H_{GG} were calculated using $\tilde{s} = .9\langle \tilde{s} \rangle$, $\langle \tilde{s} \rangle$, and $1.1\langle \tilde{s} \rangle$. The lowest eigenvalue $E(6_1)$ so obtained appears in the table.

Table 4.9. Relative energies and estimated errors for J = 8, 10 states [Method 1]. Exp. energies (46) appear in parentheses. ΔE is for points 10 above LSSL

ISOTOPE	SPIN	NMAX	$E_B(J_i) - E_B(0_1)$			ξ_B			$\Delta E(J_i)$		
			ENERGIES (MeV)			S-TILDA			EST. ERROR (MeV)		
			LEVEL #: 1	2	3	1	2	3	1	2	3
BA-128	8	25	2.1751 (2.126)	3.7658	4.8111	1.06	1.07	1.05	0.00049	0.00059	0.00052
	10	25	3.0772 (3.019)	5.0204	6.2550	1.07	1.07	1.01	0.00055	0.00056	0.00162
BA-130	8	25	2.4131 (2.396)	4.1638	5.1550	1.09	1.09	1.09	0.00015	0.00028	0.00050
	10	25	3.3626 (3.3615)	5.4938	6.7373	1.07	1.07	1.08	0.00011	0.00033	0.00051
BA-132	8	25	2.9042 (2.796)	5.0456	6.1636	1.11	1.08	1.10	0.00019	0.00072	0.00081
	10	25	4.0096 (3.729)	6.6047	8.0919	1.10	1.14	1.08	0.00049	0.00154	0.00255
TE-120	8	25	2.5098 (2.653)	3.3117	4.1279	1.02	1.08	1.06	0.00000	0.00000	0.00001
	10	25	3.2787	4.1259	4.9993	1.08	1.06	1.02	0.00001	0.00001	0.00002
TE-122	8	25	2.5336 (2.669)	3.3993	4.3606	1.06	1.05	1.05	0.00000	0.00000	0.00000
	10	25	3.2756 (3.290)	4.2203	5.2335	1.07	1.05	1.05	0.00000	0.00000	0.00001
TE-124	8	25	2.1668 (2.6643)	2.9999	3.6092	1.09	1.05	1.09	0.00011	0.00032	0.00003
	10	25	2.6325 (3.1542)	3.6601	4.1289	1.06	1.06	1.07	0.00016	0.00037	0.00157
TE-126	8	25	2.2288 (2.7654)	2.7604	3.3529	1.02	1.02	1.04	0.00103	0.00076	0.00333
	10	25	2.5146 (2.9752)	3.3222	3.6314	1.04	1.05	1.02	0.00111	0.00036	0.00813
XE-126	8	25	2.4437 (2.437)	4.0533	4.9309	1.06	1.06	1.06	0.00026	0.00040	0.00126
	10	25	3.3738 (3.317)	5.3354	6.3667	1.07	1.06	1.04	0.00025	0.00050	0.00079
XE-128	8	25	2.5722 (2.513)	4.4385	5.4837	1.04	1.06	1.05	0.00060	0.00192	0.00213
	10	25	3.5145 (3.373)	5.7710	7.1732	1.06	1.03	1.08	0.00050	0.00351	0.00343
XE-130	8	25	2.8347 (2.696)	4.7117	5.7009	1.04	1.06	1.07	0.00006	0.00034	0.00019
	10	25	3.8254	6.0742	7.3468	1.06	1.02	1.06	0.00006	0.00122	0.00042

Table 4.10. Relative energies and estimated errors for J = 8, 10 states [Method II]. Exp. energies (46) appear in parentheses. ΔE is for points 1 σ above LSSL

ISOTOPE	SPIN	NMAX	$E_B(J_1) - E_B(0_1)$			S_B			$\Delta E(J_1)$		
			ENERGIES (MeV)			S-TILDA			EST. ERROR (MeV)		
			LEVEL #:	1	2	3	1	2	3	1	2
BA-128	8	25	2.1752 (2.126)	3.7659	4.8112	1.04	1.04	1.04	0.00030	0.00019	0.00027
	10	25	3.0773 (3.019)	5.0206	6.2556	1.04	1.04	1.04	0.00021	0.00011	0.00014
BA-130	8	25	2.4131 (2.396)	4.1638	5.1551	1.05	1.05	1.05	0.00010	0.00029	0.00036
	10	25	3.3626 (3.3615)	5.4938	6.7373	1.10	1.05	1.05	0.00020	0.00026	0.00058
BA-132	8	25	2.9042 (2.796)	5.0455	6.1635	1.11	1.11	1.11	0.00020	0.00114	0.00101
	10	25	4.0056 (3.729)	6.6052	8.0923	1.11	1.11	1.11	0.00052	0.00031	0.00151
TE-120	8	25	2.5098 (2.653)	3.3117	4.1279	1.05	1.10	1.00	0.00000	0.00000	0.00000
	10	25	3.2727	4.1259	4.9993	1.10	1.00	1.10	0.00001	0.00000	0.00002
TE-122	8	25	2.5336 (2.669)	3.3993	4.3606	1.07	1.07	1.07	0.00000	0.00000	0.00001
	10	25	3.2756 (3.290)	4.2203	5.2335	1.02	1.07	1.07	0.00000	0.00001	0.00001
TE-124	8	25	2.1668 (2.6643)	2.9999	3.6094	1.06	1.06	1.06	0.00014	0.00039	0.00048
	10	25	2.6325 (3.1542)	3.6601	4.1289	1.06	1.01	1.06	0.00015	0.00036	0.00156
TE-126	8	25	2.2288 (2.7654)	2.7604	3.3529	1.03	1.03	1.03	0.00099	0.00084	0.00359
	10	25	2.5146 (2.9752)	3.3222	3.6314	1.03	1.03	1.03	0.00108	0.00056	0.00865
XE-126	8	25	2.4438 (2.437)	4.0534	4.9309	1.06	1.06	1.06	0.00025	0.00038	0.00124
	10	25	3.3738 (3.317)	5.3355	6.3665	1.06	1.06	1.06	0.00027	0.00047	0.00122
XE-128	8	25	2.5723 (2.513)	4.4382	5.4839	1.04	1.04	1.04	0.00059	0.00278	0.00184
	10	25	3.5144 (3.373)	5.7711	7.1738	1.04	1.04	1.04	0.00082	0.00358	0.00199
XE-130	8	25	2.8347 (2.696)	4.7117	5.7008	1.05	1.05	1.05	0.00007	0.00039	0.00033
	10	25	3.8254	6.0744	7.3470	1.05	1.05	1.05	0.00007	0.00054	0.00007

isotopes, though the theoretical energies are consistently high.

$V_{GG}(\beta, \gamma)$ possesses an asymmetric minimum for each of these nuclei, and any vibrational model with this feature would probably do as well.

Theoretical estimates are consistently low for the higher spin energies of the tellurium isotopes. The potential energy surfaces for these nuclei favor axial symmetry.

E. Estimating $\tilde{s}_B$ Without Diagonalizing

Considerable time and effort can be expended in the repeated diagonalization process that is used to search for the optimal value of the basis parameter. Although valuable by-products such as error estimates also result, it would be useful to have a rapid method of estimating $\tilde{s}_B$ beforehand. At the very least this would serve to limit the scope of the $\tilde{s}_B$ search. In Section C of Chapter III, the suggestion was made that

$$\frac{d}{ds} \left[\sum_{\substack{k \text{ lowest} \\ \text{energy basis} \\ \text{states}}} \langle \psi_i^s | H | \psi_i^s \rangle \right]_{s = s^{\text{best}}} = 0 \quad (4.32)$$

be used to find a basis parameter appropriate to the diagonalization of the collective Hamiltonian, H . The corresponding criterion for the reduced Schroedinger problem is simply

$$\frac{d}{d\tilde{s}} \left[\sum_{i=1}^k \langle \tilde{\psi}_i | \tilde{H} | \tilde{\psi}_i \rangle \right]_{\tilde{s} = \tilde{s}^{\text{best}}} = 0, \quad (4.33)$$

and a solution to Equation (4.33) induces a solution to Equation (4.32) by

$$s^{\text{best}} = \frac{\bar{s}}{s} \tilde{s}^{\text{best}} \quad (4.34)$$

The resulting value of s^{best} may easily be shown to be independent of the transformation which connects the original and reduced forms of the problem. The superscript $^{\text{best}}$ will be used to denote solutions to Equation (4.33), while $\tilde{s}_B$ will refer exclusively to estimates made by a repeated diagonalization process.

Before applying Equation (4.33) to the GG-model calculations, it is informative to examine the manner in which individual matrix elements of $\bar{H}_{\text{GG}}$ depend upon $\tilde{s}$. Using Equation (4.18), such a study was made for various matrix elements of the representative-isotope Hamiltonians. The $J = 0$ elements of BA-130 proved to be typical, and examples are shown in Figures 4.15 and 4.16. Because of their asymptotic properties [Equations (4.19) and (4.20)] diagonal matrix elements must possess a minimum on $0 < \tilde{s} < \infty$; however, Figure 4.16 shows that this need not be true of off-diagonal elements. Sums of diagonal elements are similar to individual diagonal elements in their dependence upon $\tilde{s}$, as illustrated in Figure 4.17. Minima of the curves in this figure correspond to solutions of Equations (4.33) for the BA-130 Hamiltonian.

Equation (4.33) may be solved by finding the real positive roots of a polynomial of degree eight. This was accomplished for each of the 23 sets of potential parameters by using the computer program ZPOLY (47). Results for the first 12 values of the summation limit k appear in Table 4.11. $J = 0$ basis states ordered by the rules of Appendix C were used. Multiple solutions were not observed, and the single $\tilde{s}^{\text{best}}$ was

Figure 4.15. Dependence on $\tilde{s}$ of $\langle \psi_i^{\tilde{s}} | \bar{H}_{GG}[\text{BA-130}] | \psi_i^{\tilde{s}} \rangle$ for selected $J = 0$ Bohr eigenstates $(i) = (N, l, v=t, J=0)$

Figure 4.16. Dependence on $\tilde{s}$ of $\langle \psi_i^s | \bar{H}_{GG}[\text{BA-130}] | \psi_j^s \rangle$ for selected $J = 0$ Bohr eigenstates ($i, j \neq 1$). For $(N \& v J)$ labels corresponding to listed values of i and j , see Figure 4.15

Figure 4.17. Dependence on $\tilde{s}$ of $\sum_{i=1}^K \langle \psi_i^{\tilde{s}} | \bar{H}_{GG} [\text{BA-130}] | \psi_i^{\tilde{s}} \rangle$ for selected values of K . For $(N \& v J)$ labels associated with each value of i , see Figure 4.15

found to slowly increase with increasing k . The $k = 12$ values of $\tilde{s}^{\text{best}}$ are also listed in the central column of Table 4.12 where they are compared with the empirically determined $\tilde{s}_B$. For a 30-phonon diagonalization, $\tilde{s}_B$ refers to that value of $\tilde{s}$ which minimizes the sum of the calculated absolute energies of the first three $J = 0$ states. For each isotope, it has been determined from the $\tilde{s}$ -sweep calculations of the previous section. The corresponding value for a 20-phonon diagonalization would be $\sim 8\%$ lower. The final column in Table 4.12 contains $\tilde{s}^{\text{HABS}}$, the reduced equivalent of the basis parameter employed by Habs et al. [see Table 4.2]. The authors claim in (29) to have determined their basis parameter by (roughly) minimizing the first few $J = 0$ eigenvalues in a small basis calculation. On the average, $\tilde{s}^{\text{best}}$ may be seen to be a better estimate of the optimal parameter ($\tilde{s}_B$) than is $\tilde{s}^{\text{HABS}}$, particularly among the marginally converged isotopes which require extra care in the selection of $\tilde{s}$. Diagonal matrix elements of $(\beta')^p (\cos 3\gamma)^q$ vanish when q is an odd integer, and consequently two terms in $\bar{V}_{GG}$ do not contribute in Equation (4.33). This loss of information may partially account for the differences between $\tilde{s}^{\text{best}}$ and $\tilde{s}_B$; the estimation method may be more accurate for other Hamiltonians.

The calculations which provide the foundation of this chapter have been reported here in great detail. It is hoped that they may aid future investigators in testing calculations, as two independent sets of results are now available for selected GG Hamiltonians. The immediate lessons are quite simple. Employing a large number of basis states in eigenfunction expansions does not in itself insure accurate results.

Table 4.11. Value of $\tilde{s}$ which minimizes the sum over $J = 0$ states of diagonal matrix

elements, $\sum_{i=1}^k \langle \psi_i | \tilde{H}_{GG} | \psi_i \rangle$

	k = 1	2	3	4	5	6	7	8	9	10	11	12
BA-128	0.50	0.62	0.64	0.69	0.73	0.77	0.77	0.79	0.82	0.83	0.85	0.85
BA-130	0.56	0.67	0.70	0.75	0.79	0.83	0.83	0.86	0.88	0.89	0.91	0.91
BA-132	0.60	0.72	0.76	0.80	0.85	0.88	0.88	0.92	0.94	0.95	0.97	0.97
BA-134	0.72	0.84	0.90	0.93	0.99	1.01	1.02	1.06	1.07	1.08	1.11	1.11
BA-134P	0.72	0.84	0.90	0.93	0.99	1.01	1.02	1.06	1.07	1.09	1.12	1.12
BA-136	0.82	0.89	0.92	0.96	0.99	1.01	1.02	1.04	1.06	1.07	1.09	1.09
CE-136	0.69	0.81	0.87	0.90	0.96	0.98	0.99	1.03	1.04	1.06	1.09	1.09
CE-138	0.64	0.74	0.78	0.82	0.86	0.89	0.89	0.92	0.94	0.95	0.97	0.97
ND-138	0.69	0.81	0.87	0.90	0.96	0.99	0.99	1.03	1.04	1.06	1.09	1.09
ND-140	0.64	0.74	0.78	0.82	0.86	0.89	0.89	0.92	0.94	0.95	0.97	0.97
SM-142	0.63	0.74	0.77	0.82	0.85	0.88	0.88	0.91	0.93	0.94	0.97	0.97
SM-142P	0.75	0.83	0.86	0.90	0.94	0.96	0.96	0.99	1.01	1.02	1.04	1.04
TE-120	0.65	0.72	0.73	0.77	0.79	0.83	0.82	0.84	0.87	0.87	0.89	0.89
TE-122	0.74	0.83	0.94	0.88	0.90	0.93	0.93	0.95	0.97	0.98	0.99	0.99
TE-124	0.89	1.00	1.03	1.07	1.10	1.13	1.13	1.16	1.18	1.19	1.21	1.21
TE-126	1.02	1.10	1.12	1.15	1.18	1.21	1.21	1.24	1.25	1.26	1.28	1.28
TE-128	0.86	0.96	0.98	1.02	1.05	1.08	1.08	1.10	1.12	1.13	1.15	1.15
TE-130	0.85	0.95	0.98	1.02	1.05	1.08	1.08	1.10	1.12	1.13	1.15	1.15
XE-126	0.56	0.68	0.71	0.76	0.80	0.84	0.84	0.87	0.89	0.90	0.93	0.93
XE-128	0.61	0.71	0.75	0.78	0.83	0.85	0.85	0.89	0.91	0.91	0.94	0.94
XE-130	0.69	0.70	0.73	0.77	0.81	0.84	0.84	0.87	0.89	0.90	0.92	0.92
XE-132	1.03	1.17	1.24	1.28	1.35	1.38	1.38	1.43	1.45	1.47	1.50	1.50
XE-134	0.84	0.92	0.95	0.98	1.02	1.04	1.04	1.07	1.09	1.09	1.12	1.12

Table 4.12. Comparison of "optimal" basis parameters

	$\tilde{s}_B^a$	$\tilde{s}_{\text{best}}^b$ (k=12)	$\tilde{s}_{\text{HABS}}^c$
BA-128	1.11	.85	1.07
BA-130	1.12	.91	.92
BA-132	1.16	.97	1.04
BA-134	1.09	1.11	.96
BA-134P	1.10	1.12	.96
BA-136	1.03	1.09	.76
CE-136	1.14	1.09	1.06
CE-138	1.00	.97	.87
ND-138	1.15	1.09	1.14
ND-140	1.00	.97	.87
SM-142	1.00	.97	.85
SM-142P	1.02	1.04	.86
TE-120	1.11	.89	1.15
TE-122	1.11	.99	1.13
TE-124	1.14	1.21	.85
TE-126	1.12	1.28	.77
TE-128	1.00	1.15	.74
TE-130	1.02	1.15	1.10
XE-126	1.12	.93	1.03
XE-128	1.11	.94	.94
XE-130	1.10	.92	.94
XE-132	1.56	1.50	1.98
XE-134	1.02	1.12	.85

^aFound by repeated diagonalization.^bFound via Equation (4.33).^cEquivalent to parameter used by Habs et al. (29, 30).

Care must also be given to the selection of an optimal basis parameter. Perhaps the most useful single step that can be taken is the selection of a reduced Hamiltonian with fixed mass parameter and asymptotic properties. This is particularly appropriate when one is investigating a class of Hamiltonians whose members differ only in their values of numerical parameters. Such a transformation serves to stabilize the value of $\tilde{s}_B$. For specific Hamiltonians, the estimation procedure based on Equation (4.33) can then be used to provide a working estimate of the optimal parameter.¹ If necessary, $\tilde{s}$ -sweep diagonalizations can be performed to further define $\tilde{s}_B$ and to indicate the magnitude of expected errors for various choices of N_{MAX} . $J = 0$ studies will suffice in this regard. These precautions coupled with a generous helping of common sense can prevent us from employing the expansion technique unprofitably.

¹The usefulness of Equation (4.33) is somewhat obscured in Table 4.12. It would appear that $\tilde{s} = 1.0$ provides as good an overall estimate as $\tilde{s}_{best}$. Of course, $\tilde{H}_{GG}$ was specifically defined so that this would be the case. Equation (4.33) can be used in the absence of such precognition.

V. QUADRATIC POTENTIAL MODEL: GENERAL PROPERTIES

In the Gneuss-Greiner model, the authors effectively chose to construct the potential energy function from two rotational scalars and their products

$$[\alpha\alpha]_0 \propto \beta^2, \quad \text{and} \quad \left[[\alpha\alpha]_2 \alpha \right]_0 \propto \beta^3 \cos 3\gamma.$$

This restriction was adopted for computational ease, and is by no means necessary. Without a priori knowledge of $V(\beta, \gamma)$, the only constraints that need be imposed are those which follow from the characteristics of quadrupole surfaces. For any values of β and γ , the pairs (β, γ) , $(\beta, \gamma + \frac{2\pi}{3})$, and $(\beta, -\gamma)$ define three distinct quadrupole surfaces in the BF coordinate system which differ only in their orientations.¹ A simple rotation will take one into another. Consequently we expect the potential energies associated with these surfaces to be equal,

$$V(\beta, \gamma) = V(\beta, \gamma - \frac{2\pi}{3}) = V(\beta, -\gamma) \quad (5.1)$$

These symmetries serve to determine $V(\beta, \gamma)$ everywhere if it is specified on

$$\begin{aligned} &0 \leq \gamma \leq \frac{\pi}{3} \\ \text{R: } &0 \leq \beta < \infty \end{aligned} \quad (5.2)$$

A quadrupole surface having deformation $\beta = 0$ is a sphere for any value

¹This topic is discussed in Appendix A.

of γ ; hence $V(0, \gamma)$ should be independent of γ . Finally we expect $V(\beta, \gamma)$ to be a smooth function of the shape coordinates and to have asymptotic properties

$$V(\beta, \gamma) \xrightarrow{\beta \rightarrow \infty} \infty \quad [\text{all } \gamma] \quad (5.3)$$

which allow "bound" or normalizable solutions of the associated Schrodinger equation. Without further constraints, a reasonable approach consists of classifying potentials according to gross features, and systematically stepping through the possibilities. At each stage allowed theoretical phenomena may be examined and compared with experimental findings. Wide ranging agreement, if found, would eventually have to be reconciled with nuclear many-body calculations.

Regarding $V(\beta, \gamma)$ as a surface above the β - γ plane, the potential energy function may be classified by the topographical features of its surface. In this chapter we take up the study of the simplest such class, which consists of surfaces possessing a single minimum on $\mathcal{R}$. Near its minimum, (b_0, g_0) a member of this class may be approximated by the leading terms in its Taylor's expansion

$$V_{QP}(\beta, \gamma) = \frac{1}{2}c_\beta(\beta - b_0)^2 + c_\gamma(\gamma - g_0)^2 + c_{\beta\gamma}(\beta - b_0)(\gamma - g_0) \quad (5.4)$$

For points far removed from the minimum, Equation (5.4) is not expected to resemble $V(\beta, \gamma)$. However we may define a quadratic potential Hamiltonian

$$H_{QP} = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V_{QP}(\beta, \gamma) \quad (5.5)$$

by assuming that Equation (5.4) defines $V_{QP}(\beta, \gamma)$ everywhere on $\mathcal{R}$. In studying the eigenfunctions and eigenvalues of this limited category of operators, we expect to observe those coarse features which are representative of the wider class of single-minimum-potential Hamiltonians.

The quadratic potential function has two undesirable features. At $\beta = 0$ V_{QP} is not independent of γ , and consequently polar graphs such as those of Figure 4.1 would contain a pinch at the origin along the ray $\gamma = g_0$. Secondly, when Equation (5.1) is used to extend V_{QP} outside of the region $\mathcal{R}$, the full surface which results is not smooth away from the origin. If $g_0 \neq \pi/3$, there will be cusps at $\gamma = 0, \pi/3, 2\pi/3, \dots$. Neither of these difficulties is serious. In the calculation of matrix elements, integrations over the shape variables are performed with respect to the measure

$$\beta^4 |\sin 3\gamma| d\beta d\gamma$$

which vanishes at the problem sites. Consequently eigenvalues and eigenvectors of H_{QP} are not sensitive to the behavior of V_{QP} near $\beta = 0$ or $\gamma = n(\frac{\pi}{3})$. Nevertheless, smoothness could be restored by modifying V_{QP} , and the resulting model calculations would be no more difficult. For example the replacements

$$c_\gamma \rightarrow \beta^2 c_\gamma, \quad c_{\beta\gamma} \rightarrow \beta c_{\beta\gamma}$$

make each term quadratic in the deformation and eliminate the origin fold. $(\cos 3\gamma - \cos 3g_0)$ could be used in place of $(\gamma - g_0)$, thus eliminating the angular cusps. Such modifications were not used,

principally for three reasons.

- 1) The topographical structure of the potential energy surface V_{QP} is easily visualized from a knowledge of the parameters $(b_o, g_o, c_\beta, c_\gamma, c_{\beta\gamma})$.
- 2) The asymptotic properties of V_{QP} for large β are specified by the first term only and are independent of γ . Changing variables to $\beta' = s\beta = [Bc_\beta/\hbar^2 c_\beta]^{1/2} \beta$ and dividing by the energy factor

$$\hbar\bar{\omega} = \frac{\hbar^2 s^2}{B} \quad (5.6)$$

casts the Schroedinger Equation, $H_{QP}\phi = E\phi$, into the reduced form¹

$$\bar{H}_{QP}\bar{\phi}(\beta', \gamma, \theta_i) = \bar{E}\bar{\phi}(\beta', \gamma, \theta_i) \quad , \quad \bar{E} = E/\hbar\bar{\omega} \quad (5.7)$$

$$\bar{H}_{QP} = -\frac{1}{2}T(\beta', \gamma, \theta_i) + \bar{V}_{QP}(\beta', \gamma) \quad (5.8)$$

$$\begin{aligned} \bar{V}_{QP}(\beta', \gamma) = & \frac{c_\beta}{2} (\beta' - \beta_o)^2 + c_\gamma (\gamma - \gamma_o)^2 \\ & + c_{\beta\gamma} (\beta' - \beta_o)(\gamma - \gamma_o) \quad . \quad (5.9) \end{aligned}$$

For moderate values of β_o , the optimal basis parameter $\bar{s}_B$ will be on the order of $(c_\beta)^{1/2}$ which may be chosen to be unity.

- 3) Techniques for treating H_{QP} analytically by employing approximations which lead to separation of variables have been developed by Davydov (14), and by Williams, Western, Gregerson and myself (48). The validity of such techniques could be judged by comparing their results against those obtained by the large basis diagonalization of H_{QP} . The work in this chapter represents the first attempt to treat H_{QP} without approximation. The only errors introduced are

¹For a given value of c_β , the remaining parameters of Equation (5.9) are given by

$$\beta_o = \bar{s}b_o \quad , \quad \gamma_o = g_o \quad , \quad c_\gamma = \frac{B}{s^2 \hbar^2} c_\gamma \quad , \quad c_{\beta\gamma} = \frac{B}{s^3 \hbar^2} c_{\beta\gamma} \quad .$$

those due to truncation. These may be controlled and estimated by varying the basis size.

In Chapter VI, the quadratic potential Hamiltonian will be applied to specific nuclei, with model parameters adjusted to reproduce experimental energy spectra. Before beginning this process it is invaluable to attain a larger view of the possibilities pregnant within H_{QP} . Such is the goal of the present chapter. In the initial section the scope of the present investigation is defined. Computational details of $\bar{H}_{QP}$ diagonalizations are briefly addressed, as well as the problems of convergence and optimal $\tilde{s}$ selection. On the basis of simple arguments, Section B then provides a framework of theoretical expectations against which the $\bar{H}_{QP}$ spectra may be viewed. As a sharp non-spherical minimum develops in $\bar{V}_{QP}$, rotations and shape vibrations can be expected to decouple. Consequently the $\bar{H}_{QP}$ spectrum may be conveniently investigated by considering in turn

- 1) the behavior of $J = 0$ shape-vibrational states, and
- 2) the development of rotational bands based upon such states.

Relevant characteristics of rigid rotor eigenstates of the proper symmetry are also reviewed in Section B. The investigation of $\bar{H}_{QP}$ properties is then begun in earnest. The behavior of $J = 0$ energies under variations of $(\beta_0, C_\gamma, C_\beta)$ leads in Section C to the identification of β and γ -vibrational states. The development of rotational bands based upon these states is then traced as $\bar{H}_{QP}$ is systematically obtained from H_B' [Section D]. The rotational band based upon the ground state is singled out for additional study in the final section, where the effects of varying the $\bar{V}_{QP}$ parameters are illustrated.

A. Computational Details

Results presented in this chapter have been obtained by diagonalizing the reduced form of the quadratic potential Hamiltonian, $\bar{H}_{QP}$. For each value of $J \leq 20$, standard reduced matrix elements of the five operators β^2 , β , $\beta\gamma$, γ , and γ^2 were found between states of the maximal expansion basis [Table 2.3]. This permitted the matrix $[\bar{H}_{QP}]$ to be rapidly assembled for any set of values of the parameters $\{C_\beta, \beta_0, \gamma_0, C_\gamma, C_{\beta\gamma}\}$. It suffices to fix C_β and vary the remaining parameters. In this manner we obtain all of the reduced spectra and accompanying sets of B(E2) ratios which can be generated by varying the six constants appearing in the original Hamiltonian H_{QP} . Unless stated otherwise, C_β is understood to be fixed at unity. [In Section C it will prove instructive to observe the effect of increasing C_β .]

Although γ_0 will usually be specified by stating its equivalent in degrees, both γ and γ_0 in the expression $(\gamma - \gamma_0)$ are understood to be in radians. $(\gamma - \gamma_0)^2$ is then generally small compared to unity on $0 \leq \gamma \leq \frac{\pi}{3}$, and typical values of $C_\gamma \approx 10$ should not be unexpected. In the calculation of matrix elements, the factor $|\sin 3\gamma|(\gamma - \gamma_0)^2$ appears in the γ -integral of the C_γ term. The magnitude of its variation on $0 \leq \gamma \leq \frac{\pi}{3}$ may be seen in Figure 5.1 to be strongly dependent upon the value of γ_0 . Consequently, for fixed C_γ , the intrinsic strength of the "perturbation" $C_\gamma(\gamma - \gamma_0)^2$ increases as γ_0 decreases from 30° . As γ_0 tends to zero, the effect of $C_\gamma(\gamma - \gamma_0)^2$ on the energy spectrum is expected to grow and an enlarged expansion basis will be required for converged results.

Figure 5.1. $(\gamma - \gamma_0)^2$ and $|\sin 3\gamma|(\gamma - \gamma_0)^2$ as functions of γ for three values of γ_0

The effect of the $(\beta' - \beta_0)(\gamma - \gamma_0)$ term has been reserved for future investigation; in the present work $C_{\beta\gamma} = 0$ has been imposed. [This elimination of the crossing term does not allow separation of variables. Dynamically, through the kinetic energy operator T , the β and γ degrees of freedom are mixed with the rotations and with one another.] With this constraint it proves sufficient to investigate only those potential minima whose angular part is in the range of $0 \leq \gamma_0 \leq 30^\circ$. If $C_{\beta\gamma} = 0$, reflection of $\bar{V}_{QP}(\beta', \gamma)$ about $\gamma = 30^\circ$ returns $\bar{V}_{QP}(\beta', \gamma)$ with γ_0 replaced by $(60^\circ - \gamma_0)$. As noted in Appendix A, such an alteration in the Schroedinger equation leaves the energies and (first order) $B(E2)$ transition rates unchanged; (first order) quadrupole moments are multiplied by (-1) . This point is borne out in 20-phonon model calculations as shown in Figure 5.2. Three Hamiltonians $\{\bar{H}_{QP}^i: i = 1, 2, 3\}$ have been treated which are expected to have the same reduced structure. $B(E2)$'s and quadrupole moments are given in units of $[D_1/\bar{s}]^2$ and $[16\pi/5]^{1/2} D_1/\bar{s}$ respectively. [As always $\bar{s}$ specifies the transformation linking H_{QP} and $\bar{H}_{QP}$]. The results illustrate that $C_\beta = 1$ and $0 \leq \gamma_0 \leq 30^\circ$ may be adopted with no loss of generality in the reduced spectra or transition scheme. In particular, if

$$\bar{\phi}^2 = \sum_i a_i \psi_i^{\bar{s}_2} \quad (5.10)$$

is an eigensolution of $\bar{H}_{QP}^2$, then

$$\bar{\phi}^1 = \sum_i a_i \psi_i^{\bar{s}_1} \quad ; \quad \bar{s}_1 = \sqrt{3} \bar{s}_2 \quad (5.11)$$

Figure 5.2. Three quadratic potential Hamiltonians possessing common reduced energies and B(E2) ratios. Making the change of variable $\beta'' = \sqrt{3}\beta'$ in $\bar{H}_{QP}^1(\beta', \gamma, \theta_i)$ and dividing by 3 results in $\bar{H}_{QP}^2(\beta'', \gamma, \theta_i)$. $\bar{H}_{QP}^1$ and $\bar{H}_{QP}^2$ are related by a reflection of $\bar{V}_{QP}(\beta', \gamma)$ about $\gamma = 30^\circ$. The value of $\tilde{s}$ used in each diagonalization is indicated

and

$$\bar{\phi}^3 = \sum_i a_i (-1)^{\ell_i} \bar{\psi}_i^{\tilde{s}_2} \quad (5.12)$$

are the corresponding solutions of $\bar{H}_{QP}^1$ and $\bar{H}_{QP}^3$ respectively. If γ_0 were 30° , reflection about $\gamma = 30^\circ$ would leave $\bar{V}_{QP}(\beta', \gamma)$ unaltered. $\bar{H}_{QP}^2$ and $\bar{H}_{QP}^3$ would then be identical with $\bar{\phi}^2$ and $\bar{\phi}^3$ referring to the same solution. Consequently $\bar{\phi}^2$ would equal $\bar{\phi}^3$ to within a phase, and all $\bar{\psi}_i^{\tilde{s}_2}$ appearing in Equation (5.10) would have a common value of $(-1)^{\ell_i}$. [Recall that if $V(\beta, \gamma)$ is a function of β only, ℓ remains a good quantum number. This is no longer the case when γ -dependence is added. However, if $V(\beta, \gamma)$ has reflection symmetry about $\gamma = 30^\circ$, basis states of even and odd ℓ will not be mixed, and eigenfunctions of $H = -\frac{1}{2}AT(\beta, \gamma, \theta_i) + V(\beta, \gamma)$ will possess a definite ℓ -parity, $(-1)^\ell$. See Section E of Appendix A.]

For our purposes high accuracy is not required, and the majority of the results in this chapter have been obtained by using 20-phonon expansion bases. A region of $(\beta_0, \gamma_0, C_\gamma)$ parameter space large enough to indicate general tendencies, yet small enough that 20-phonon calculations were sufficiently converged, was selected for study. A mesh was imposed on this region, as shown in Figure 5.3, and for each of the $7 \cdot 13 \cdot 8$ values of $(\beta_0, \gamma_0, C_\gamma)$ $[\bar{H}_{QP}]$ was assembled and diagonalized. The eigenvalue and eigenvector information obtained has been used in the preparation of many of the figures and tables, and will be herein referred to as the GRID data. Its further use in fitting applications will be described in Chapter VI.

PARAMETER-SPACE REGION EXPLORED BY GRID CALCULATIONS

For each of the $7 \cdot 13 \cdot 8 = 728$ values of
 $(\beta_0, \gamma_0, C_\gamma)$ the following diagonalizations were performed:

J :	0	2	3	4	5	6	7	8	10
$N_{MAX}(J)$:	22	20	20	20	20	20	20	20	20
# states in basis:	52	77	33	100	57	114	72	121	121
# eigenvalues calculated:	7	9	7	9	7	7	6	7	7
# eigenvectors calculated:	5	7	3	6	3	4	4	4	4

Figure 5.3. Particulars of GRID calculations for $\bar{H}_{QP}(\beta_0, \gamma_0, C_\gamma)$ eigenvalues and eigenvectors [$C_\beta = 1, C_{\beta\gamma} = 0$]

Table 5.1. Comparison of calculated relative energies for 20 [GRID] (above) and 25-phonon (below) calculations. States are $J_i = 0_4, 2_2, 3_1$ and 10_1 (CW from top left)

β_o	C_Y	γ_o	0°		10°		20°		30°	
0	10		4.551	2.414	4.074	2.321	3.895	2.075	3.963	1.960
			-	-	-	-	3.894	-	-	-
			4.239	3.115	4.540	2.928	4.793	2.808	4.894	2.766
	40		-	-	-	2.929	-	-	4.895	-
			5.294	2.068	5.426	2.256	4.948	2.111	4.684	1.649
			5.283	2.066	5.418	-	4.949	2.112	4.687	1.652
			3.272	4.115	3.815	3.237	4.297	2.500	4.413	2.199
			3.273	-	-	3.238	4.299	2.502	4.416	2.202
	70		5.332	2.001	5.493	2.178	5.518	1.980	5.402	1.352
			5.308	1.993	5.482	2.176	5.509	1.984	5.390	1.356
			2.892	4.827	3.541	3.468	4.017	2.291	3.986	1.804
			2.893	4.822	-	3.469	4.022	2.294	3.991	1.808
3	10		2.536	1.252	2.190	1.006	2.152	.675	2.139	.496
			-	-	-	-	-	-	-	-
			1.560	1.464	1.643	1.140	1.698	.857	1.701	.732
	40		-	-	-	-	-	-	-	-
			3.608	1.280	3.277	1.280	2.559	.668	2.502	.366
			3.603	1.279	3.276	1.279	2.558	-	2.501	-
			1.342	2.460	1.515	1.550	1.583	.788	1.508	.525
			-	2.457	-	1.549	-	-	-	-
	70		3.712	1.304	3.613	1.294	3.180	.600	3.195	.316
			3.691	1.295	3.610	1.291	3.178	.599	3.193	-
			1.249	3.087	1.463	1.714	1.503	.709	1.416	.458
			1.243	3.053	1.460	1.712	-	.708	1.415	.457
6	10		2.025	.750	1.975	.458	1.607	.208	1.432	.110
			2.024	-	1.974	-	-	-	-	-
			.525	.781	.543	.493	.540	.250	.517	.163
	40		-	-	-	-	-	-	-	-
			2.876	1.074	2.051	.653	2.030	.174	2.036	.093
			2.832	1.066	2.046	.651	2.028	-	2.033	-
			.498	1.501	.530	.684	.517	.211	.491	.138
			.494	1.471	.528	.681	.516	-	.490	-
	70		3.255	1.121	2.165	.709	2.055	.161	2.059	.091
			3.179	1.079	2.155	.706	2.044	.158	2.049	.089
			.503	2.074	.531	.740	.509	.198	.487	.139
			.480	1.915	.522	.735	.504	.194	.481	.132

The degree of convergence of the GRID data at various limiting points of the parameter region is indicated in Table 5.1. Twenty and twenty-five phonon calculations are compared. Within each rectangle, calculated relative energies of the states $J_i = 0_4, 2_2, 3_1$ and 10_1 have been arranged clockwise beginning at top left. The 25-phonon value, when different, appears below the corresponding 20-phonon result. Notice that for fixed (β_0, C_Y) , differences are generally larger for the smaller values of γ_0 and amount to several percent near the bottom of the table. As β_0 and C_Y increase, the relative energy of the 2_1 state drops rapidly; hence small relative errors translate into large percentage errors. Near the β_0 and C_Y extrema, the 20-phonon value of $\Delta = [\bar{E}(2_1) - \bar{E}(0_1)]$ is in error by as much as 10%. Consequently reduced energies there [obtained by dividing relative energies by Δ] are somewhat suspect.

As always, the question of optimizing $\tilde{s}$ must be addressed. For calculations upon $\bar{H}_{0p}$, the lessons of Chapter IV have been taken to heart, and $\tilde{s}_B$ is chosen in two stages. Initially Equation (4.33) is used to obtain the estimate $\tilde{s}^{\text{best}}$. $\tilde{s}$ is then swept through a series of values near $\tilde{s}^{\text{best}}$ with the absolute energies of the lowest few $J = 0$ states determined by diagonalization. $\tilde{s}_B$ is chosen to approximately minimize their sum. Table 5.2 contains the information used in selecting $\tilde{s}_B$ for $(\beta_0, \gamma_0, C_Y) = (3, 15^\circ, 30)$. Eighteen and 25-phonon $J = 0$ diagonalizations were performed; $\tilde{s}_B$ was estimated at .925 for a 20-phonon calculation. This procedure was not repeated for every one of the GRID points. Rather for each pair (β_0, C_Y) , $\tilde{s}_B$ was determined only at $\gamma_0 = 0^\circ, 15^\circ$, and 30° . An approximate linear relationship

Table 5.2. $\tilde{s}$ selection process for $(\beta_0, \gamma_0, C_\gamma) = (3, 15^\circ, 30)$. Calculated absolute energies of $J = 0$ states are given (minus the constant $\frac{1}{2}\beta_0^2 + C_\gamma\gamma_0^2$). The average appears in the rightmost column, and $\leftarrow$ indicates the selected value of $\tilde{s}_B = .925$ used in ensuing calculations

$N_{\max}$	$\tilde{s}$	$J_i = 0_1$	0_2	0_3	0_4	0_5	$\frac{1}{5} \sum_{K=1}^5 \bar{E}(0_K^+)$
18	.5	-4.94551	-3.80383	-2.56749	-2.18108	-0.75517	-2.85062
	.6	-4.96057	-3.83557	-2.68070	-2.37023	-1.47874	-3.06520
	.7	-4.97098	-3.84496	-2.69417	-2.38591	-1.51601	-3.08241
	.8	-4.97546	-3.85096	-2.70179	-2.39648	-1.52333	-3.08960
	.9	-4.97707	-3.85386	-2.70527	-2.40365	-1.52891	-3.09375 $\leftarrow$
	1.0	-4.97762	-3.85501	-2.70380	-2.40570	-1.50377	-3.08918
	1.1	-4.97738	-3.84715	-2.63948	-2.39378	-1.27219	-3.02600
	1.2	-4.97126	-3.78686	-2.41605	-2.33119	-0.79670	-2.86041
25	.7	-4.97608	-3.85190	-2.70338	-2.40165	-1.52583	-3.09177
	.8	-4.97746	-3.85445	-2.70640	-2.40609	-1.53076	-3.09503
	.9	-4.97785	-3.85542	-2.70785	-2.40725	-1.53273	-3.09622 $\leftarrow$
	1.0	-4.97799	-3.85578	-2.70853	-2.40755	-1.53367	-3.09671
	1.1	-4.97805	-3.85589	-2.70838	-2.40761	-1.52826	-3.09564
	1.2	-4.97802	-3.85432	-2.69208	-2.40546	-1.44359	-3.07469

$$\tilde{s}_B \approx a + b\gamma_0$$

was deduced and used to determine $\tilde{s}_B$ for all γ_0 . For fixed (β_0, γ_0, C_Y) , a single value of $\tilde{s}$ was used to treat all angular momenta. From Table E.4 the value of $\tilde{s}$ used for each of the GRID calculations may be found. For example in the thirteen calculations having $(\beta_0, C_Y) = (4, 30)$, $\tilde{s}$ ranged linearly from .78 to .82 as γ_0 ran through the list $0^\circ, 2.5^\circ, 5^\circ, \dots, 30^\circ$.

No attempt has been made to tabulate GRID or any of the other data sets which contribute to the figures of this chapter. The amount of information involved is simply too vast, and graphical portrayal has been used. When energies or $B(E2)$'s appear plotted against one of the potential parameters [e.g., Figure 5.6] the ISU Simplotter routines (49) were used; calculated points have consequently been replaced by a smooth (spline) curve. Detailed information concerning the density of points, and the particulars ($N_{MAX}(J)$, $\tilde{s}$, etc.) of the figure calculations may be found in Table E.5.

B. An Interpretive Framework

Before examining the spectra of $\bar{H}_{QP}$ it is useful to formulate some simple expectations that may be of help in correlating and interpreting the calculated results. Consider a classical liquid droplet which, at any instant, is restricted to a quadrupole shape. If its potential energy function $V(\beta, \gamma)$ possesses a minimum at $(\beta_0 \neq 0, \gamma_0)$, the droplet will have a non-spherical equilibrium shape. The stability of this equilibrium shape, as viewed from the BF frame, will of course

increase as the minimum of $V(\beta, \gamma)$ is sharpened. For a strong minimum, we can expect to "rotate" the droplet¹ without greatly affecting its BF frame appearance, although some centripetal stretching should occur. Similarly, low-energy oscillations in the β and γ coordinates would not severely alter the principal moments of inertia. The rotational and shape-vibrational degrees of freedom are then effectively decoupled by a sharp non-spherical minimum in $V(\beta, \gamma)$.

Though the energies and angular momenta involved will be discrete, the same effect should appear in quantum mechanical calculations. As β_0 , C_β and C_γ are slowly increased from zero, the spectra of $\bar{H}_{QP}$ should exhibit the development of rotational sequences based upon β and γ

¹The "rotation" of the classical droplet here refers to the rotation of the confining surface, as viewed from the LAB frame when β and γ are fixed at β_0 and γ_0 respectively. Individual fluid elements do not rotate about the center of mass with the angular velocity of the confining surface. Such a rigid motion would violate the irrotational flow condition $\nabla \times \mathbf{v} = 0$ which the classical velocity field, $\mathbf{v}$, was assumed to satisfy. Effective moments of inertia, I_k , for the irrotational droplet may be deduced by writing the classical kinetic energy, T , [with $\dot{\beta} = \dot{\gamma} = 0$] in the form

$$T = \frac{1}{2} \sum_k I_k \omega_k^2,$$

where ω_k is the projection of the angular velocity upon the BF k -axis. For a fluid of mass density ρ_0 , we find [to lowest order in β_0]

$$I_k = 4B\beta_0^2 \sin^2(\gamma_0 - \frac{2\pi k}{3}) \quad ; \quad B \equiv \frac{\rho_0 R_0^5}{2}.$$

These may be compared with the inertia moments appropriate to the rigid rotation of the entire droplet:

$$I_k^{RQ} = [16\pi B/15] [1 - (5/4\pi)^{1/2} \beta_0 \cos(\gamma_0 - \frac{2\pi k}{3})]$$

In this work the term "rigid quadrupole rotor" will be used exclusively to refer to a rigid rotor with moments of inertia I_k .

vibrations. From the figures of Appendix A, it is clear that the changes

$$\beta \rightarrow \beta + \Delta\beta$$

$$\gamma \rightarrow \gamma + \Delta\gamma$$

carry no net angular momentum in the BF coordinate system. Consequently pure β and γ vibrations (as well as their sums) will be associated with $J = 0$ states. The rotational bands built upon such vibrations should resemble those of a rigid quadrupole rotor as C_β and C_γ tend to infinity [or equivalently as β_0 and $C_\gamma \rightarrow \infty$ with fixed $C_\beta = 1$]. In light of these expectations, it will prove expeditious to analyze the spectra of $\bar{H}_{QP}$ by asking:

- 1) what happens to the $J = 0$ states as the parameters of $\bar{H}_{QP}$ are varied; and
- 2) how do rotational bands develop from the (unperturbed) eigenstates of H_B , and how does each compare with the asymmetric rotor band (ARB) of a rigid rotor having the Bohr moments of inertia?

It is necessary for us to recall several features of quantum mechanical rotors.¹ The Hamiltonian for a general rigid rotor may be written as

$$H_R = \frac{\hbar^2}{2} \sum_{k=1}^3 \frac{L_k^2}{I_k} \quad (5.13)$$

¹The mathematical details of the summary presented here may be found in Chapter 3 of the text by J. P. Davidson (5).

I_k is the moment of inertia about the k^{th} BF axis, and $\hbar L_k$ is the operator for the projection of the total angular momentum upon this axis. In the case $I_1 = I_2 \neq I_3$, eigenfunctions of H_R are the rotation matrix elements $D_{MK}^{J*}(\theta_i)$ when the Euler angles specifying the LAB $\rightarrow$ BF rotation are used as coordinates. J and M are good quantum numbers as is K , the projection of J upon the BF z -axis (in units of $\hbar$). The eigenvalue of H_R associated with $D_{MK}^{J*}(\theta_i)$ is

$$E_R = \frac{\hbar^2}{2} \left[\frac{J(J+1)}{I_1} + \left(\frac{1}{I_3} - \frac{1}{I_1} \right) K^2 \right], \quad [I_1 = I_2] \quad (5.14)$$

When $I_1 \neq I_2$, K is no longer a classical constant of the motion, and eigenfunctions of H_R are linear combinations of rotation matrix elements:

$$\phi_{JM} = \sum_{K=-J}^J A_K D_{M,K}^{J*}(\theta_i) \quad (5.15)$$

The constants A_K will depend upon the moments of inertia.

In general, the eigenfunctions of H_R may be classified into four types $\{A, B_1, B_2, B_3\}$ according to their transformation properties under operations which relabel the BF axes. The A-type states have only even values of K appearing in Equation (5.15), and further obey

$$A_{-K} = (-1)^J A_K \quad (5.16)$$

Their transformation properties consequently mirror those of the ψ_α [see Equation (2.27)], and they will be the only rotor states of

interest to us. A-type eigenfunctions for $l_1 = l_2$ are¹

$$\phi_{JM|K|} = \left[\frac{2J+1}{2(1+(-1)^J \delta_{K,0})} \right]^{\frac{1}{2}} \left[D_{M,K}^{J*}(\theta_i) + (-1)^J D_{M,-K}^{J*}(\theta_i) \right], \quad (5.17)$$

$$|K| = 0, 2, 4, \dots, J \text{ or } J-1$$

and these develop smoothly into the A-type states of an asymmetric rotor as l_2 moves away from l_1 . [Matrix elements of H_R between rotor states of different symmetry types vanish for all values of the l_k .] Enumeration of the $\phi_{JM|K|}$ then serves to enumerate the A-type states of any rigid rotor. J may assume the values

$$\begin{aligned} J &= 0, 2, 4, 6, \dots & ; & \quad |K| = 0 & , \\ J &= |K|, |K|+1, |K|+2, \dots & ; & \quad |K| \neq 0 & , \end{aligned} \quad (5.18)$$

and consequently be tabulated as in Figure 5.4a.

When $l_1 = l_2$, $|K|$ is a good quantum number, and can be used to partition the A-type rotational "band" into K-sequences [Figure 5.4b]. E2 transitions between such states of a symmetric rotor must satisfy the selection rule

$$\Delta|K| = 0, +2 \quad (5.19)$$

For the A-type states of an asymmetric top, $|K|$ is of course no longer a good label. However I will continue to refer to a set of levels with spins $0, 2, 4, \dots$ or $K, K+1, K+2, \dots$ as a "K-sequence". Such

¹These are normalized over the range of the Euler angles [Equation (2.15)] with respect to the volume element $[\sin \theta_2 d\theta_1 d\theta_2 d\theta_3 / 8\pi^2]$.

Figure 5.4. Quantum states of an A-type rotor
 (a) Using Equation (5.18) to count the states of an A-type rotor
 (b) Energy eigenvalues of a symmetric rotor grouped into K sequences

Figure 5.5. Comparison of spectra for H_R and $\bar{H}_{Qp}$. The drawing at left has been taken from Reference (5) and has vertical units of $\hbar\omega = \hbar^2/4B\beta_{O_2}^2$. The drawing at right, formed from the GRID data, depicts the relative eigenvalue $\bar{E}(J_i) - \bar{E}(0_1)$ of $H_{Qp}(\beta_0=4, C_\gamma=30)$ as a function of γ_0 . J is labeled on each curve

sequences are assumed to have developed smoothly from those of a symmetric rotor as the symmetry $I_1 = I_2$ is broken. The sum rules [Reference (50)]

$$\begin{aligned} E_R(3_1) &= E_R(2_1) + E_R(2_2) \\ E_R(5_1) &= 4E_R(2_1) + E_R(2_2) \\ E_R(5_2) &= E_R(2_1) + 4E_R(2_2) \end{aligned} \quad \left[\begin{array}{l} E_R(J_i) = \text{relative} \\ \text{energy (above the GS)} \\ \text{of the } J_i \text{ (A-type)} \\ \text{eigenstate of } H_R \end{array} \right] \quad (5.20)$$

hold for all A-type rotors, independent of the values of the I_k .

For the rigid quadrupole rotor, the effective moments of inertia appearing in H_B [Equation (2.11)] are used with β and γ considered fixed:

$$I_k = 4B\beta_0^2 \sin^2(\gamma_0 - \frac{2\pi k}{3}) \quad (5.21)$$

Energies for low-lying A-type states are shown as functions of γ_0 in the left portion of Figure 5.5. Notice that β_0 enters only in the overall scale factor. When $\gamma_0 = 0^\circ$, the quadrupole surface has a peanut-like appearance which is unchanged by rotations about the BF z-axis. I_1 , I_2 , and I_3 are $3B\beta_0^2$, $3B\beta_0^2$, and 0 respectively; and the $K \neq 0$ sequences occur at infinite energy [Equation (5.14)]. As γ_0 and consequently I_3 increase, axial symmetry is broken and these energies are lowered. Portions of the $K = 2$ and $K = 4$ sequences are shown in Figure 5.5. The $J = 6$ and 7 members of $K = 2$ may be seen to cross near $\gamma_0 = 25^\circ$.

A-type eigenstates of the rigid quadrupole rotor may be written as

$$\phi_{JMK'} = \sum_{\substack{K=0 \text{ or } 2 \\ \text{even}}}^J A_{K'K}(\gamma_0) \phi_{JM|K|} \quad ,$$

where K' is the sequence label appearing in Figure 5.4a, and $\phi_{JM|K|}$ are the symmetric rotor eigenfunctions of Equation (5.17). At $\gamma_0 = 0^\circ$ the coefficients satisfy

$$A_{K'K} = \delta_{K',K}$$

As γ_0 is increased from 0° , the $A_{K'K}$ ($K' \neq K$) grow in absolute values at the expense of the $A_{K'K'}$. For example at $\gamma_0 = 30^\circ$, ϕ_{2M0} has $A_{00} = \sqrt{3}/2$, $A_{20} = \frac{1}{2}$, and may be said to be 75% $|K| = 0$ and 25% $|K| = 2$ (9). Correspondingly, ϕ_{2M2} is 75% $|K| = 2$ and 25% $|K| = 0$. The off-diagonal $A_{K'K}$ are generally found to be appreciable only for $\gamma_0 > 15^\circ$ (51).

The right hand portion of Figure 5.5 has been constructed using the GRID data and illustrates the dependence upon γ_0 of selected energies of $\bar{H}_{QP}$. The similarity with the rigid rotator¹ spectrum is striking. The additional $J = 0, 2$ states above .9 are evidently connected with a β or γ vibration. As the parameters of $\bar{H}_{QP}$ are varied, energy eigenvalues are generally forbidden to cross for states of like spin (39). [Such a degeneracy, if it occurred, would be associated with a symmetry of $\bar{H}_{QP}$.] Rather, the approaching levels strongly repel one another and the associated wavefunctions interchange their characteristics. This phenomenon occurs for the 2_2 and 2_3 levels in Figure 5.5 and will be considered later in more detail.

¹ Throughout the remainder of this work, the only rigid rotor of interest is the "rigid quadrupole rotor", i.e., a rigid rotor with principal moments of inertia given by Equation (5.21). Unless context indicates otherwise, the term "rigid rotor" can be taken to refer to the A-type quantum states of the rigid quadrupole rotor.

C. The Identification of Vibrational States [$J = 0$]

The quantized excitations of a one-dimensional harmonic oscillator
(52)

$$H_{os}\phi(x) = E_{os}\phi(x) \quad (5.22a)$$

$$H_{os} = \frac{1}{2}m(\dot{x})^2 + \frac{1}{2}k(x - x_0)^2 = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2}k(x - x_0)^2, \quad (5.22b)$$

subject to the boundary condition

$$\phi(x) \xrightarrow{|x - x_0| \rightarrow \infty} 0, \quad (5.23)$$

have absolute energies which are half-integral multiples of $\hbar\sqrt{k/m}$

$$E_{os} = (n + \frac{1}{2}) \hbar\sqrt{k/m} \quad n = 0, 1, 2, \dots \quad (5.24)$$

As the restoring constant k is increased, the relative energies rise like $\sqrt{k}$. With this in mind, we may attempt to identify shape vibrational states in the spectrum of $\bar{H}_{QP}$ by varying the constants C_β and C_γ . If the potential minimum is sharp, excitations associated with harmonic oscillations in the β or γ coordinate should rise in energy roughly like $\sqrt{C_\beta}$ or $\sqrt{C_\gamma}$ respectively. This in fact is the prediction of strong-deformation collective models [such as the rotation-vibration model of Faessler et al. (11)] in which both β and γ degrees of freedom are treated. In the special case $C_\gamma = \beta_0 = 0$, the Bohr Hamiltonian is recovered from $\bar{H}_{QP}$; increasing C_β then causes the entire energy spectrum to rise in a manner proportional to $\sqrt{C_\beta}$. However as a non-spherical, γ -stable minimum develops, the relative energies of the β and

γ -vibrational band heads are expected to become independent of C_γ and C_β respectively. For $J = 0$ states of $\bar{H}_{QP}$, $\bar{\phi}(\beta', \gamma, \theta_i) = \bar{\phi}(\beta', \gamma)$ and from Equations (2.11) and (5.8) we have effectively [$C_{\beta\gamma} = 0$]

$$\begin{aligned} \bar{H}_{QP}(\beta', \gamma) = -\frac{1}{2} \left[\frac{1}{\beta'^4} \frac{\partial}{\partial \beta'} \beta'^4 \frac{\partial}{\partial \beta'} + \frac{1}{\beta'^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} \right] \\ + \frac{1}{2} C_\beta (\beta' - \beta_0)^2 + C_\gamma (\gamma - \gamma_0)^2, \quad 0 \leq \gamma \leq \frac{\pi}{3}. \end{aligned} \quad (5.25)$$

For large β_0 and C_β , the approximation $\frac{1}{\beta'^2} \approx \frac{1}{\beta_0^2}$ in the second term is expected to be valid, and permits separation of variables. The energy of $\bar{\phi}(\beta', \gamma) = F(\beta') G(\gamma)$ is then the simple sum of contributions from β and γ excitations:

$$\bar{E} = \bar{E}_\beta + \bar{E}_\gamma. \quad (5.26)$$

The separated equations may be made to resemble Equation (5.22a), if the substitution

$$\bar{\phi}(\beta', \gamma) = \frac{f(\beta')}{\beta'^2} \frac{g(\gamma)}{|\sin 3\gamma|^{\frac{1}{2}}} \quad (5.27)$$

is used in Equation (5.25). In that event we obtain

$$\left[-\frac{1}{2} \frac{d^2}{d\beta'^2} + \frac{1}{2} C_\beta (\beta' - \beta_0)^2 \right] f(\beta') = \left[\bar{E}_\beta - \frac{1}{\beta'^2} \right] f(\beta') \quad (5.28a)$$

$$\left[\frac{-1}{2\beta_0^2} \frac{d^2}{d\gamma^2} + C_\gamma (\gamma - \gamma_0)^2 \right] g(\gamma) = \left[\bar{E}_\gamma + \frac{1}{2\beta_0^2} \frac{9}{4} \left(1 + \frac{1}{\sin^2 3\gamma} \right) \right] g(\gamma). \quad (5.28b)$$

The boundary conditions appropriate to Equations (5.28) follow from the finiteness of $\bar{\phi}$:

$$f(0) = 0 \quad \text{and normalizeable} \quad (5.29a)$$

$$g(n \frac{\pi}{3}) = 0, \quad n = 0, 1, 2 \dots \quad \text{and normalizeable.} \quad (5.29b)$$

Equations (5.25) and (5.28b) specify the problem only on $0 \leq \gamma \leq \pi/3$;

Equation (5.1) must be used to obtain the potential energy function elsewhere. However, it is sufficient to consider only this range as $\bar{H}_{QP}(\beta', \gamma)$, $\bar{\phi}(\beta', \gamma)$, and the boundary condition (5.29b) are all unaffected by the transformations

$$\gamma \rightarrow -\gamma \quad ; \quad \gamma \rightarrow \gamma - 2\pi/3$$

If we replace the last terms in Equations (5.28) by their equilibrium values, and substitute boundary conditions of the form Equation (5.23) for Equations (5.29) we obtain

$$\bar{E}_\beta = [C_\beta]^{1/2} [n_\beta + \frac{1}{2}] + \frac{1}{\beta_o^2}, \quad n_\beta = 0, 1, 2, \dots \quad (5.30a)$$

$$\bar{E}_\gamma = \left[\frac{2C_\gamma}{\beta_o^2} \right]^{1/2} [m_\gamma + \frac{1}{2}] - \frac{9}{8\beta_o^2} \left[1 + \frac{1}{\sin^2 3\gamma_o} \right], \quad m_\gamma = 0, 1, 2, \dots \quad (5.30b)$$

Although these approximations cannot be trusted in all cases (particularly near $\gamma_o = 0$), the leading terms in Equations (5.30) indicate how the vibrational character of a given $J = 0$ state may be determined from the effects of varying $(\beta_o, C_\beta, C_\gamma)$ in $\bar{H}_{QP}$. The calculation of expectation values such as $\langle (\gamma - \langle \gamma \rangle)^2 \rangle$ and $\langle (\beta - \langle \beta \rangle)^2 \rangle$ would also be of aid in identifying shape-vibrational states, but has not been attempted in this work. As we shall see, the energy method is quite sufficient.

If we wish to observe the effect of smoothly obtaining $\bar{H}_{QP}$ from the standard reduced Bohr Hamiltonian, it is convenient to proceed in three stages.

Stage I. C_β and C_γ are fixed at 1 and 0 respectively; β_0 is slowly increased from zero to its desired value. At each point in this process, ℓ remains a good quantum number. Members of each ℓ -multiplet are easily traced to the "seed" states of H_B^I from which they originate.

Stage II. With $(\beta_0, C_\beta, \gamma_0)$ fixed, C_γ is slowly increased from zero to its desired value, breaking the ℓ degeneracy. $J = 0$ γ -vibrational states may be identified by the rise of their relative energies. Remaining $J = 0$ states, by default, are to be associated with β vibrations.

Stage III. With $(\beta_0, \gamma_0, C_\gamma)$ fixed, C_β is increased from unity to its desired value to verify the identifications made during Stage II.

The possible reduced spectra of $\bar{H}_{QP}$ may of course be investigated without recourse to Stage III calculations.

The results of Stage I calculations are shown in Figures 5.6-5.8. In the first of these figures, the ℓ -multiplets may be seen to be grouping into tightly spaced bands as β_0 is increased. Members of a given band originate from seed states having a common value of $N - \ell$. [Such behavior is not unexpected in light of the radial probability densities depicted in Figure (2.7).] In the second two figures, the $\ell = N$ and $\ell = N - 2$ bands of multiplets have been isolated. Though ℓ remains a good quantum number, N does not. At $\beta_0 = 5.1$ the $\ell = J = 0$ ground state which originates from $[N, \ell] = [0, 0]$ is only .03% $N = 0$.

Figure 5.6. $\bar{H}_{QP}$ Stage I calculations [$C_\gamma = C_{\beta\gamma} = 0$, $C_\beta = 1$]. $\bar{H}_{QP} = H_B^I$ at $\beta_0 = 0$, and states of like N are degenerate. At $\beta_0 \neq 0$, ℓ and J remain good quantum numbers and states originating from Bohr states of like $[N, \ell]$ remain degenerate

Figure 5.7. $\bar{H}_{0p}$ Stage I calculations. Relative energies of states originating ($\beta_0 = 0$) with $[N, l] = [N, N]$ and $[N, N-2]$

Figure 5.8. $\bar{H}_{0p}$ Stage I calculations. Reduced energies of states originating ($\beta_0 = 0$) with $[N, \ell] = [N, N]$ and $[N, N-2]$

That is, in the expansion¹

$$\bar{\phi} = \sum_i a_i \psi_i^{\tilde{s}} \quad (5.31)$$

we find

$$\sum_i (a_i)^2 \delta_{N_i, 0} = .00026 \quad (5.32)$$

Similarly, the ground state consists of $N = 2, 4, 6, \dots, 20$ in the following percentages respectively: .4, 3, 9, 17, 22, 21, 15, 8, 4 and 1. At $\beta_0 = 5.1$ the expectation value of N defined by

$$\langle N \rangle = \sum_i (a_i)^2 N_i \quad (5.33)$$

is 11.1 for the ground state. It is $\sim 12, 13$, and 14 for the $J = 0$ states originating from $[N, \ell] = [2, 0], [4, 0]$, and $[6, 0]$ respectively. As the relative energies of these states approach multiples of $\sqrt{C_\beta} = 1$ for large β_0 , it is tempting to associate them with the first three β vibrations.

Credence may be given to this association by considering an approximate analytical treatment of Equation (5.7) for $C_\gamma = C_{\beta\gamma} = 0$ and large β_0 .² The substitution $\bar{\phi} = \frac{1}{\beta^{1/2}} f(\beta') \Phi(\gamma, \theta_i)$ permits separation of

¹The values of the sums in Equations (5.32) and (5.33) will of course depend upon the value of $\tilde{s}$ used in the expansion of Equation (5.31). In this case $\tilde{s} = 1$ is used, for which the unperturbed ground state would be 100% $N = 0$. The figures quoted result from a 30 phonon diagonalization.

²The mathematical development summarized here parallels that contained in (14).

variables with the resulting radial equation

$$\left[-\frac{1}{2} \frac{d^2}{d\beta'^2} + W_{\Lambda}(\beta') \right] f(\beta') = \bar{E} f(\beta') \quad (5.34)$$

$$W_{\Lambda}(\beta') = \frac{1}{2} C_{\beta} (\beta' - \beta_0)^2 + \frac{1}{2\beta'^2} [2 + \Lambda] \quad (5.35)$$

The separation constant Λ may be determined from the angular portion of the problem to be

$$\Lambda = \ell(\ell + 3) \quad ; \quad \ell = 0, 1, 2, \dots \quad (5.36)$$

[The $\Phi(\gamma, \theta_i)$ are the angular factors of the ψ_{α} ; ℓ in Equation (5.36) is the usual R(5) IR label.] If $W_{\Lambda}(\beta')$ is expanded about its minimum, β_{Λ} , the resulting approximation

$$W_{\Lambda}(\beta') \approx W_{\Lambda}(\beta_{\Lambda}) + \frac{1}{2} C_{\Lambda} (\beta' - \beta_{\Lambda})^2$$

may be used in Equation (5.34). Solutions $f(\beta')$ obeying the boundary condition of Equation (5.29a) are found to be parabolic cylinder functions (53). Energy eigenvalues are

$$\bar{E} = \sqrt{C_{\beta}} \left\{ (v_{n_{\beta}} + \frac{1}{2}) \left(\frac{Z_1}{Z} \right)^2 + \frac{\Lambda + 2}{2Z^2} \left[1 + \frac{(\Lambda + 2)}{Z^4} \right] \right\} \quad (5.37)$$

$$Z = (C_{\beta})^{\frac{1}{4}} \beta_{\Lambda}$$

$$Z_1 = [Z^4 + 3(\Lambda + 2)]^{\frac{1}{4}}$$

where $v_{n_{\beta}}$ ($n_{\beta} = 0, 1, 2, \dots$) are the (ordered) values which make the parabolic cylinder function

$$D_{v_{n_\beta}}(-\sqrt{2} z_1)$$

zero. In the limit of large β_0 ,

$$z \rightarrow (C_\beta)^{\frac{1}{4}} \beta_0$$

$$\frac{z_1}{z} \rightarrow 1 + \frac{3(\Lambda + 2)}{4z^4}$$

$$v_{n_\beta} \rightarrow n_\beta$$

$$\bar{E} \rightarrow \sqrt{C_\beta} (n_\beta + \frac{1}{2}) + \frac{\Lambda + 2}{2\beta_0^2} ; \quad \begin{array}{l} n_\beta = 0, 1, 2, \dots \\ \ell = 0, 1, 2, \dots \end{array} \quad (5.38)$$

and the energy spectrum decomposes into ℓ sequences ($\ell = 0, 1, 2, \dots$) based upon equally spaced β vibrations. The integer n_β is interpreted as the number of β -excitational quanta. For the ground state band ($n_\beta = 0$), reduced energies approach

$$\frac{\bar{E}(n_\beta = 0, \ell) - \bar{E}(0, 0)}{\bar{E}(0, 1) - \bar{E}(0, 0)} = \frac{\ell(\ell + 3)}{4} \quad [\beta_0 \rightarrow \infty]$$

The reduced energies shown in the left portion of Figure 5.8 are then expected to converge to 0, 1, 2.5, 4.5, 7, 10, and 13.5 for $\ell = 0, 1, 2, 3, 4, 5$, and 6 respectively. At $\beta_0 = 5.1$, the calculated values are 0, 1, 2.47, 4.40, 6.74, 9.46, and 12.55.

If the n_β -th β -vibrational band head originates from the $J = 0$ Bohr eigenstate having

$$[N, \ell, J] = [2n_\beta, 0, 0] \quad \begin{array}{l} \text{seed state for} \\ n_\beta\text{-th } \beta\text{-vibration} \end{array} \quad (5.39)$$

what can be said of the γ vibrations? When $C_\gamma = 0$, rotations and γ vibrations are strongly coupled, and the seeds of pure γ vibrations are evidently buried within the $n_\beta = 0$ [i.e., $N = \ell$] spectrum of Figure 5.7. As $\ell \neq 0$, $J = 0$ states of H_β occur only for $\ell = 3, 6, 9, \dots$, we may tentatively assume that the m_γ -th γ -vibrational band head will eventually develop from

$$[N, \ell, J] = [3m_\gamma, 3m_\gamma, 0] \quad \begin{array}{l} \text{seed state for} \\ m_\gamma\text{-th } \gamma\text{-vibration} \end{array} \quad (5.40)$$

as the γ coordinate stabilizes. Under this assumption the angular momentum spectrum for the case $\beta_0 = 3$, $C_\gamma = 0$ has been partitioned as indicated in Figure 5.9. Above each of the low-lying $J = 0$ states a complete set of A-type rotor levels may be assembled, as has been shown explicitly for the ground state (GS) and in less detail for the first β and γ vibrations. All members of the GS and γ bands originate from $N = \ell$ seed states, while those of the first β band develop from $\ell = N - 2$ seeds. As the γ coordinate has not been stabilized about an equilibrium value, each of these bands of "rotational" states bears little resemblance to those shown in Figures 5.4 and 5.5. In particular, within a given K-sequence adjacent even and odd spin members are pairwise degenerate. This situation is expected to change as C_γ moves off of zero.

In Equations (5.39) and (5.40), $J = \ell = 0$ states have been associated with β band heads only. On the basis of Equation (5.30a), the relative energies of such states are expected to remain approximately constant during Stage II calculations. That this is actually the case may be seen in Figure 5.10 [25-phonon calculations for $C_\gamma = 0, 1, 2, \dots, 80$]. This figure may be interpreted in terms of β and γ vibrations

Figure 5.10. $\bar{H}_{0p}$ Stage II calculations [$\beta_0 = 2$, $C_\beta = 1$, $C_{\beta\gamma} = 0$] for $J = 0$ states. At $C_Y = 0$, ℓ is a good quantum number, and the ℓ labels at left apply to each panel. Vibrational labels ($m_Y\gamma + n_\beta\beta$) at large C_Y have been assigned from energy considerations

Figure 5.11. Reduced energies for the eight lowest $J = 0$ states of Figure 5.10.

and their superpositions. The quantum number ℓ , valid at $C_Y = 0$, has been labeled for each state of the left panel. The bottommost of the steeply rising curves in each panel originates from the $\ell = 3$ state of lowest energy. This curve, identified with the lowest γ vibration, resembles

$$\bar{E}(0_Y) - \bar{E}(\text{GS}) = a_1 \sqrt{C_Y} + a_2 \quad (5.41)$$

for $C_Y \geq 10$, with the constants a_1 and a_2 depending upon γ_0 .¹ Parallel curves, also originating from $\ell = 3$ states, have been labeled as representing β vibrations superimposed upon the first γ vibration. The

¹The boundary condition (BC) approximation leading to Equation (5.30b) is expected to be most valid if γ_0 lies in the center of the interval $[0, \pi/3]$. From the GRID calculations

$$v \equiv \frac{\bar{E}(0_Y) - \bar{E}(\text{GS})}{\left[\frac{2C_Y}{\beta_0^2} \right]^{\frac{1}{2}}} = \begin{cases} 1 & \text{when Equation (5.30b) holds} \end{cases}$$

is found to have the values [$C_Y = 30$]

	$\beta_0 =$	2	4	6
$\gamma_0 = 0^\circ$		1.23	1.71	1.92
15°		.85	1.04	1.02
30°		.72	.92	.98

Hence as β_0 grows, the calculated ratio v is approximately given by Equation (5.30b) if γ_0 is not near 0° . An approximate treatment of Equation (5.25) with BC appropriate to $\gamma_0 = 0^\circ$ [pp. 37-39 of (6)] results in the replacement of Equation (5.30b) by

$$\bar{E}_Y = \left[\frac{2C_Y}{\beta_0^2} \right]^{\frac{1}{2}} [2m_Y + 1] \quad , \quad m_Y = 0, 1, 2, \dots$$

The ratio v then assumes the value 2.

vertical separation between such curves is very nearly equal to the relative energy of the lowest β vibration. The 2γ band head originates from the lowest $\ell = 6$ state and lies at approximately twice the energy of the first γ excitation. It rises rapidly "through" the $m_\gamma = 0, 1$ levels as C_γ increases. True crossing of the energies in Figure 5.10 is forbidden with the exception of the $\gamma_0 = 30^\circ$ panel within which states of opposite ℓ -parity can cross. However the short-range repulsion effects are not always visible on the scale of the figure. For low values of C_γ , the modulation by γ_0 of the effective strength of $C_\gamma(\gamma - \gamma_0)^2$ is obvious. The value of γ_0 also has a striking effect upon the associated reduced spectra, shown in Figure 5.11. As C_γ increases, thus stabilizing the intrinsic shape, the relative energy of the rotational state $J_1 = 2_1$ falls slightly. The reduced energies of all vibrational band heads consequently rise.

The vibrational identifications labeled in Figures 5.11 and 5.12 may be further verified by performing Stage III calculations. As C_β is increased, β -vibrational energies should rise, while those of γ vibrations are expected to be relatively unchanged. The results of such a series of calculations are shown in Figure 5.12 [25-phonon; $C_\beta = 1, 1.1, 1.2, \dots, 10$]. The starting values of the potential parameters correspond to the dashed line in Figure 5.10, and the vibrational labels at $C_\beta = 1$ have been taken from there. As before, the points corresponding to a given relative eigenvalue $[\bar{E}(0_1) - \bar{E}(0_1)]$ have been smoothly connected and the curves so obtained are forbidden to cross. If the repulsion effects are ignored, the β and γ -vibrational band heads behave as

Figure 5.12. $\bar{H}_{Qp}$ Stage III calculations for $J = 0$ states. Vibrational labels at $C_\beta = 1$ are those at the dashed line in Figure (5.10)

expected when C_β is increased. Initially all energies rise (as would be the case if C_β were increased in H_β) but those of the purely γ -vibrational states begin to level off. Furthermore, the relative energy of the n_β -th β vibration approaches $n_\beta \sqrt{C_\beta}$ (from above). For $n_\beta = 1, 2, 3, 4$ and 5, the quantity

$$\frac{\bar{E}(n_\beta^{\text{th}} \beta\text{-vib.}) - \bar{E}(\text{GS})}{n_\beta \sqrt{C_\beta}}$$

has the calculated values 1.278, 1.300, 1.321, 1.341, and 1.361 at $C_\beta = 1$ in Figure 5.12. However at $C_\beta = 10$, we find 1.052, 1.058, 1.065, 1.074 and 1.086 respectively.

D. Rotational Band Development

The $J = 0$ energy calculations of the previous section may be summarized by the following statements. As a non-spherical, γ -stable minimum develops, the $J = 0$ spectrum of $\bar{H}_{Qp}$ may be interpreted as being comprised of β and γ vibrations and their superpositions. The two types of shape excitations may be identified by their behaviors under variations of the potential parameters. β -vibrational states rise in energy like $\sqrt{C_\beta}$ but are fairly insensitive to changes in C_γ . The reverse is characteristic of the γ -vibrational states. If $\bar{H}_{Qp}$ is obtained from H_B^I by proceeding sequentially through calculational Stages I, II and III, the hybrid band head consisting of n_β β vibrations and m_γ γ vibrations develops smoothly from the H_B^I state with quantum numbers

$$[N, \ell, J] = [2n_\beta + 3m_\gamma, 3m_\gamma, 0] \quad (5.42)$$

The relative energy¹

$$\bar{e}(n_{\beta}, m_{\gamma}, J_i) \equiv \bar{E}(n_{\beta}, m_{\gamma}, J_i) - \bar{E}(0, 0, 0_1) \quad (5.43)$$

of this state is given approximately by

$$\bar{e}(n_{\beta}, m_{\gamma}, 0_1) \sim n_{\beta} \cdot \bar{e}(1, 0, 0_1) + m_{\gamma} \cdot \bar{e}(0, 1, 0_1) \quad (5.44)$$

Equations (5.30) are useful for estimating shape-vibrational energies [$J = 0$] when the potential minimum is sharp and $\gamma_0 \approx 0^\circ$.

We expect that statements similar to these can be made for states of other spins. Figure 5.6 indicates that all states originating with $(N - 2)/2 = n_{\beta}$ should be associated with the n_{β} -th β vibration. As a γ -stable minimum develops, these states are expected to arrange themselves into A-type rotor bands. Each such band should resemble that of Figure 5.5 in its dependence upon γ_0 . Figure 5.13, formed from the GRID data, indicates that such a partitioning does indeed occur. Accompanying each of the low-lying $J = 0$ states is a $J = 2, 2, 3$ sequence similar to that in Figure 5.5. [As only the nine lowest $J = 2$ states were stored during the GRID calculations, the second $J = 2$ level of the $\gamma + \beta$ band, $(n_{\beta}, m_{\gamma}, J_i) = (1, 1, 2_2)$, does not appear.] The first sum rule of Equations (5.20) may be seen to be approximately obeyed within each band.

The development of each low-lying state may be traced by pursuing the Stage I and II calculations used to identify developing band heads. Such calculations have been carried out, and a sampling of Stage II

¹Here $(n_{\beta}, m_{\gamma}, J_i)$ denotes the i^{th} state of spin J associated with the shape vibration specified by n_{β} and m_{γ} .

Figure 5.13. $\bar{H}_{Qp}$ [$\beta_0 = 5$, $C_\gamma = 30$] reduced energies of the states $J_i = 0_1, 0_2, \dots, 0_5; 2_1, 2_2, \dots, 2_9; 3_1, 3_2, \dots, 3_5$ [GRID data]

Figure 5.14. $\bar{H}_{QP}$ [$\beta_0 = 3$, $\gamma_0 = 15^\circ$] Stage II calculations. l is a good quantum number at $C_\gamma = 0$ and may be found in the bracket $[N, l]$. N denotes the principal quantum number of the H_B^I seed state from which the state developed during the preceding Stage I calculations [Figure 5.6]. $(n\beta + m\gamma)_i$ denotes the i th state of the spin in question belonging to the $(n\beta + m\gamma)$ vibrational band

Figure 5.15. $\bar{H}_{QP}$ [$\beta_0 = 3$, $\gamma_0 = 15^\circ$] Stage II calculations. See caption of Figure 5.14

Figure 5.16. $\bar{H}_{QP}$ [$\beta_0 = 3$, $\gamma_0 = 30^\circ$] Stage II calculations. See caption of Figure 5.14.

Figure 5.17. $\bar{H}_{QP}$ [$\beta_0 = 3, \gamma_0 = 30^\circ$] Stage II calculations. See caption of Figure 5.14

energies appears in Figures 5.14-5.17. Two fixed values of γ_0 were considered: $\gamma_0 = 30^\circ$ for which $(-1)^L$ is well-defined; and $\gamma_0 = 15^\circ$ which represents the more typical situation. 20-phonon diagonalizations were performed for each of $J = 0, 2, 3, \dots, 7$ as C_γ ranged over 0, 2, 4, ..., 24. The calculated relative energy of the state J_i^1 appears as a smooth curve in the figures.

As C_γ is increased, $J = 0$ energies behave as expected; developing β and γ -vibrational band heads may be easily identified and have been so labeled. The energy spectrum for $J = 3$ may be roughly obtained by adding the relative energy of the 3_1 state to the $J = 0$ spectrum. The resemblance improves as C_γ increases, and the band assignments for $J = 3$ states in Figures 5.14 and 5.16 have been made accordingly. Recall that an A-type rotor possesses a single state of spin 3. For $J = 2$ there are two such rotor states and the situation becomes slightly more complicated. The entire $J = 2$ spectrum may be approximately obtained by adding the full $J = 0$ spectrum to each of 2_1 and 2_2 . Again the resemblance improves as C_γ increases, and results in the labeled band assignments. Two $J = 2$ levels have been assigned to each band, and they are distinguished by the subscripts 1 and 2. For each of the two values of γ_0 , the $(2_1, 2_2, 3_1)$ sequence within each band approximately satisfies the rotor sum rule [Equation (5.20)].

¹Two distinct methods of identifying states H_{0p} are employed in the remainder of this work. J_i refers to the i -th lowest energy state of spin J in the entire H_{0p} spectrum. (n_β, m_γ, J_k) is the k -th lowest energy state of spin J belonging to the rotation band based upon the (n_β, m_γ) shape vibration.

In a similar manner we may bootstrap our way to band assignments for higher spins, guided by the A-type rotor spectrum of Figure 5.5.

Initially, as C_Y and β_O are increased, the energies of $GS_1, GS_2, \dots$

GS_p [$p = \frac{J-1}{2}$ (J odd); $p = \frac{J+2}{2}$ (J even)] adapt their spacings to

resemble the rigid rotor situation. Once this has been obtained further

increases in the two parameters have little effect on the reduced

energies of these states. For states not belonging to the GS band, we

then have

$$\bar{e}(n_\beta, m_Y, J_i) \approx \bar{e}(0, 0, J_i) + n_\beta \cdot \bar{e}(1, 0, 0_1) + m_Y \cdot \bar{e}(0, 1, 0_1) \quad (5.45)$$

Having made the band assignments in Figures 5.14-5.17, it is but a simple matter to discover a rule relating the members of a given band with their states of origin. The rule may be stated in two parts.

- 1) The unperturbed spectrum (i.e., that of H_0^1) may be collected into bands based upon $J = 0$ states^B (band heads) and distinguished by two integers

$$n_\beta = 0, 1, 2, \dots$$

$$m_Y = 0, 1, 2, \dots$$

The N and ℓ quantum numbers of a band head are given by

$$N = 3m_Y + 2n_\beta$$

$$\ell = 3m_Y$$

and these determine $[N, \ell]$ for every other member of the band as shown in Figure 5.18. Each band consists of $(J+2)/2$ members for each even J together with $(J-1)/2$ members for each odd J , as is the case for an A-type rotor. For a fixed value of N , the allowed spins within a band form a "k-series"

$$J = 2k, 2k - 2, 2k - 3, \dots, k \quad (5.46)$$

where k may be thought of as the number of phonons of excitation above the band head energy. In Figure 5.18 the prototype band of seed states has been further divided (horizontally) into K-sequences [see Figure 5.4].

- 2) The unperturbed band identified by the pair (n_β, m_γ) contains the seed states of a rotational band of $H_{\beta\gamma}^{QP}$ based upon the superposition of n_β β vibrations and m_γ γ vibrations. That is, when a sharp, non-spherical minimum is formed by proceeding sequentially through Stages I, II and III, the energy spectrum which develops from each seed band comes to resemble that of an A-type rotor with moments of inertia given by Equation (5.21). For large β_0 , the entire band tends to rise in relative energy like

$$n_\beta \sqrt{C_\beta} \quad \text{or} \quad m_\gamma a \sqrt{\frac{2C_\gamma}{\beta_0^2}}$$

as C_β or C_γ is varied respectively. The constant a ranges from ~ 2 for $\gamma_0 = 0^\circ$ to ~ 1 for $\gamma_0 = 30^\circ$.

Two points should be raised in clarification of this summary. The first concerns the lack of reference to the quantum number ν in the new partitioning of H_β states. The second deals with the attempted crossing of energy levels. We will consider each in turn.

The new partitioning scheme correctly counts the number of H_β states of given N , ℓ and J . Recall the rule given in Chapter II: for fixed $[N, \ell] = [N_0, \ell_0]$ the multiplicity label assumes the values

$$\nu = 0, 1, 2, \dots, [\ell_0/3]_{GI} \quad (5.47)$$

and with each is associated the k-series of angular momenta

$$J = 2k, 2k - 2, 2k - 3, \dots, k \quad [k = \ell_0 - 3\nu] \quad (5.48)$$

N, ℓ , and J Quantum Numbers of H_B
Eigenstates Assigned to the (n_β, m_γ) Band

N	ℓ	k	J's						
-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-
$2n_\beta + 3m_\gamma + k$	$3m_\gamma + k$	k	2k	2k-2	2k-3	.	.	.	k
-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-
-	-	-	-	-	-	-	-	-	-
-	-	6	12	10	9	8	7	6	
-	-	5	10	8	7	6	5		
-	-	4	8	6	5	4			
$2n_\beta + 3m_\gamma + 3$	$3m_\gamma + 3$	3	6	4	3				
$2n_\beta + 3m_\gamma + 2$	$3m_\gamma + 2$	2	4	2					
$2n_\beta + 3m_\gamma + 1$	$3m_\gamma + 1$	1	2						
$2n_\beta + 3m_\gamma$	$3m_\gamma$	0	0						
K label:			0	2		4		6	

Figure 5.18. Quantum numbers for the prototype H_B band. As H_B^I is driven to H_{QP} , these states develop into an A-type rotor band based upon a shape-vibrational $J = 0$ state. n_β and m_γ are the numbers of β and γ -vibrational quanta respectively in the limit of large β_0 and C_γ [Equations (5.26) and (5.30)]

DECOMPOSITION OF UNPERTURBED SPECTRUM ($N \leq 9$) INTO BANDS

N	GROUND STATE BAND	FIRST β BAND	FIRST γ BAND	2β
	$\lambda=N$	$\lambda=N-2$	$\lambda=N$	$\lambda=N-4$
9	18 16 15 14 13 12 11 10 9	14 12 11 10 9 8 7	12 10 9 8 7 6	10 8 7 6 5
8	16 14 13 12 11 10 9 8	12 10 9 8 7 6	10 8 7 6 5	8 6 5 4
7	14 12 11 10 9 8 7	10 8 7 6 5	8 6 5 4	6 4 3
6	12 10 9 8 7 6	8 6 5 4	6 4 3	4 2
5	10 8 7 6 5	6 4 3	4 2	2
4	8 6 5 4	4 2	2	0
3	6 4 3	2	0	
2	4 2	0		
1	2			
0	0 = J			

SELECTION RULE
FOR 1ST ORDER
E2 TRANSITIONS

$\Delta N = \pm 1$
 $\Delta \lambda = \pm 1$

N	$\beta+\gamma$	3β	2γ	$\gamma+2\beta$	4β	$2\gamma+\beta$	$\gamma+3\beta$	3γ
	$\lambda=N-2$	$\lambda=N-6$	$\lambda=N$	$\lambda=N-4$	$\lambda=N-8$	$\lambda=N-2$	$\lambda=N-6$	$\lambda=N$
9	8 6 5 4	6 4 3	6 4 3	4 2	2	2	0	0
8	6 4 3	4 2	4 2	2	0	0		
7	4 2	2	2	0				
6	2	0	0					
5	0							

THE BAND HEAD FOR
 $M_\gamma \gamma + M_\beta \beta$
HAS QUANTUM NUMBERS
 $N = 2M_\beta + 3M_\gamma$
 $\lambda = 3M_\gamma$
 $J = 0$

Figure 5.19. Decomposition of the H_B spectrum [$N \leq 9$] into bands of the type shown in Figure 5.18

Hence $([\ell_o/3]_{G1} + 1)$ k-series contribute to the degenerate spectrum specified by $[N_o, \ell_o]$. Consider now the counting of $[N_o, \ell_o]$ states from the band viewpoint with Figure 5.18 in mind. If the (n_β, m_γ) unperturbed band head lies at or below N_o in relative energy, the associated band will make a contribution to the collection of H_B states having $N = N_o$. This will be the case if

$$3m_\gamma + 2n_\beta \leq N_o, \quad (5.49)$$

i.e., for those (n_β, m_γ) pairs enumerated by

$$n_\beta = 0, 1, 2, \dots, \left[\frac{N_o}{2} \right]_{G1} \quad (5.50a)$$

$$m_\gamma = 0, 1, 2, \dots, \left[\frac{N_o - 2n_\beta}{3} \right]_{G1} \quad (5.50b)$$

When Equation (5.49) is satisfied, the k-series at N_o arising from the (n_β, m_γ) band is characterized by

$$\begin{aligned} N &= N_o \\ k &= N_o - 3m_\gamma - 2n_\beta \\ \ell &= 3m_\gamma + k = N_o - 2n_\beta \end{aligned} \quad (5.51)$$

If we restrict our attention to those k-series in Equation (5.51) for which $\ell = \ell_o$ also holds, then

$$n_{\beta} = \frac{1}{2}(N_0 - \ell_0)$$

$$m_{\gamma} = 0, 1, 2, \dots, \left[\frac{N_0 - 2N_{\beta}}{3} \right]_{GI} = \left[\frac{\ell_0}{3} \right]_{GI} \quad (5.52)$$

$$k = \ell_0 - 3m_{\gamma}$$

The counting rule of Equations (5.47) and (5.48) is recovered with m_{γ} now playing the role of ν . Rather than using (N, ℓ, ν, J, M) to label H_B eigenfunctions, we can use $(N, \ell, m_{\gamma}, J, M)$ or the slightly redundant $(N, \ell, n_{\beta} = \frac{N - \ell}{2}, m_{\gamma}, J, M)$.

The complete band decomposition of the $N \leq 9$ H_B spectrum is shown in Figure 5.19. In those cases where the ν quantum number is required to distinguish states with a common set (N, ℓ, J, M) , we might ask how the (n_{β}, m_{γ}) seed states are related to the $\psi_{N\ell\nu JM}$. In particular for $N = \ell = J = M = 6$, which linear combination of ψ_{66066} and ψ_{66166} is the seed of the $K = 6$ member of the GS band, and which is the seed of the $K = 0$ member of the γ band? In all cases it is natural to define seed states, ${}^0\psi_i$, by the following property: If H_B^I is perturbed by the addition of ϵV , the eigenfunctions, ϕ_i , of $H = H_B^I + \epsilon V$ should obey

$$\phi_i \xrightarrow[\epsilon \rightarrow 0]{} {}^0\psi_i \quad (5.53)$$

For n degenerate seed states, ${}^0\psi_i$ ($i = 1, 2, \dots, n$), each having principal quantum number N and angular momentum character JM , we may write

$${}^0\psi_i = \sum_{j=1}^n a_{ij} \tilde{\psi}_{\alpha_j}^s \quad [N_j = N, J_j = J, M_j = M] \quad (5.54)$$

Equation (5.53) may be satisfied¹ by choosing the expansion coefficients in Equation (5.54) such that

$$\langle {}^0\psi_i | V | {}^0\psi_j \rangle = 0 \quad i, j = 0, 1, 2, \dots, n, \quad (5.55)$$

$$i \neq j$$

Hence the a_{ij} which specify the seed states will depend upon the nature of V . In Stage I calculations, $V = \beta'$ and $\epsilon = -2\beta_0$. For arbitrary $h(\beta')$

$$\langle \tilde{\psi}_{N\ell\nu JM}^{\tilde{s}} | h(\beta') | \tilde{\psi}_{N\ell'\nu' JM}^{\tilde{s}} \rangle \propto \delta_{\ell\ell'}$$

holds. Hence Equation (5.55) may be satisfied by choosing degenerate seed states to be orthogonal states of good $[N, \ell]$. For example

$${}^0\psi_i = \tilde{\psi}_{N\ell, t_i JM}^{\tilde{s}}$$

will do, as would

$${}^0\psi_i = \sum_j A_{ij} \tilde{\psi}_{N\ell, t_j JM}^{\tilde{s}} \quad (5.56)$$

with $[A]$ any unitary matrix. Thus without further characterizing the degenerate ϕ_i we are unable to make any statement about the ν (or t) content of their seed states when only Stage I calculations are considered. When Stage II calculations are begun, appropriate seed states are eigenfunctions of $H = -\frac{1}{2}T + \frac{1}{2}(\beta' - \beta_0)^2$. The degenerate seed states may be denoted ${}^0\psi_{\ell JMj}$ where j distinguishes multiple occurrences of (ℓJM) .

¹ See Chapter 16, Section G of the text by Merzbacher (39) regarding this point.

They will satisfy

$$\langle {}^0\psi_{\ell JM_i} | (\gamma - \gamma_0)^2 | {}^0\psi_{\ell JM_j} \rangle = 0 \quad i \neq j,$$

and this condition may be used together with

$${}^0\phi_{\ell JM_i} \xrightarrow{\beta_0 \rightarrow 0} {}^0\psi_i$$

to determine the coefficients A_{ij} in Equation (5.56). Unfortunately these coefficients depend upon the value of γ_0 . For this reason the relationship between the seed states $\psi_{N\ell n_{\beta} m_{\gamma} JM}$ and the $\psi_{N\ell \nu JM}$ has been left somewhat ambiguous.

In the course of Stage II or III calculations, states of like spin may attempt to cross in energy. This has been observed in the present work only when the two states involved belong to different bands. Some typical examples, taken from Figures 5.14-5.17, are shown in detail in Figures 5.20-5.22. At each calculated point information relating to the ℓ -decomposition of the $\tilde{H}_{QP}$ eigenfunction

$$\tilde{\phi} = \sum_i a_i \tilde{\psi}_i \quad (5.57)$$

has been given. This may include one or both¹ of

$$\langle \ell \rangle \equiv \sum_i (a_i)^2 \ell_i \quad (5.58)$$

¹ $\langle \ell \rangle$ and $[\% \ell = \ell']$ are independent of the value of $\tilde{s}$ used in Equation (5.57) if truncation effects are ignored.

$$[\% \ell = \ell'] \equiv 100\% \cdot \sum_i (a_i)^2 \delta_{\ell_i, \ell'} \quad (5.59)$$

For $C_Y = 0$, ℓ is well-defined and $\langle \ell \rangle$ is an integer. The observed general trend is for $\langle \ell \rangle$ to increase slowly as C_Y increases from 0 to 24. States having the same J , K , and γ -vibrational character begin with identical ℓ -decompositions, and this equality is approximately maintained as C_Y increases. This may be seen for the $J = K = 0$ β and 2β levels in Figure 5.20, which each begin with $\ell = 0$ and slowly gain higher ℓ components. At $C_Y = 24$ their ℓ -decompositions are approximately equal even though each has interacted with the rising γ -vibration. The latter state begins with 100% $\ell = 3$ and rather rapidly spreads its strength over several ℓ values.

In the vicinity of an attempted crossing, energy levels strongly repel one another and the two wavefunctions involved essentially interchange their characters over the course of this repulsion. Even though the energy levels may not actually cross, it thus makes good sense to consider, for example, the γ -vibrational levels as rising through and above their β counterparts. In fact near a close interaction, which we may symbolize by

Figure 5.20. $\langle l \rangle$ for $J_i = 0_2, 0_3, 0_4$ states of $\bar{H}_{0p}$ [$\beta_0 = 3, \gamma_0 = 15^\circ$]. Dots denote values of C_γ [0, 2, 4, ... 24] for which eigenvalues and eigenvectors were calculated. [$\%l = l'$] is given for selected states. The energy curves also appear in Figure [5.14]

Figure 5.21. $\langle l \rangle$ and $[\% \ell = \ell']$ for $J_i = 24$ and 25 states for $\bar{H}_{0p}$. States have well-defined ℓ -parity. Energy curves also appear in Figure [5.16]

Figure 5.22. $\langle l \rangle$ for $J_i = 2_{13}, 2_{14}, 2_{15}, 2_{16}$ states of $\bar{H}_{0p}$. Energy curves also appear in Figure 5.16. The states 2_{15} and 2_{16} have opposite l -parity and cross in energy

one finds

$$|\langle \bar{\phi}_1 | \bar{\phi}_4 \rangle| \approx |\langle \bar{\phi}_3 | \bar{\phi}_2 \rangle| \approx 1$$

$$|\langle \bar{\phi}_1 | \bar{\phi}_2 \rangle| \approx |\langle \bar{\phi}_3 | \bar{\phi}_4 \rangle| \approx 0$$

On either side of the interaction region, the vibrational character of each state is well-established. The nearest approach distance, $\Delta E(i, i + 1)$, is empirically found to be large if $\langle \ell \rangle$ is not too different for the two approaching levels. The $2_4 - 2_5$ interaction in Figure 5.21 is a good example of a long-range repulsion and its resulting slow interchange of characteristics. In the region $8 \lesssim C_Y \lesssim 12$ it is difficult to distinguish the γ_1 and β_2 $J = 2$ states [i.e., the states $(0, 1, 2_1)$ and $(1, 0, 2_2)$ in the notation of Equation (5.43)]. As the density of states increases, so does the likelihood of interactions. In Figure 5.22, the $(3\beta)_2$ level interacts with $(\gamma + 2\beta)_1$ and $(2\gamma)_2$ in its attempt to parallel the β_2 energy curve.

For $\gamma_0 = 15^\circ$ and 30° , energy trends and ℓ -decompositions were used to track several hundred levels through Stage I and Stage II calculations. Final states were then grouped according to the unperturbed bands from which they originated.¹ The situations at $(\beta_0, \gamma_0, C_Y) = (3, 15^\circ, 18)$ and $(3, 30^\circ, 24)$ are shown in Figures 5.23-5.26. The first two figures locate the $J = 0$ band heads while the latter two give the energies of band members relative to their corresponding heads. The following points

¹ Attempted crossings were treated as true crossings for the purposes of tracking levels. For example at $\gamma_0 = 15^\circ$, $C_Y = 24$ in the left panel of Figure 5.14, the state 0_4 is considered to have developed from $[N, \ell] = [3, 3]$. Strictly speaking 0_4 at $C_Y = 24$ develops continuously from 0_4 at $C_Y = 0$.

Figure 5.23. $\bar{H}_{QP}$ J = 0 energies at $C_\gamma = 18$ in Figure 5.14: Vibrational characters, energy differences and $\langle l \rangle$ are indicated for the eigenfunctions

Figure 5.24. $\bar{H}_{QP} J = 0$ energies at $C_\gamma = 24$ in Figure 5.16. Vibrational characters, energy differences and $\langle l \rangle$ are indicated for the eigenfunctions

Figure 5.25. Energies of traced $\bar{H}_{0p}$ states relative to the appropriate band-head energy [Figure 5.23]. Energies of the rigid quadrupole rotor are eigenvalues of H_R [Equations (5.13) and (5.21)] with $\hbar^2/B = 1$, $\beta_0 = 3$ and $\gamma_0 = 15^\circ$

$\beta_0 = 3$. DECOMPOSITION
 $C_\gamma = 24$. OF SPECTRUM
 $\gamma_0 = 30^\circ$ INTO BANDS

RIGID ROTOR	GROUND STATE	β	2β	3β	4β	γ	$\gamma+\beta$	$\gamma+2\beta$	2γ	$2\gamma+\beta$
3. ENERGY										
				-7						
			-7		7-			-7	-7	
		-7		7-6			-7			7-
7-6	-7		7-6	6-	5-7	-7		7-	7-	
6-		7-6	6-	5-67		7-6	7-6		6-	5-7
2. ENERGY	7-6	6-	5-67		4-5	6-	6-	5-7	5-7	
	6-	5-7		4-5		5-7	5-6		5-6	
5-6	5-6	4-5		6-4	6-4	4-5	4-5	4-5	4-5	-5
5-7	5-7	4-5	6-4		-3	4-	4-5		-4	
4-	4-	6-4	6-4	-3		-5	-4	-4	-4	-3
6-4	6-4	-3	4-2	4-2	4-2	6-	-3	6-	6-3	6-
1. ENERGY	6-	-3	4-2			-3	6-	4-2	4-2	4-2
	4-3	4-2		2-	2-	4-2	4-2		2-	2-
4-3	4-2	2-	2-			2-	2-	2-	2-	2-
2-2	2-									
0-	0-	0-	0-	0-	0-	0-	0-	0-	0-	0-

Figure 5.26. Energies of traced $\bar{H}_{qp}$ states relative to the appropriate band-head energy [Figure 5.24]. Energies of the rigid quadrupole rotor are eigenvalues of H_R [Equations (5.13) and (5.21)] with $\hbar^2/B = 1$, $\beta_0 = 3$ and $\gamma_c = 30^\circ$

Table 5.3. ℓ -decomposition of $J = 0$ states of $\bar{H}_{0p}$ for $(\beta_0, \gamma_0, C_\gamma) = (3, 15^\circ, 18)$. Within each rectangle the $[\% \ell = \ell']$ of Equation (5.59) are given for the state specified by the row and column labels

		ℓ'	$+\beta$	$+2\beta$	$+3\beta$	$+4\beta$	$+5\beta$	$+6\beta$
GS	0	64.8	65.2	63.1	50.1	55.0	52.8	48.4
	3	34.3	33.1	32.2	27.7	30.5	31.4	31.5
	6	.6	1.4	3.9	19.2	12.6	13.7	17.1
	9	.2	.2	.8	2.8	1.6	1.8	2.5
γ	0	20.3	31.9	24.8	24.6	26.7	28.6	
	3	17.4	24.5	23.7	23.7	23.2	22.3	
	6	55.9	33.9	37.0	34.9	32.3	31.4	
	9	6.4	9.4	14.0	15.9	16.7	16.4	
	12	.0	.3	.5	.7	1.0	1.1	
2γ	0	16.3	14.9	13.6	12.6			
	3	14.1	14.7	14.4	14.1			
	6	5.0	10.6	13.3	12.9			
	9	51.3	35.9	27.9	25.6			
	12	13.2	22.3	27.5	30.2			
	15	.1	1.5	3.2	4.5			
3γ	0	10.4	9.4					
	3	18.6	15.4					
	6	5.9	10.0					
	9	10.6	17.1					
	12	40.0	18.7					
	15	14.3	26.2					

Table 5.4. ℓ -decomposition of $J = 0$ states of $\bar{H}_{0p}$ for $(\beta_0, \gamma_0, c_\gamma) = (3, 30^\circ, 24)$. [See caption for Table 5.3.]

ℓ'		$+\beta$	$+2\beta$	$+3\beta$	$+4\beta$	$+5\beta$	$+6\beta$
GS	0	90.4	89.4	88.1	86.7	85.1	83.6
	6	9.5	10.5	11.6	12.9	14.2	15.5
	12	.1	.1	.3	.4	.6	.9
γ	3	86.7	83.6	80.6	77.6	57.3	
	9	13.2	16.2	18.8	21.5	38.6	
	15	.1	.3	.6	.9	4.1	
2γ	0	14.9	15.4	15.7	16.2		
	6	72.4	67.8	63.3	59.7		
	12	12.7	16.6	20.2	23.1		
	18	.1	.3	.7	1.0		
3γ	3	21.9	42.1				
	9	66.7	46.0				
	15	11.4	11.8				
	21	.0	.1				

may be made

- 1) For the two situations shown, the energy separation between adjacent β vibrations increases slightly with energy, while that of adjacent γ vibrations falls. [When the expansion basis is enlarged, the energies of the higher states drop slightly, but, in the absence of interference effects, these separation trends continue to hold]. For H_B^1 , β -vibrational band heads are equally spaced in energy; the same is true for γ vibrations. As β_0 is increased from zero in Stage 1 calculations, the relative energies of all excited states fall. For both the β and γ -vibrational $J = 0$ states, the separation between adjacent levels rises with increasing energy. For example at $\beta_0 = 2.4$, the relative energies of the first three β band heads are in the proportion 1:2.06:3.18, and for the γ vibrations we have 1:2.34:3.86. As β_0 tends to infinity these proportions approach 1:1:1 and 1:3:6 respectively. Only the γ -vibrational $J = 0$ energies are greatly affected by changing C_γ ; the separation between adjacent γ levels may rise or fall with increasing energy depending upon the values of β_0 and C_γ . For the parameter sets considered during the GRID calculations, the energy separation between adjacent β vibrations was found to increase with energy.
- 2) $\langle \ell \rangle$ has been given for each state in Figures 5.23 and 5.24. In the absence of crossing effects, $\langle \ell \rangle$ rises slightly as β -excitations are added, and rises greatly as γ -vibrations are added. Recall that in H_B^1 , β and γ -vibrational "phonons" are defined as carrying 0 and 3 units of ℓ respectively. In general, the ℓ -decomposition of a state is not greatly affected by the addition of a β -vibration. This may be seen in Tables 5.3 and 5.4 respectively for the $J = 0$ states shown in Figures 5.23 and 5.24.
- 3) The energy spectrum relative to the appropriate band head is similar for all bands. Furthermore, this common spectrum resembles that of an A-type quadrupole rotor. The latter is shown for $\gamma_0 = 15^\circ$ and 30° at the extreme left of Figures 5.25 and 5.26 respectively. Rotor energies have been taken from Reference (54) and are those appropriate to $\hbar^2/B = 1$, $\beta_0 = 3$. As β and γ excitations are added to the GS band,¹ the "rotor" spectrum spreads,

¹"Missing" energies in the excited bands of Figures 5.25 and 5.26 correspond to levels whose developments were not traced, usually because i in $(J_i \text{ of } H_{Qp})$ exceeded 25 for these states.

indicating that the effective moments of inertia are decreasing. As C_β is smaller than $2C_\gamma/\beta_0^2$, this effect is more pronounced for the deformation vibrations than for the asymmetry ones.

First order B(E2) rates for transitions between $\bar{H}_{QP}$ states were calculated for the $\gamma_0 = 15^\circ$ and 30° parameter sets. The results are presented in Figures 5.27-5.31 and Tables 5.5-5.6. Comparison with the H_B^1 decay scheme [Figures 3.3-3.4; Tables 3.1-3.2] leads to the following conclusions.

- 1) $\Delta K = 0$ transitions within the GS band [Figure 5.27] are enhanced over their H_B^1 counterparts; $\Delta K > 2$ transitions [Figures 5.28-5.29] are much smaller, particularly for $\gamma_0 = 15^\circ$. The validity of interpreting the label K as the BF z-component of J, and hence the validity of the symmetric rotor selection rule

$$\Delta K = 0, 2, \dots$$

is expected to increase as γ_0 approaches zero. This is observed. For $\gamma_0 = 30^\circ$, $(-1)^L$ is well-defined and first order E2 transitions between states of the same L-parity are forbidden. Also first order quadrupole moments are zero for all states.

- 2) B(E2) rates for transitions within a shape-vibrational band tend to mirror those of the GS band, with some enhancement. [In Tables 5.5-5.6, J_i and J_f are the GS band labels (as they appear in Figure 5.27). The transition rate between these levels appears in the "GS" column. The transition between corresponding levels belonging to the first β -vibrational band appears in the column labeled " β ", and so forth.] Anomalies in the tables may be traced to crossing effects. For example in the $\gamma_0 = 15^\circ$ case, the $(\gamma + \beta)$ - band head is in the process of crossing that of the 3β band at $C_\gamma = 18$. Consequently the B(E2) rate for the $2_1 \rightarrow 0_1$ transition within the $(\gamma + \beta)$ band is modified.
- 3) Transitions between bands [Figures 5.30-5.31] are hindered, particularly if the two states involved differ in their γ -vibrational character.

Figure 5.27. Selected first-order B(E2) transition rates for two instances of $\bar{H}_{QP}$ [$C_\beta = 1$, $C_{\beta\gamma} = 0$]. J_i denotes the i^{th} highest energy state of H_{QP} having spin J . Transitions shown above connect GS-band states belonging to the same K-sequence

Figure 5.28. First-order $B(E2)$ transition rates for $\bar{H}_{0p}$ transitions connecting GS-band states of different K -sequences. [Vertical position does not indicate the energy of the state J_i ; see Figure 5.27]

Figure 5.29. First-order $B(E2)$ transition rates for $\bar{H}_{0p}$ transitions connecting GS-band states of different K -sequences. [Vertical position does not indicate the energy of the state J_i ; see Figure 5.27]

Figure 5.30. First-order $B(E2)$ rates for $2 \rightarrow 0$ transitions between selected $\bar{H}Qp$ states. State labels are J_i (i^{th} lowest energy state with spin J) and vibrational band assignments are indicated. Each $J = 2$ level shown is the first spin 2 level ($n_\beta, m_\gamma, 2_1$) associated with the underlying band head ($n_\beta, m_\gamma, 0_1$). Transitions with non-zero values of $\Delta\beta \equiv \Delta n_\beta$ and/or $\Delta\gamma \equiv \Delta m_\gamma$ are inhibited

$\beta_0=3$
 $\gamma_0=30^\circ$
 $C_\gamma=24$

$B(E2: J_i \rightarrow J_f)$ rates for $2 \rightarrow 0$ transitions
 between states of low-lying bands of $\bar{H}_{QP}$
 (units of $[D_1/\bar{s}]^2$).

Figure 5.31. $B(E2: 2_i \rightarrow 0_f)$ for $\bar{H}_{QP}$ states. See caption of Figure 5.30

Table 5.5. First-order $B(E2)$ rates for corresponding intraband transitions, and quadrupole moments for corresponding $J = 2$ states. $(\beta_0, \gamma_0, C_\gamma) = (3, 15^\circ, 18)$. J_i and J_f labels for the GS band members are taken from Figure 5.27. Units for $B(E2)$'s and QM's are $[D_1/\xi]^2$ and $[16\pi/5]^{1/2}[D_1/\xi]$ respectively

J_i	J_f	band:	GS	β	2β	γ	$\gamma+\beta$	2γ
$2_1 \rightarrow 0_1$			2.05	2.19	2.29	2.48	1.59	2.61
$4_1 \rightarrow 2_1$			3.18	3.39	3.62	3.79	3.97	2.58
$3_1 \rightarrow 2_2$			4.17	4.51	4.87	4.86	4.72	5.32
$5_1 \rightarrow 3_1$			2.48	2.66	2.85	2.89	3.08	3.08
$5_1 \rightarrow 4_1$			.18	.14	.10	.34	.27	.14
$5_2 \rightarrow 3_1$			.18	.14	.11	.26	.20	.33
$5_2 \rightarrow 4_1$			.0005	.0004	.0003	.0003	.0002	.0001
$5_2 \rightarrow 4_4$			4.24	4.55	4.88	4.79	5.01	5.20
$7_1 \rightarrow 5_1$			3.75	4.00	4.25	4.25	4.48	3.94
$7_2 \rightarrow 5_2$			1.88	2.01	2.14	2.17	2.25	2.36
$7_2 \rightarrow 5_1$			.050	.038	.029	.074	.053	.095
<hr/>								
$Q(2_1)$			- .89	- .91	- .91	- .99	- .99	- .78
$Q(2_2)$			.93	.93	.91	1.01	.75	1.05

Table 5.6. First-order B(E2) rates for corresponding intraband transitions, and quadrupole moments for corresponding $J = 2$ states. $(\beta_0, \gamma_0, C_\gamma) = (3, 30^\circ, 24)$. [See caption for Table 5.5]

$J_i \rightarrow J_f$	band:	GS	β	2β	γ	$\gamma+\beta$	2γ
$2_1 \rightarrow 0_1$		2.15	2.20	2.25	2.68	2.80	2.91
$4_1 \rightarrow 2_1$		3.27	3.43	3.58	3.94	4.10	3.53
$3_1 \rightarrow 2_2$		4.25	4.52	4.82	5.00	5.00	5.60
$5_1 \rightarrow 3_1$		2.53	2.67	2.71	3.02	3.18	3.29
$5_1 \rightarrow 4_1$		0.	0.	0.	0.	0.	0.
$5_2 \rightarrow 3_1$		0.	0.	0.	0.	0.	0.
$5_2 \rightarrow 4_1$		.064	.030	.012	.044	.011	.061
$5_2 \rightarrow 4_3$		4.47	4.77	5.06	5.05	5.10	5.87
$7_1 \rightarrow 5_1$		3.78	3.99	4.14	4.36	4.56	4.29
$7_2 \rightarrow 5_2$		2.01	2.10	2.16	2.42	2.51	2.62
$7_2 \rightarrow 5_1$		0.	0.	0.	0.	0.	0.
$Q(2_1)$		0.	0.	0.	0.	0.	0.
$Q(2_2)$		0.	0.	0.	0.	0.	0.

E. Characteristics of the Ground State Band

We have seen that the energy spectrum of $\bar{H}_{QP}$ may be regarded as a collection of rotational bands each of which is based upon a $J = 0$ shape-vibrational state. To a first approximation, the entire spectrum may be constructed by placing the GS band atop each of the $J = 0$ energies. This approximation is exact when $\bar{H}_{QP} = H_B^1$; it is also accurate when $\bar{V}_{QP}$ possesses a sharp non-spherical minimum. In this section we examine further the effect upon the GS band of varying the potential parameters ($\beta_0, \gamma_0, C_\gamma$). $C_\beta = 1$ is assumed.

Energy information for GS band yrast states¹ (n_β, m_γ, J_1) = (0, 0, J_1) is presented in Figures 5.32-5.39 for spins 0, 2, 3, ..., 8. The energy of a given state, regarded as a function of two parameters, appears as a surface in these figures. The GRID data has been used with energy values at intermediate points obtained by fitting a bicubic spline² through the calculated results. The following points are evident.

Ground state energy. For $\bar{H}_{QP} = H_B^1$, the absolute energy of 0_1 [Figure 5.32] takes the value

$$\bar{E}(0_1) = 2.5$$

As β_0 increases, in effect widening the potential well radially, $\bar{E}(0_1)$ falls, and for $C_\gamma = 0$ approaches the value given by Equation (5.30a):

¹Here the term "yrast state" is used to denote the lowest energy state of $\bar{H}_{QP}$ possessing a given value of J . For $\bar{H}_{QP}$, yrast states belong to the GS band.

²The IMSL programs IBCICU and IDCEVU (47) were applied.

Absolute energy of the ground state of $\bar{H}_{QP}, O_1^+$

Figure 5.32. The eigenvalue $\bar{E}(0_1)$ of $\bar{H}_{QP}$ as a function of (β_0, c_γ) for three values of γ_0 . The height above the base plane is the value of $\bar{E}(0_1)$. The spike of height 8.0 sets the vertical scale. The numerical values of $\bar{E}(0_1)$ are labeled at the four corners of each surface

Calculated energy of the 2_1^+ eigenstate of $\bar{H}_{QP}$
(relative to the ground state)

Figure 5.33. The relative eigenvalue $[\bar{E}(2_1) - \bar{E}(0_1)]$ of $\bar{H}_{QP}$ as a function of (β_0, c_γ) for three values of γ_c .

Calculated energy of the 2_1^+ eigenstate of $\bar{H}_{QP}$
(relative to the ground state)

Figure 5.34. The relative eigenvalue $[\bar{E}(2_1) - \bar{E}(0_1)]$ of $\bar{H}_{QP}$ as a function of (γ_0, C_γ) for three values of β_0

Calculated energies of the 2_1^+ , 4_1^+ , and 6_1^+ states of $\bar{H}_{0P}$
(relative to the ground state) $C_Y=40$

Figure 5.35. $[\bar{E}(J_1) - \bar{E}(0_1)]$ as a function of (β_0, γ_0) for $J_1 = 2_1, 4_1, 6_1$, and $C_Y = 40$

Reduced energy of the 4_1^+ state of $\bar{H}_{QP}$

Figure 5.36. $[\bar{E}(4_1) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ as a function of (β_0, γ_0) for three values of C_γ . The rigid quadrupole rotor value of this ratio, which depends only upon γ_0 , appears in brackets for $\gamma_0 = 0^\circ, 15^\circ, 30^\circ$

Reduced energies of the 4_1^+ , 6_1^+ and 8_1^+ states of $\bar{H}_{QP}$
 $\gamma_0 = 15^\circ$

Figure 5.37. $[\bar{E}(J_i) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ as a function of (β_0, C_γ) for $J_i = 4_1, 6_1, 8_1$, and $\gamma_0 = 15^\circ$. The rigid quadrupole rotor ratio at $\gamma_0 = 15^\circ$ appears in brackets

Figure 5.38. $[\bar{E}(3_1) - \bar{E}(0_1)]$ (bottom row) and $[\bar{E}(3_1) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ (top row) as functions of (γ_0, c_γ) for three values of β_0

Reduced energies of the 3_1^+ , 5_1^+ and 7_1^+ eigenstates of $\bar{H}_{QP}$: $C_\gamma = 30$

Figure 5.39. $[\bar{E}(J_i) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ as a function of (β_0, γ_0) for $J_i = 3_1, 5_1, 7_1$, and $C_\gamma = 30$

$$\bar{E}(0_1) = \frac{1}{2} + \frac{1}{\beta_0^2} \quad [C_Y = 0; \text{large } \beta_0] \quad (5.60)$$

At $\beta_0 = 6$, the calculated absolute energy is .529, while Equation (5.60) yields .528. Narrowing the potential well in the γ direction by increasing C_Y from zero causes $\bar{E}(0_1)$ to rise, particularly for small γ_0 . Near $\gamma_0 = 30^\circ$, Equation (5.30b) is expected to become accurate as the intrinsic shape stabilizes: at $(\beta_0, \gamma_0, C_Y) = (5, 30^\circ, 50)$ Equations (5.30) together predict $\bar{E}(0_1) = 1.450$; diagonalization gives 1.448.

2_1 energy. Increasing β_0 raises the effective moments of inertia [Equation (5.21)] and rapidly lowers the relative energy of the rotational state 2_1 [Figure 5.33]. On the basis of Equation (5.38) we expect this energy to approach

$$\bar{e}(0, 0, 2_1) = \frac{2}{\beta_0^2} \quad [C_Y = 0; \text{large } \beta_0] \quad (5.61)$$

when $C_Y = 0$. At $\beta_0 = 6$, the relative energies obtained by diagonalization and by way of Equation (5.61) are .0576 and .0555 respectively.

Increasing C_Y then stabilizes the intrinsic shape. This evidently has the effect of further increasing the I_K and lowering the rotational energies; the rigid approximation becomes accurate. A rigid quadrupole rotor with $\hbar^2/B = 1$ and $\beta_0 = 6$ has relative 2_1 energies of .028, .032 and .042 for $\gamma_0 = 0^\circ, 15^\circ$ and 30° respectively. Diagonalization of $\bar{H}_{QP}$ for $(\beta_0, C_Y) = (6, 40)$ in the GRID expansion basis yields .029, .032 and .045. Further increasing C_Y has little effect. The contribution of the $C_Y(\gamma - \gamma_0)^2$ term to the 2_1 relative energy may be seen explicitly in Figure 5.34.

Even-spin yrast states. As shown in Figure 5.35, the 4_1 and 6_1 relative energies behave similarly to that of 2_1 under changes of the potential parameters. Although the relative energies fall as β_0 and C_Y increase, the reduced energies rise [Figures 5.36, 5.37] approaching the rigid values. The rigid rotor reduced energies which appear in the figures are independent of β_0 .

Odd-spin yrast states. Belonging to a $K = 2$ rotor sequence, these states exhibit a different dependence upon (β_0, γ_0, C_Y) than do the even-spin yrast levels. In particular the rigid rotor reduced energies are infinite at $\gamma_0 = 0^\circ$, and $\bar{H}_{QP}$ reduced energies of $J_i = 3_1, 5_1, 7_1, \dots$ similarly become large as a spheroidal minimum develops. As before, increasing β_0 lowers the relative energies but raises the reduced ones. This effect is shown for the 3_1 state in Figure 5.38. Reduced energy surfaces for odd-spin yrast states are seen in Figure 5.39 to have a similar appearance. For $\gamma_0 = 30^\circ$, rigid rotor reduced energies are 3.00, 6.00 and 9.67 for the $3_1, 5_1$ and 7_1 states respectively. $\bar{H}_{QP}$ at $(\beta_0, \gamma_0, C_Y) = (5, 30^\circ, 30)$ has 3.1, 5.9 and 9.1 for the corresponding reduced eigenvalues. However the $\bar{H}_{QP}$ reduced energies of $K = 2$ states can rise significantly above their rigid rotor counterparts for intermediate values of the asymmetry parameter. For example at $\gamma_0 = 15^\circ$, reduced energies of $(3_1, 5_1, 7_1)$ are (7.85, 10.85, 15.15) and (11.1, 14.0, 18.0) for $\bar{H}_R$ and $\bar{H}_{QP}$ $[(\beta_0, \gamma_0, C_Y) = (5, 15^\circ, 30)]$ respectively. This effect is also indicated in Figure 5.5 where 3_1 crosses 6_1 near $\gamma_0 = 17^\circ$ for $\bar{H}_R$ and near 20° for $\bar{H}_{QP}$.

It is interesting to note that even when $\beta_0 = 0$ in $\bar{H}_{QP}$, the expectation value of β is non-zero, and increasing C_γ effects the development of rotational bands. This phenomenon is demonstrated by Figure 5.40 in which the splittings of the $N \leq 4$ H_B^1 energies are shown. For fixed C_γ , the degree of splitting increases as γ_0 decreases. This is expected on the basis of Figure 5.1. Notice that as C_γ increases, the γ -vibrational band head, which develops from $[N, \ell] = [3, 3]$, rises rapidly above other members of its ℓ -multiplet. This also occurs for non-zero values of β_0 .

Trends in the $\bar{H}_{QP}$ energy spectrum are further illustrated in Figures 5.41-5.46. The behaviors of selected eigenvalues under parameter variations are shown, with the lowest β and γ -vibrational energies appearing as dashed curves. The figures have been constructed on the basis of the GRID calculations and may be briefly summarized as follows.

Variations of β_0 . Increasing β_0 with (γ_0, C_γ) fixed increases the effective moments of inertia, thus lowering GS band relative energies. Beyond $\beta_0 = 3$, the energies of the β -vibrational band heads are not greatly effected; however, γ -vibrational relative energies drop rapidly with increasing β_0 . [Recall the $1/\beta_0$ dependence of $\bar{E}_\gamma$ in Equation (5.30b).] The decline in the relative energy of 2_1 [$\sim 1/\beta_0^2$] causes the reduced energies of all shape-vibrational states to rise rapidly. For large β_0 further increases of the parameter have little effect upon the reduced spectrum of the GS band.

Variations of C_γ . Increasing C_γ with (β_0, γ_0) fixed lowers the relative energies of GS band $K = 0$ states; other GS band members generally have their relative energies raised for $\gamma_0 \lesssim 20^\circ$. $\bar{e}(1, 0, 0_1)$ is quite

Figure 5.40. Removal of H_B degeneracy by increasing C_γ from zero in $\bar{H}_{Qp}$. The l and J quantum numbers at left apply to each panel at $C_\gamma = 0$. Each curve represents $[E(J_i) - E(0_i)]$ for fixed J and i . The value of J is indicated for each curve. Notice the rise of the γ -vibrational band head originating from $(l, J) = (3, 0)$

Figure 5.41. $[\bar{E}(J_i) - \bar{E}(0_1)]$ as a function of γ_0 for selected $\bar{H}_{0p}$ states [$J_i = 0_1, 2_1 - 2_4, 3_1, 4_1 - 4_4, 5_1, 6_1, 8_1$; energies of the β and γ vibrational band heads (0_β and 0_γ of Equation (6.13)) appear as dashed curves]. Note how the increase of β_0 compresses the GS-band energies

Figure 5.42. $[\bar{E}(J_i) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ as a function of γ_c for selected $\bar{H}_{0p}$ states [$J_i = 0_1, 2_1, \dots, 8_1, 10_1; 0_\beta, 0_\gamma$]. Increasing β_0 raises the reduced energies

Figure 5.43. Relative and reduced energies as functions of β_0 for selected $\bar{H}_{Qp}$ states [$J_i = 0_1, 2_1-2_3, 3_1, 4_1-4_3, 5_1-5_2, 6_1, 8_1; 0_\beta, 0_\gamma$]

Figure 5.44. $[\bar{E}(J_i) - \bar{E}(0_1)]$ as a function of γ_0 for selected $\bar{H}_{0p}$ states [$J_i = 0_1, 2_1-2_4, 3_1, 4_1-4_4, 5_1, 6_1, 8_1; 0_\beta, 0_\gamma$]. The dependence upon γ_0 of GS-band $K = 2$ energies sharpens as C_γ is increased. The relative energy of 0_β is seen to be quite insensitive to changes in γ_0 and C_γ .

Figure 5.45. Reduced-energy version of Figure 5.44. $[\bar{E}(J_i) - \bar{E}(0_1)] / [\bar{E}(2_1) - \bar{E}(0_1)]$ is shown as a function of γ_0 for $J_i = 0_1, 2_1, 3_1, \dots, 8_1, 10_1$, and for the β and γ -vibrational band heads

Figure 5.46. Relative and reduced energies as functions of C_γ for selected states of $\bar{H}_{QP}$ [$J_i = 0_1, 2_1-2_4, 3_1, 4_1-4_3, 5_1, 6_1, 8_1; 0_\beta$ and 0_γ].

insensitive to the term $C_Y(\gamma - \gamma_0)^2$. $\bar{e}(0, 1, 0_1)$ rises as either C_Y is increased or γ_0 is decreased. Reduced energies of all states above 2_1 generally rise as C_Y is increased; those of the GS band approach rigid rotor values when β_0 is also large.

For intermediate values of β_0 and C_Y , the GS band spectrum may differ significantly from that of an A-type rigid rotor. In such cases centripetal stretching does not act simply to increase the effective value of β_0 . This may be seen in Table 5.7. For four GS band members [$n_\beta = m_Y = 0$; $J_i = 2_1, 4_1, 2_2, 3_1$] and for several values of (β_0, γ_0) , the quantity

$$\beta_R(J_i) \equiv \text{value of deformation for which } H_R \text{ [with } \hbar^2/B = 1] \text{ has the same relative eigenvalue as } \bar{H}_{QP} \text{ for the state } J_i \quad (5.62)$$

has been computed. C_Y was fixed at 40, and the value of γ_0 used in H_R was that appearing in $\bar{V}_{QP}$. As enlarging the expansion basis changes $\bar{H}_{QP}$, calculated eigenvalues and hence alters β_R , 20 and 25-phonon diagonalizations are compared in the table. $K = 0$ rotations of an axially-symmetric prolate nucleus can be expected to enlarge the mean deformation: for the 2_1 and 4_1 states [$K = 0$] at $\gamma_0 = 0^\circ$ we find

$$\beta_R > \beta_0 \quad ; \quad \beta_R \xrightarrow[\beta_0 \rightarrow \infty]{} \beta_0$$

For asymmetric shapes however, β_R may be larger or smaller than β_0 , and the different categories of rotation [$K = 0$, $K = 2$] evidently lead to different stretching effects. Of course small changes in $\langle \gamma \rangle$ can dramatically effect $K \neq 0$ rotor energies. Thus the calculation of $\langle \beta \rangle$

Table 5.7. Calculated value of $\beta_R(J_i)$ [Equation 5.62] for four H_{0p} states belonging to the GS band. $C_Y=40$ in all cases.

γ_0	J_i^a	$N_{\max}$	$\beta_0=0$		$\beta_0=3$		$\beta_0=6$	
			20	25	20	25	20	25
0°	2_1		1.88	1.88	3.41	3.42	5.87	6.01
	4_1		1.99	1.99	3.46	3.47	5.94	6.02
	2_2		∞	∞	∞	∞	∞	∞
	3_1		∞	∞	∞	∞	∞	∞
10°	2_1		1.63	1.63	3.18	3.18	5.83	5.92
	4_1		1.79	1.79	3.25	3.26	5.89	5.93
	2_2		2.38	2.38	3.40	3.40	5.09	5.10
	3_1		2.36	2.36	3.41	3.41	5.13	5.14
20°	2_1		1.42	1.42	3.03	3.03	5.85	5.87
	4_1		1.63	1.63	3.11	3.11	5.85	5.86
	2_2		1.50	1.50	2.66	2.66	5.21	5.22
	3_1		1.55	1.55	2.76	2.76	5.33	5.34
30°	2_1		1.32	1.32	2.92	2.92	5.77	5.78
	4_1		1.52	1.52	3.06	3.06	5.84	5.84
	2_2		1.82	1.82	2.86	2.86	5.68	5.69
	3_1		1.43	1.43	2.93	2.93	5.70	5.72

^aFull state labels are $(n_\beta, m_Y, J_i) = (0, 0, J_i)$.

and $\langle \gamma \rangle$ for $\bar{H}_{QP}$ eigenstates would be helpful in clarifying the stretching phenomenon.

The GRID calculations indicate that the A-type rotor sum rules hold for $\bar{H}_{QP}$ GS-band states in the limit of large β_O and C_Y . For example the first sum rule in Equations (5.20) may be written as

$$r = 1 \quad (5.63a)$$

$$r \equiv \frac{\bar{e}(0, 0, 2_1) + \bar{e}(0, 0, 2_2)}{\bar{e}(0, 0, 3_1)} \quad (5.63b)$$

Equation (5.63a) holds for H_B^1 . Over the course of Stage I calculations r decreases, approaching .77 from above as β_O tends to infinity. As $C_Y(\gamma - \gamma_O)^2$ is added to the Hamiltonian, r rises and may exceed unity for intermediate values of C_Y [at $(\beta_O, \gamma_O, C_Y) = (3, 30^\circ, 40)$, $r = 1.03$].

$B(E2)$ values for representative transitions between eigenstates of $\bar{H}_{QP}$ are presented in Tables 5.8-5.11 for twenty-seven sets of the parameters (β_O, γ_O, C_Y) . The GRID data set has been employed in the construction of these tables. Calculated values are consequently not always converged to the three decimal places listed; however, they will be sufficient for our purposes. The thirteen tabulated transitions are schematically indicated in Figure 5.47. Those connecting GS-band members may be classified according to their dependency upon γ_O for large (β_O, C_Y) .

- 1) Type I transitions have values of $B(E2:J_+ \rightarrow J_-)$ which are on the order of one [in units of $B(E2:2_1 \rightarrow 0_1)$] for all γ_O on $[0^\circ, 30^\circ]$. These transitions have strong counterparts in H_B , and obey the selection rules

TABULATED TRANSITION RATES

Figure 5.47. Transitions for which $B(E2; J_i \rightarrow J_f)$ is tabulated as a function of $(\beta_0, \gamma_0, C_\gamma)$ [Tables 5.8-5.11]

$$\Delta K = 0 \quad , \quad (5.64a)$$

$$\Delta l = \pm 1 \quad [H_B \text{ seed states}] \quad (5.64b)$$

In addition to the six GS-band transitions indicated in Figure 5.47, $(4_2 \rightarrow 2_2)$ and $(5_1 \rightarrow 4_2)$ are also of type I.

- 2) Type II transitions are characterized by a strong dependence upon γ_0 . One or the other of Equations (5.64) is not satisfied, and $B(E2)$ ranges from ~ 1 at one extreme of γ_0 to ~ 0 at the other. Recall that at $\gamma_0 = 30^\circ$ the first order transition is forbidden unless the l -parity changes sign:

$$\Delta[(-1)^l] = \pm 2 \quad (\gamma_0 = 30^\circ) \quad (5.65)$$

Near $\gamma_0 = 0^\circ$ only transitions obeying Equation (5.64a) are found to be appreciable. $(4_2 \rightarrow 4_1)$ and $(4_2 \rightarrow 3_1)$ are of type II. The first of these, like $(4_1 \rightarrow 3_1)$ and $(2_2 \rightarrow 2_1)$ in Figure 5.47, violates only Equation (5.64a) and is large only near $\gamma_0 = 30^\circ$. $(4_2 \rightarrow 3_1)$ exhibits the opposite behavior.

- 3) Type III transitions violate each of Equations (5.64). $(3_1 \rightarrow 2_1)$, $(2_2 \rightarrow 0_1)$, $(4_1 \rightarrow 2_2)$, $(4_2 \rightarrow 2_1)$, and $(6_1 \rightarrow 4_2)$ of the GS band are all of this type. Their $B(E2)$ values are ~ 0 near the γ_0 extremes and achieve only moderate values elsewhere.

The effect of violating either of Equations (5.64) may also be gauged by reconsulting Figures 5.27-5.29.

The dependence upon γ_0 may be explicitly seen in Figures 5.48 and 5.49 for several of the tabulated transitions. For fixed $(\beta_0, C_\gamma \gg 1)$, the 2_2 member of the GS band $[(0, 0, 2_2)]$ will rise in energy above the β -vibrational state $(1, 0, 2_1)$ as γ_0 is decreased from 30° . [For example, see Figure 5.41.] Interference effects in the vicinity of the attempted crossing alter each of the two states and consequently affect transitions to them. This leads, for example, to the kinks observable in the $(2_2 \rightarrow 0_1)$.

Rates for E2 transitions within the ground state band
(first order)

Figure 5.48. $B(E2)$ values and ratios for selected transitions connecting GS-band eigenstates of H_{QP} . Full state labels are $(n_\beta=0, m_\gamma=0, J_i)$

First order B(E2) ratios for transitions
within the ground state band

Figure 5.49. B(E2) ratios for selected $\bar{H}_{0p}$ GS-band transitions [Type II ($2_2 \rightarrow 2_1$, $4_1 \rightarrow 3_1$) and Type III ($2_2 \rightarrow 0_1$, $3_1 \rightarrow 2_1$)]

Table 5.8. $B(E2:J_i \rightarrow J_f)$ for GS-band H_{qp} transitions in units of $[D_1/\bar{s}]^2$

J_i	J_f	β_0	C_Y γ_0	0	20	20	20	20	40	40	40	40
			γ_0	0°	0°	10°	20°	30°	0°	10°	20°	30°
$2_1 \rightarrow 0_1$	0			0.500	0.749	0.621	0.527	0.518	0.941	0.744	0.583	0.561
	2			1.148	1.591	1.381	1.203	1.227	1.837	1.527	1.288	1.359
	4			3.308	3.677	3.404	3.164	3.447	3.921	3.529	3.257	3.576
$4_1 \rightarrow 2_1$	0			1.000	1.271	1.136	1.048	1.030	1.492	1.251	1.095	1.093
	2			1.973	2.451	2.203	2.037	2.067	2.761	2.363	2.120	2.205
	4			4.902	5.368	5.023	4.815	5.003	5.697	5.175	4.939	5.133
$6_1 \rightarrow 4_1$	0			1.500	1.699	1.589	1.546	1.577	1.891	1.671	1.584	1.674
	2			2.693	3.000	2.793	2.738	2.892	3.284	2.914	2.810	3.068
	4			5.977	6.128	5.824	5.865	6.384	6.453	5.947	6.001	6.578
$4_1 \rightarrow 3_1$	0			0.333	0.072	0.126	0.277	0.483	0.042	0.081	0.244	0.594
	2			0.598	0.082	0.154	0.432	0.997	0.051	0.104	0.402	1.197
	4			1.328	0.104	0.212	0.830	2.533	0.068	0.156	0.860	2.785
$3_1 \rightarrow 2_1$	0			0.000	0.089	0.099	0.079	0.000	0.073	0.094	0.105	0.000
	2			0.000	0.141	0.181	0.204	0.000	0.107	0.157	0.227	0.000
	4			0.000	0.227	0.348	0.535	0.000	0.168	0.293	0.538	0.000
$5_1 \rightarrow 3_1$	0			1.050	1.204	1.098	1.050	1.058	1.436	1.218	1.076	1.074
	2			1.766	2.064	1.868	1.756	1.786	2.385	2.046	1.803	1.826
	4			3.592	3.957	3.664	3.476	3.639	4.316	3.865	3.527	3.706
$7_1 \rightarrow 5_1$	0			1.714	1.914	1.791	1.730	1.725	2.181	1.919	1.762	1.749
	2			2.747	3.101	2.878	2.760	2.774	3.487	3.069	2.807	2.823
	4			5.218	5.664	5.315	5.136	5.269	6.130	5.546	5.188	5.346

Table 5.9. $B(E2:J_i \rightarrow J_f)/B(E2:2_1 \rightarrow 0_1)$ for GS-band, H_{qp} transitions. See caption of Table 5.11 for an explanation of values in () and "a"

$J_i \rightarrow J_f$	β_0	$C_Y: 0$	20	20	20	20	40	40	40	40
		$\gamma_0: 0^\circ$	0°	10°	20°	30°	0°	10°	20°	30°
$4_1 \rightarrow 2_1$	0	2.000	1.698	1.830	1.988	1.990	1.585	1.681	1.877	1.949
	2	1.718	1.540	1.595	1.694	1.685	1.503	1.547	1.647	1.623
	4	1.482	1.460	1.476	1.522	1.451	1.453 (1.43)	1.466 (1.44)	1.516 (1.52)	1.435 (1.38)
$6_1 \rightarrow 4_1$	0	3.000	2.269	2.559	2.934	3.045	2.008	2.247	2.716	2.985
	2	2.345	1.885	2.023	2.277	2.357	1.788	1.908	2.182	2.258
	4	1.807	1.667	1.711	1.854	1.852	1.646 (1.57)	1.685 (1.59)	1.843 (1.74)	1.839 (1.73)
$4_1 \rightarrow 3_1$	0	0.667	0.096	0.202	0.526	0.932	0.045	0.109	0.419	1.058
	2	0.521	0.052	0.111	0.359	0.813	0.028	0.068	0.312	0.881
	4	0.401	0.028	0.062	0.262	0.735	0.017 (0.0)	0.044 (0.005)	0.264 (0.338)	0.779 (0.78)
$3_1 \rightarrow 2_1$	0	0.000	0.119	0.160	0.149	0.000	0.077	0.126	0.180	0.000
	2	0.000	0.088	0.131	0.169	0.000	0.058	0.103	0.176	0.000
	4	0.000	0.062	0.102	0.169	0.000	0.043 (0.0)	0.083 (0.014)	0.165 (0.13)	0.000 (0.0)
$5_1 \rightarrow 3_1$	0	2.100	1.607	1.768	1.992	2.042	1.525	1.637	1.845	1.916
	2	1.538	1.297	1.353	1.460	1.456	1.298	1.340	1.400	1.344
	4	1.086	1.076	1.076	1.098	1.056	1.101 (0.955 ^a)	1.095 (0.955)	1.083 (0.955)	1.036 (0.955)
$7_1 \rightarrow 5_1$	0	3.429	2.556	2.886	3.284	3.332	2.317	2.580	3.020	3.119
	2	2.392	1.949	2.084	2.295	2.261	1.898	2.010	2.180	2.077
	4	1.577	1.540	1.561	1.623	1.529	1.563 (1.319 ^a)	1.571 (1.321)	1.593 (1.346)	1.495 (1.310)

Table 5.10. $B(E2:J_i \rightarrow J_f)$ for H_{QP} transitions in units of $[D_1/\bar{\epsilon}]^2$. [$\bar{\epsilon}$ specifies the $H_{QP} \rightarrow \bar{H}_{QP}$ transformation.] Values marked by * are influenced by the energy crossing of GS $2_2 = (0, 0, 2_2)$ with other $J = 2$ states

		$C_Y: 0$		20	20	20	20	40	40	40	40
		$\gamma_O: 0^\circ$		0°	10°	20°	30°	0°	10°	20°	30°
$J_i \rightarrow J_f$	β_O										
GS GS $2_2 \rightarrow 0_1$	0	0.000	0.046	0.050*	0.032	0.000	0.039*	0.048	0.044	0.000	
	2	0.000	0.077	0.109*	0.099	0.000	0.059*	0.086	0.114	0.000	
	4	0.000	0.128	0.189	0.295	0.000	0.093	0.154*	0.297	0.000	
β GS $2_1 \rightarrow 0_1$	0	0.000	0.009	0.000*	0.002	0.000	0.021	0.010	0.005	0.000	
	2	0.006	0.037	0.015*	0.018	0.007	0.045	0.034	0.023	0.011	
	4	0.051	0.069	0.071	0.059	0.050	0.071	0.077*	0.059	0.056	
GS GS $2_2 \rightarrow 2_1$	0	1.000	0.114	0.134*	0.502	1.025	0.074*	0.121	0.351	1.090	
	2	1.973	0.149	0.202*	0.647	2.059	0.102*	0.175	0.520	2.214	
	4	4.902	0.215	0.394	1.128	5.035	0.149	0.316*	1.099	5.213	
$\bar{E}$ GS $2_1 \rightarrow 2_1$	0	0.000	0.083	0.139*	0.017	0.000	0.078	0.079	0.034	0.000	
	2	0.000	0.111	0.155*	0.066	0.000	0.106	0.109	0.080	0.000	
	4	0.000	0.133	0.123	0.108	0.000	0.129	0.112*	0.106	0.000	
GS GS $3_1 \rightarrow 2_2$	0	1.071	1.945	1.459*	1.457	1.440	2.486*	2.008	1.685	1.618	
	2	1.923	3.586	2.962*	2.740	2.769	4.278*	3.563	2.991	3.021	
	4	4.269	7.184	6.535	5.929	6.352	7.933	7.036*	6.217	6.623	
GS β $3_1 \rightarrow 2_1$	0	0.000	0.041	0.232*	0.001	0.000	0.029	0.056	0.005	0.000	
	2	0.000	0.032	0.185*	0.013	0.000	0.026	0.054	0.045	0.000	
	4	0.000	0.018	0.009	0.037	0.000	0.017	0.003*	0.047	0.000	

Table 5.11. $B(E2:J_i \rightarrow J_f)/B(E2:2_1 \rightarrow 0_1)$ for H_{QP} transitions. Values in () are rigid rotor ratios (9, 51, 55). Values in < > are those of the Davydov-Chaban (DC) model (55) with $1/\mu = 4$ [which corresponds to $\beta_0 = 4$ in H_{QP}]. Rotor and DC ratios are evaluated at the appropriate value of γ_0 , with the exception of entries marked "a" which correspond to $\gamma_0 = 3^\circ$

			$C_Y: 0$	20	20	20	20	40	40	40	40
J_i	J_f	β_0	$\gamma_0: 0^\circ$	0°	10°	20°	30°	0°	10°	20°	30°
GS	GS	0	0.000	0.062	0.081	0.061	0.000	0.041	0.065	0.075	0.000
$2_2 \rightarrow 0_1$		2	0.000	0.049	0.079	0.082	0.000	0.032	0.056	0.089	0.000
		4	0.000	0.035	0.056	0.093	0.000	0.024	0.044	0.091	0.000
								(0.0	.029	.072	0.0)
β	GS	0	0.000	0.012	0.000	0.003	0.000	0.023	0.014	0.008	0.000
$2_1 \rightarrow 0_1$		2	0.005	0.023	0.011	0.015	0.005	0.024	0.022	0.018	0.008
		4	0.015	0.019	0.021	0.019	0.015	0.018	0.022	0.018	0.016
								< .024 a	.023	.022	.021 >
GS	GS	0	2.000	0.153	0.215	0.953	1.980	0.078	0.162	0.602	1.943
$2_2 \rightarrow 2_1$		2	1.718	0.094	0.146	0.538	1.678	0.055	0.115	0.404	1.629
		4	1.482	0.058	0.116	0.357	1.461	0.038	0.090	0.338	1.458
								(0.0	.052	.383	1.43)
β	GS	0	0.000	0.111	0.224	0.032	0.000	0.083	0.107	0.058	0.000
$2_1 \rightarrow 2_1$		2	0.000	0.070	0.112	0.055	0.000	0.058	0.071	0.062	0.000
		4	0.000	0.036	0.036	0.034	0.000	0.033	0.032	0.033	0.000
								< .043 a	.043	.035	0.0 >
GS	GS	0	2.143	2.598	2.351	2.785	2.782	2.640	2.700	2.889	2.885
$3_1 \rightarrow 2_2$		2	1.675	2.253	2.145	2.278	2.257	2.329	2.333	2.323	2.223
		4	1.290	1.954	1.920	1.874	1.843	2.023	1.994	1.909	1.852
								(1.786	1.821	1.790	1.786)
GS	β	0	0.000	0.055	0.374	0.003	0.000	0.030	0.075	0.009	0.000
$3_1 \rightarrow 2_1$		2	0.000	0.020	0.134	0.011	0.000	0.014	0.035	0.035	0.000
		4	0.000	0.005	0.003	0.012	0.000	0.004	0.001	0.015	0.000
								< .003 a	.010	.009	0.0 >

and $(2_2 \rightarrow 2_1)$ curves of Figure 5.49.¹ Tabulated values of transition rates which are strongly influenced by crossing phenomena have been marked by asterisks.

With C_Y fixed at zero, increasing β_0 results in an increase in the $B(E2)$ value of any transition obeying Equation (5.64b). The increase is particularly marked for $(2_1 \rightarrow 0_1)$ and results in ratios $B(E2:J_i \rightarrow J_f) / B(E2:2_1 \rightarrow 0_1)$ which fall as β_0 rises. When both J_i and J_f belong to the GS band, this ratio approaches the rigid rotor value as β_0 and C_Y increase. $B(E2)$ ratios for the rigid quadrupole rotor (9, 51, 55) are independent of β_0 and appear within parentheses in Tables 5.9 and 5.11.

Three transitions connecting the GS band with the 2_1 β -vibrational state have also been tabulated: $[2_1(\beta) \rightarrow 0_1(\text{GS})]$, $[2_1(\beta) \rightarrow 2_1(\text{GS})]$, and $[3_1(\text{GS}) \rightarrow 2_1(\beta)]$. These have no counterpart in the rigid rotor model and are [to first order] forbidden when $H_{QP} = H_B$. For other values of (β_0, γ_0, C_Y) , $B(E2)$ values for the three transitions may be seen to be relatively small. Only the $[2_1(\beta) \rightarrow 0_1(\text{GS})]$ transition satisfies Equation (5.65) and is allowed at $\gamma_0 = 30^\circ$. As might be expected, its $B(E2)$ value is fairly independent of γ_0 for large (β_0, C_Y) . The same is true of $[2_1(\beta) \rightarrow 2_1(\text{GS})]$ if γ_0 is not near 30° .

There are many other topics deserving of pursuit which could rightfully be included in this chapter. As already mentioned, calculations

¹ In Figures 5.48 and 5.49 the full state labels are $(0, 0, J_i)$. (n_β, m_Y) are also deleted in Tables 5.8-5.11. There the symbols "GS" and " β " are used to denote the bands involved.

of the expectation values $\langle\beta\rangle$, $\langle\gamma\rangle$, $\langle(\beta - \langle\beta\rangle)^2\rangle$ and $\langle(\gamma - \langle\gamma\rangle)^2\rangle$ would be useful in detailing the manner in which rotational energies approach the rigid spectrum. K-decompositions of the (n_β, m_γ, J_i) as functions of $(\beta_0, \gamma_0, C_\gamma)$ could indicate the relationship between the label K employed within this chapter and the rotational quantum number of the same name. The effect of the parameter $C_{\beta\gamma}$, particularly upon $J = 0$ energies, remains to be investigated. A thorough comparison of $\bar{H}_{QP}$ model properties with those of the Davydov-Chaban (10), Davydov (14) and rotor-vibrator (11) models would be an ambitious undertaking, yet necessary to a truly complete discussion of H_{QP} . A first step in the study of double-minima potentials could be taken by simply allowing C_γ in $\bar{H}_{QP}$ to be negative. The potential symmetries [Equation (5.1)] then force simultaneous prolate and oblate minima at $\gamma = 0^\circ$ and 60° respectively if $\gamma_0 \neq 0^\circ, 60^\circ$.

The time has come, however, to make some contact with reality. In the present chapter we have achieved a sufficient overview of H_{QP} properties to permit the intelligent application of the quadratic potential model. This new phase begins in the final chapter.

VI. QUADRATIC POTENTIAL MODEL: APPLICATIONS

In a given application of the quadratic potential model, the three parameters of $\bar{H}_{QP}$ [$C_\beta = 1$, $C_{\beta\gamma} = 0$] may be determined by optimizing the agreement between model and experimental reduced energies. This may be accomplished by coupling the diagonalization procedure to a suitable fitting routine. In the present work, the optimal set $(\beta_o, \gamma_o, C_\gamma)$ is defined as that for which

$$\chi^2 = \frac{1}{n} \sum_{q=1}^n \frac{[e_q - \hbar\bar{\omega} \bar{e}_q]^2}{e_q^2} \quad (6.1)$$

is a minimum. Here q distinguishes the n experimental excited states which contribute to the fitting process, and the definitions

$$\begin{aligned} e_q &\equiv \text{exp. energy of state } q \text{ relative to the GS,} \\ \bar{e}_q &\equiv \bar{E}_q - \bar{E}_{GS} = \text{relative } \bar{H}_{QP} \text{ eigenvalue of the corresponding} \\ &\quad \text{model state,} \end{aligned}$$

are assumed. $\hbar\bar{\omega}$ is an overall energy scale factor for the model spectrum.

For a given set $(\beta_o, \gamma_o, C_\gamma)$, $\hbar\bar{\omega}$ is determined by the requirement

$$\frac{\partial[\chi^2]}{\partial[\hbar\bar{\omega}]} = 0 \quad (6.2)$$

to be

$$\hbar\bar{\omega} = \frac{\sum_q [e_q \bar{e}_q / e_q^2]}{\sum_q [\bar{e}_q^2 / e_q^2]} \quad (6.3)$$

Hence χ^2 is regarded as a function of $(\beta_o, \gamma_o, c_\gamma)$ only, and the fitting process reduces to a search for its absolute minimum. The search is performed by the computer code STEPIT (56), and terminates when variations of the three parameters become sufficiently small between successive evaluations of χ^2 . The fitting process is described schematically by Figure 6.1a.

Locating the χ^2 minimum to within .1% in each of the three parameters can require the computation of as many as 150 model spectra. This can be quite costly if diagonalization is used to calculate model energies. For this reason an alternative method of obtaining $\bar{H}_{QP}$ eigenvalues was developed. Approximate relative energies are calculated by interpolating between model eigenvalues gathered during the GRID computations of Chapter V. The method is illustrated by Figure 6.1b. There the calculation of $\bar{e}(J_i)$ is described for the case $(\beta_o, \gamma_o, c_\gamma) = (.5, 1^\circ, 7) = p$. In the situation shown, p is located near a corner of the GRID lattice. In general as many as four planes, S_i , and sixteen points in each plane may contribute to the evaluation of $\bar{e}(J_i)$ at p . The IMSL codes IBCICU and ICSICU (47) were used in the calculation of the bicubic and cubic spline functions which replaced portions of the GRID data. The entire fitting procedure, incorporating the interpolation process, requires ~45 seconds of IBM 370/158 computing time in a typical application [150 evaluations of χ^2 ; $n = 20$]. The search for the optimal set $(\beta_o, \gamma_o, c_\gamma)$ is always preceded by the evaluation of χ^2 at each of the 728 GRID lattice points. The resulting map proves invaluable in locating valleys and relative minima in the χ^2 hypersurface.

(b) ENERGY INTERPOLATION METHOD: AN EXAMPLE

To find $\bar{e}(J_i)$ at the point
 $p = (\beta_0, \gamma_0, C_\gamma) = (.5, 2^\circ, 7)$:

- (1) It is assumed that the value of $\bar{e}(J_i)$ is known for the $(\beta_0, \gamma_0, C_\gamma)$ parameter sets associated with each lattice point shown.
 [Provided by the GRID calculations.]
- (2) Within each plane, S_k , a bicubic spline function, $BCS_k(\beta_0, \gamma_0)$, is determined. Its values at lattice points in the plane are the appropriate $\bar{e}(J_i)$ of step (1).
- (3) The approximate value of $\bar{e}(J_i)$ at point A_k is found by evaluating BCS_k at $(\beta_0, \gamma_0) = (.5, 2^\circ)$.
- (4) A cubic spline function, $CS(C_\gamma)$, is constructed to represent $\bar{e}(J_i)$ for parameter sets on the dashed line. Its values at the A_k are those found in step (3).
- (5) $CS(C_\gamma)$ evaluated at point p [i.e., at $C_\gamma = 7$] is taken to be $\bar{e}(J_i)$ at p .

Figure 6.1. Energy fitting procedure (a) and theoretical energy interpolation method (b)

Furthermore, starting values of $(\beta_o, \gamma_o, C_\gamma)$ for the parameter search can be wisely chosen on the basis of this information.

Extrapolation outside of the GRID lattice [Figure 5.3] was not attempted. Within the lattice, test calculations indicated that interpolated eigenvalues usually differed from their diagonalized counterparts by less than 1%. The largest differences occurred in the calculation of nearly degenerate energies of states of like spin. The errors were particularly large when the minimum of

$$\Delta \bar{e} = \bar{e}(J_{i+1}) - \bar{e}(J_i)$$

occurred well between lattice points. [Small values of $\Delta \bar{e}$ are associated with the attempted crossing (in energy) of two states of differing shape-vibrational characters.] When the GRID interpolation procedure was considered unreliable, model spectra were determined from 15-phonon diagonalizations. At the conclusion of every fitting process, final values for the $\bar{e}_q$ were obtained from a large basis diagonalization of $\bar{H}_{QP}$. The associated optimal value of $\hbar\bar{\omega}$ was then found from Equation (6.3).

Referring to Equations (5.4)-(5.9) [or to Figure 3.2 in the more general case] it is clear that the original Hamiltonian $[H_{QP}]$ may be recovered from its reduced form $[\bar{H}_{QP}]$ if the energy factor $[\hbar\bar{\omega}]$ and deformation scaling constant $[\bar{s}]$ are known. That is, from

$$\mathbf{s}_1: \{\beta_o, \gamma_o, C_\gamma, [C_\beta = 1, C_{\beta\gamma} = 0], \hbar\bar{\omega}, \bar{s}\}$$

we may find

$$\mathbf{s}_2: \{b_o, g_o, c_\gamma, c_\beta, [c_{\beta\gamma} = 0], B\}$$

All members of $\mathbf{s}_1$, with the exception of $\bar{s}$, are determined by the energy-level fitting process. The latter constant appears in the factor $D_k/\bar{s}^k$ which connects matrix elements of the k-th order E2 operator with dimensionless matrix elements whose values depend only on the $\bar{H}_{QP}$ problem [Equation (3.57)]. Hence if $\bar{H}_{QP}$ is fixed, $\bar{s}$ may be found by equating one model $B(E2)$ or quadrupole moment to the experimental value.

The determination of the $\mathbf{s}_2$ constants is particularly straightforward if the theoretical value of $B(E2:2_1 \rightarrow 0_1)$ in first order is set equal to the experimental reduced transition rate. In this case it is useful to define the dimensionless quantities:

$$b_{ex} \equiv \text{experimental value of } B(E2:2_1 \rightarrow 0_1) \text{ in units of } (e \cdot \text{barn})^2 \quad (6.4a)$$

$$b_{th} \equiv \text{first order model value of } B(E2:2_1 \rightarrow 0_1) \text{ in units of } [D_1/\bar{s}]^2 \quad (6.4b)$$

$$F \equiv \text{value of } \hbar\omega \text{ in units of MeV} \quad (6.4c)$$

$$D'_1 \equiv \text{value of } \left[D_1 = \frac{3ZeR_o^2}{4\pi} \right] \text{ in units of } (e \cdot \text{barn}) \quad (6.4d)$$

If we obtain R_o from the nuclear mass number A by

$$R_o = 1.2A^{1/3} \text{ Fermi} \quad , \quad (6.5)$$

then

$$D'_1 = \frac{.0108}{\pi} ZA^{2/3} \quad , \quad (6.6)$$

and

$$\bar{s} = \left[\frac{b_{th}}{b_{ex}} \right]^{\frac{1}{2}} D_1' \quad (6.7)$$

The five non-trivial members of $\mathfrak{g}_2$ are then found to be given by

$$b_0 = \beta_0 / \bar{s} \quad (6.8a)$$

$$g_0 = \gamma_0 \quad (6.8b)$$

$$c_Y = c_Y F \cdot [1 \text{ MeV}] \quad (6.8c)$$

$$c_\beta = \bar{s}^2 F \cdot [1 \text{ MeV}] \quad (6.8d)$$

$$B = .43325133 \frac{\bar{s}^2}{F} \cdot [10^{-42} \text{ MeV} \cdot \text{sec}^2] \quad (6.8e)$$

If both first and second order terms are retained in the model expression for $B(E2:2_1 \rightarrow 0_1)$, only Equation (6.7) requires modification. In that event, equating model and experimental values leads to

$$\sqrt{5b_{ex}} = \frac{D_1' m_1}{\bar{s}} + \frac{D_2' m_2}{\bar{s}^2} \quad (6.9)$$

as the determining relationship for $\bar{s}$, where the additional definitions

$$m_k \equiv \text{model value of } \langle \bar{\phi}_{J_f=0_1} || \Omega_k^{LAB} || \bar{\phi}_{J_i=2_1} \rangle \quad ; \quad k = 1, 2 \quad (6.10)$$

[computed from Equation (3.60) for the $\bar{H}_{QP}$ problem]

$$D_2' \equiv \frac{-10}{\sqrt{70\pi}} D_1' \quad (6.11)$$

have been introduced. Equation (6.9) reduces to Equation (6.7) when m_2 is neglected and the identity

$$b_{th} = \frac{2J_f + 1}{2J_i + 1} [m_1]^2 \quad (6.12)$$

is used.

Experimental $B(E2)$ values and quadrupole moments do not directly contribute to the determination of the optimal $(\beta_0, \gamma_0, C_\gamma)$ set. During the energy-fitting process, allowed model asymmetry extends only over $0^\circ \leq \gamma_0 \leq 30^\circ$. When fitting has been concluded, the sign of the experimental $Q(2_1)$ determines if reflection of $\bar{V}_{QP}(\beta', \gamma)$ about $\gamma = 30^\circ$ is necessary. [Such a reflection leaves model energies unaltered but reverses the sign of (first order) model quadrupole moments.] Having fixed $\bar{H}_{QP}$, (first order) $B(E2)$ transition rates are determined to within a factor which depends upon $\bar{s}$. This final constant may be found by employing either of Equations (6.7) or (6.9). As always $B(E2: J_i \rightarrow J_f)$ will be specified for the $J_i \geq J_f$ transition unless otherwise indicated.

With the aforementioned computational techniques as prologue, the final three sections of the thesis proper report on applications of the quadratic potential (QP) model to eight nuclei. ^{106}Pd , which originally motivated the Chapter V study of model properties, is considered in Section A. Within the framework of the QP model, it proves impossible to account for the entire low-energy spectrum of ^{106}Pd . When attention is restricted to the S_1 levels in Figure 1.1, the Davydov-Chaban (DC) model fit to the experimental energies may be improved, but γ -vibrational energies are then found to be quite high. High- C_γ [^{166}Er , ^{182}W] and low- C_γ [^{122}Te] applications of $\bar{H}_{QP}$ are discussed in Section B. For the first two nuclei, QP model applications encounter parameter ambiguities,

and the DC model appears to be slightly superior. In ^{122}Te , however, γ vibrations prove necessary for an adequate accounting of the low-energy experimental spectrum. QP and Gneuss-Greiner (GG) model parameters and predictions are compared for this nucleus. The final section treats four osmium isotopes which lie in the transition region dividing deformed [$150 \lesssim A \lesssim 180$] and spherical [near ^{208}Pb] nuclei. For each of $^{186}, ^{188}, ^{190}, ^{192}\text{Os}$, DC and QP model applications are compared; the latter offers an improved reckoning of experimental energies, but neither model proves to be very satisfactory. For each of the four isotopes, the most effective version of the QP model interprets the states 0_2 and 0_3 as β and γ vibrations respectively. These model calculations indicate that nuclear deformation decreases and BF z-axis asymmetry increases as neutron pairs are added to ^{186}Os .

QP and DC model results are compared for seven of the eight nuclei treated in this chapter. DC model calculations for ^{166}Er , ^{182}W and $^{186}, ^{188}, ^{190}, ^{192}\text{Os}$ were performed by Dr. Stanley A. Williams (55), and the ^{106}Pd results have been taken from (12, 57). In each case the three DC parameters of Equation (1.2) were determined from experimental energies by minimizing an expression similar to that of Equation (6.1). Since $[\hbar^2/Bc_\beta]$ is effectively unity in $\bar{H}_{QP}$, the nonadiabaticity parameter μ may be directly compared with $1/\beta_0$; γ_0 and the energy scale factor play identical roles in each model. Energy ratios for A-type states of the rigid quadrupole rotor are occasionally cited for purposes of comparison. In all cases, the ratios have been deduced from the tables of R. B. Moore and W. White (54).

A. ^{106}Pd

In Chapter I the hope was expressed that the theoretical interpretation of the ^{106}Pd spectrum, offered in (12), could be completed by an application of the QP model. In particular it was hoped that γ vibrations could supply the additional $J = 0$ states at 1134 and 1706 keV in Figure 1.1. It would be necessary for the energy separation between adjacent γ -vibrational band heads to decrease as m_γ rises. Furthermore, the collection of rotational and β -vibrational states [Davydov-Chaban sequence] based upon a γ vibration would be required to have a similar energy structure to that based upon the ground state. Both features have been observed in the $\bar{H}_{QP}$ studies of Chapter V [see Figures 5.23-5.26].

The result of the initial application of the QP model to the ^{106}Pd experimental spectrum is summarized by Figure 6.2. The GRID fitting procedures were used to adjust the $\bar{H}_{QP}$ parameters and overall scale factor so as to provide a best fit to the $J = 0, 2, 2, 4, 3, 6, 8$ sequence shown. These seven states were presumed to belong to the GS rotational band [$n_\beta = m_\gamma = 0$]. The optimal set $(\beta_0, \gamma_0, C_\gamma, \bar{\omega})$ was found to equal (2.24, 27.46°, 44.74, 1.953 MeV), and a subsequent 20-phonon, $\tilde{s} = 1$ diagonalization of the corresponding Hamiltonian produced the theoretical portion of Figure 6.2. The lowest β vibration was predicted to lie at 2257 keV, within 1% of the 2278 keV $J = 0$ state designated in (12) as the experimental β vibration. The first γ -vibrational $J = 0$ state was predicted to have an energy of 6033 keV,

Figure 6.2. Application of $\tilde{H}_{op}$ to ${}^{106}\text{Pd}$ [$\beta_0=2.24$, $\gamma_0=27.46^\circ$, $C_\gamma=44.74$, $\hbar\omega=1.953$ MeV]. The experimental levels used in the determination of model parameters are shown at left. Some of the other experimental levels are also indicated as well as the model predictions for shape-vibrational energies

considerably above the second β vibration, and several times the energy of the 1134 keV experimental state.

From the calculations of Chapter V, it is clear that the first excited $J = 0$ state of $\bar{H}_{QP}$ will be a γ vibration only if β_0 is relatively large and $C_Y(\gamma - \gamma_0)^2$ is small. The smallest value of β_0 for which this is possible may be found from Figure 5.6. The $J = 0$ state originating from $[N, \ell] = [2, 0]$ intersects that from $[3, 3]$ near $\beta_0 = 2.63$. At larger values of β_0 it is therefore possible to satisfy

$$\bar{e}(0_\gamma) \leq \bar{e}(0_\beta) \quad (6.13)$$

$$0_\gamma \equiv (0, 1, 0_1) \text{ [in the } (n_\beta, m_\gamma, J_1) \text{ notation]} ,$$

$$0_\beta \equiv (1, 0, 0_1) .$$

The (β_0, γ_0, C_Y) parameter region within which Inequality (6.13) holds is the topic addressed by Figure 6.3. There the necessarily non-negative energy difference between the first and second excited $J = 0$ states,

$$\Delta \equiv \bar{E}(0_3) - \bar{E}(0_2) ,$$

is displayed as a function of (γ_0, C_Y) for three values of β_0 . $\Delta = 0$ would correspond to the exact degeneracy of the lowest β and γ -vibrational energies. This may be realized only for the special cases of $\gamma_0 = 30^\circ$ or $C_Y = 0$. More generally, the "crossing" of vibrational energies will be indicated by small but non-zero values of Δ . On the basis of the behavior of Δ under an increase of C_Y , we may determine whether 0_β or 0_γ has the lower energy. For example in the $\beta_0 = 6$ surface of Figure 6.3, three distinct regions may be discerned. Their descriptions and

Figure 6.3. $\Delta \equiv [\bar{E}(O_3) - \bar{E}(O_2)]$ for $\bar{H}_{Op}$ as a function of (γ_0, c_γ) . From the behavior of Δ under an increase of c_γ , one may determine whether O_β or O_γ is lower in energy

interpretations are as follows:

- 1) Δ decreases as C_Y rises [$0_Y = 0_2$ lies below $0_\beta = 0_3$ in energy and the former is rising to meet the latter];
- 2) Δ increases as C_Y rises [$0_Y = 0_3$ lies above $0_\beta = 0_2$ and is rising]; and
- 3) Δ unchanged by variations in C_Y and γ_0 [0_2 and 0_3 are the first and second β vibrations respectively].

The first region has no observable counterpart in either the $\beta_0 = 0$ or the $\beta_0 = 3$ surface. Actually, at the $C_Y = 0$ boundary of the central surface, 0_Y lies below 0_β in energy. As C_Y is increased from zero Δ consequently falls, achieving zero near $C_Y = 3$ [$\gamma_0 = 30^\circ$, $\beta_0 = 3$]. This behavior is not evident in Figure 6.3 which reflects the results of the GRID calculations. The large C_Y step size [$\Delta C_Y = 10$] prevents the resolution of all but the coarsest surface features. For this reason the crossing of $\bar{e}(0_\beta)$ and $\bar{e}(0_Y)$ near $(\beta_0, \gamma_0, C_Y) = (6, 0^\circ, 5)$ has also been obscured in the figure.

The 0_Y energy clearly rises rapidly as C_Y is increased; hence β_0 must be simultaneously increased if $\bar{e}(0_Y) < \bar{e}(0_\beta)$ is to be maintained. As the $\bar{V}_{QP}$ minimum sharpens, we may make use of

$$\bar{e}(0_\beta) \approx 1 \quad [C_\beta = 1] \quad ; \quad \text{and} \quad (6.14a)$$

$$\bar{e}(0_Y) \approx a \left[\frac{2C_Y}{\beta_0^2} \right]^{\frac{1}{2}}, \quad (6.14b)$$

$$a \approx 1 \quad \text{at} \quad \gamma_0 = 30^\circ \quad ,$$

$$a \approx 2 \quad \text{at} \quad \gamma_0 = 0^\circ \quad ;$$

to replace Inequality (6.13) by the more useful relationship,

$$C_\gamma \lesssim \frac{\beta_0^2}{2a^2} \quad \text{in order that} \quad \bar{e}(0_\gamma) \leq \bar{e}(0_\beta) \quad . \quad (6.15)$$

The energy spacings of the experimental $J = 0, 2, 2, 4, 3, 6, 8$ sequence in ^{106}Pd strongly resemble those occurring for a rigid quadrupole rotor with $\gamma_0 \approx 30^\circ$ [Figure 5.5]. The appearance of a similarly spaced sequence in the $\bar{H}_{QP}$ spectrum requires a fair amount of γ -stability [$C_\gamma \approx 20$] at moderate deformation, $1 \lesssim \beta_0 \lesssim 3$. A slightly smaller value of C_γ may be tolerated if β_0 is larger [see Figures 5.44 and 5.41]. If we fix $(C_\gamma, \gamma_0) = (15, 30^\circ)$ and further insist that $\bar{e}(0_\beta) \approx 2\bar{e}(0_\gamma)$ [as would be the case if the 1134 and 2278 keV levels in ^{106}Pd were interpreted as γ and β vibrations respectively], Equations (6.14) require $\beta_0 \approx 2\sqrt{30} \approx 11$. The reduced spectrum of a similar QP Hamiltonian is displayed in Figure 6.4. The $J = 0, 2, 2, 4, 3, 6$ sequence in the GS band resembles that in ^{106}Pd , and $\bar{e}(0_\beta)/\bar{e}(0_\gamma) = 2$ is approximately satisfied. The reduced energies of the vibrational states are, however, much too high to permit their association with ^{106}Pd experimental levels.

In a given application of the QP model, an upper limit on β_0 may be deduced from the energies of the even-spin yrast states. We begin by noting that increasing either β_0 or C_γ causes the reduced energies of these GS-band states to rise. For H_B the reduced energies of the $J_i = 4_1, 6_1, 8_1$ states are 2, 3, and 4 respectively, while in ^{106}Pd they are 2.40, 4.05, and 5.79. If the entire increase of any one of the latter energies [above its H_B counterpart] is attributed to the

Figure 6.4. Reduced $\bar{H}_{QP}$ spectrum for a large β_0 example. Rotational bands resemble those of a rigid rotor with $\gamma_0 = 30^\circ$.
 $\bar{e}(0_\beta) \approx 2\bar{e}(0_\gamma)$

$\frac{1}{2}(\beta' - \beta_0)^2$ term of $\bar{V}_{QP}$, β_0 may be deduced. For example if $(\beta_0, C_Y) = (3.6, 0)$ in $\bar{H}_{QP}$, $\bar{e}(4_1)/\bar{e}(2_1) = 2.40$. Similarly $(\beta_0, C_Y) = (3.36, 0)$ leads to $\bar{e}(6_1)/\bar{e}(2_1) = 4.05$, and $(3.11, 0)$ yields $\bar{e}(8_1)/\bar{e}(2_1) = 5.79$. Hence in the case of ^{106}Pd , we expect that $\beta_0 \approx 3$ will be necessary if we are to adequately account for GS-band energies. At $(\beta_0, C_Y) = (3, 0)$, $\bar{e}(0_Y)$ is indeed below $\bar{e}(0_\beta)$ as shown in Figure 6.5. However 0_Y rises above the second β vibration when the required γ -stability is supplied. As noted previously, the best fit to the ^{106}Pd GS-band states occurs when $(\beta_0, \gamma_0, C_Y) = (2.24, 27.46^\circ, 44.74)$.

The case against treating the 1134 keV experimental state as a γ vibration may be further strengthened by considering the $J = 0, 3, 4, 6$ multiplet which arises from $[N, \ell] = [3, 3]$. These states are degenerate for $\bar{H}_{QP}$ whenever C_Y is zero. In Chapter V, $J = 3, 4, 6$ were assigned to the GS band while $J = 0$ was designated as the lowest γ -vibrational band head. These assignments were based on the knowledge that the $J = 0$ energy rises rapidly above those of $J = 3, 4, 6$ when C_Y is increased for any value of γ_0 . This phenomenon is demonstrated in Figure 5.40 for $\beta_0 = 0$, and in Figure 6.6 for $\beta_0 = 4$. The low-energy portion of the ^{106}Pd spectrum is also shown in the latter figure. [The energy of the second $J = 4$ state (dashed line) has been taken from the DC calculation of Reference (12)]. Not one of the first four excited $J = 0$ states in ^{106}Pd lies above all of the circled levels. Consequently not one can be adequately represented by an $\bar{H}_{QP}$ γ vibration. The only alternative within the QP model is to treat all four of these $J = 0$

Figure 6.6. Low-energy reduced spectra for four instances of $\bar{H}_{QP} [B_0=4]$. For $C_\gamma \neq 0$, 0_β , 0_γ and selected $K=0, 2$ GS-band levels are shown. The circled spins denote levels originating from $[N, l] = [3, 3]$ states of H_B . For $C_\gamma > 0$, the $J=0$ state $[0_\gamma]$ lies above the other $[3, 3]$ levels

states [1134, 1706, 2001 and 2278 keV] as β vibrations. This approach would not be fruitful because of the obvious decrease in $E(0_{i+1}) - E(0_i)$ with increasing i . In the model studies of Chapter V, such an effect was not observed for successive β vibrations.

Even if we choose to treat only the experimental 0_2 as a β vibration, ignoring all higher $J = 0$ states, grave problems arise. Such an assumption was used in a fit to the $J_i = 0_1, 2_1, 2_2, 0_2, 4_1, 3_1, 6_1, 8_1$ experimental sequence. It was found that β_0 had to be restricted to very small values in order to hold 0_2 near 2_2 and 4_1 . In fact the best fits occurred for $(\beta_0, \gamma_0, c_\gamma) \sim (0, 26^\circ, 26)$, and the resulting model spectra resembled that appearing at the right hand edge of Figure 5.40. The model energies of the 6_1 and 8_1 states were much too low, and the proper ordering of the $2_2, 0_2, 4_1$ triplet could not be achieved. For experimental states contributing to the fitting process, the average value of

$$\left| \frac{e_q - \hbar\omega \bar{e}_q}{e_q} \right| = 100\% \quad (6.16)$$

was $\sim 11\%$. This may be compared with .6% for the fit depicted in Figure 6.2. We conclude that interpreting the 1134 keV state in ^{106}Pd as either a β or γ vibration leads to substantial disagreements between experimental and QP model energies. The 1134 keV $J = 0$ state, as well as those at 1706 and 2002 keV, is evidently associated with other nuclear degrees of freedom.

In the initial application of $\bar{H}_{QP}$ to the ^{106}Pd spectrum [Figure 6.2] $\bar{e}(0_\gamma)$ was quite large. Its precise value, which could be altered

by small changes of C_Y , was found to have little influence on the low-energy portion of the model spectrum. We might expect the DC model, which discounts γ vibrations entirely, to offer similar predictions for the low-energy states. Energies and $B(E2)$ ratios for the two models are compared with measured values in Tables 6.1 and 6.2. References (12) and (57) are the source of the experimental and DC results. QP results are based on $(\beta_0, \gamma_0, C_Y, \hbar\bar{\omega}) = (2.24, 27.46^\circ, 44.74, 1.953 \text{ MeV})$. QP model energies are seen to be generally nearer the experimental ones, while the DC model has a slight edge in accounting for measured $B(E2)$ ratios. The strength of the angular perturbation, $C_Y(\gamma - \gamma_0)^2$, is similar to that encountered in upcoming applications. For this reason I have taken the opportunity, in Tables 6.1 and 6.2, to compare to results of employing 20 and 25-phonon diagonalizations at the conclusion of the GRID fitting process. $\bar{H}_{QP}$ energies were lowered slightly when the larger basis was used, resulting in a .005% increase in the optimal value of $\hbar\bar{\omega}$. QP model calculations leading to Table 6.2 included the effect of the first-order E2 operator only. In the ^{106}Pd application, 20-phonon results were found to be sufficiently converged. Throughout the remainder of this chapter, 25-phonon bases are employed exclusively.

Taking the experimental value of $B(E2:2_1 \rightarrow 0_1)$ in ^{106}Pd to be 1.53 (e.barn)² (58), we may use Equations (6.6)-(6.8) to recover the H_{QP} parameters. We find

$$\bar{s} = 12.442$$

$$c_\beta = 302.28 \text{ MeV}$$

$$b_0 = .1800$$

$$c_Y = 87.36 \text{ MeV}$$

Table 6.1. Model and experimental relative energies [in MeV] for selected states in ^{106}Pd . Experimental and DC values are taken from References (12) and (57)

State (n_β, m_γ, J_i)			Exp. Energy	DC Model	QP Model 20-phonons ($\hbar\omega=1.95262$ MeV) ($\tilde{s}=1$)	QP Model 25-phonons ($\hbar\omega=1.95272$ MeV) ($\tilde{s}=1$)
0 0	[GS]	0_1	0.0	0.0	0.0	0.0
		2_1	.512	.512	.514	.514
		2_2	1.128	1.120	1.132	1.132
		4_1	1.229	1.305	1.228	1.228
		3_1	1.556	1.522	1.552	1.553
		6_1	2.076	2.234	2.053	2.053
		4_2	(2.350)	2.299	2.316	2.316
		5_1		2.593	2.541	2.541
		4_3			2.907	2.907
1 0	[β]	8_1	(2.962)	3.272	2.976	2.976
		0_1	2.278	2.270	2.257	2.256
		2_1		2.912	2.928	2.925
0 1	[γ]	2_2			3.687	3.686
		0_1			6.033	6.034
		2_1			6.458	6.458
		2_2			7.139	7.139

Table 6.2. Model and experimental values of $B(E2:J_i \rightarrow J_f)/B(E2:J_i' \rightarrow J_f')$. Experimental and DC values are taken from References (12) and (57)

Transition Ratio ^a	¹⁰⁶ Pd Experiment	DC Model	QP Model 25 phonons (20 phonons)
$\frac{2_2 \rightarrow 2_1}{2_1 \rightarrow 0_1}$	$.96 \pm .14$	1.04	1.31781 (1.31736)
$\frac{4_1 \rightarrow 2_1}{2_1 \rightarrow 0_1}$	$1.55 \pm .23$	1.58	1.59
$\frac{2_2 \rightarrow 2_1}{2_2 \rightarrow 0_1}$	38 ± 6	24.3	50.422 (50.349)
$\frac{4_1 \rightarrow 2_1}{2_2 \rightarrow 2_1}$	$1.62 \pm .31$	1.52	1.21
$\frac{3_1 \rightarrow 4_1}{3_1 \rightarrow 2_2}$	$.33 \pm .07$	.50	.49
$\frac{0_2 \rightarrow 2_2}{0_2 \rightarrow 2_1}$	.85	.07	.05
$\frac{2_3 \rightarrow 2_1}{2_3 \rightarrow 0_1}$	6.76	1.28	1.1784 (1.1779)

^aState labels are $J_i \equiv i$ -th state of spin J in the QP model spectrum (ordered by increasing energy). See Figures 1.1 and 6.2.

$$g_0 = 27.46^\circ \quad B = 34.345 \cdot 10^{-42} \text{ MeV} \cdot \text{sec}^2$$

To help visualize the equilibrium deformation of the model droplet, we compute the origin-to-surface distances along the body-fixed x, y and z axes. From Equations (2.2) and (2.6) these are given by

$$R_k = R_0 \left\{ 1 + \left[\frac{5}{4\pi} \right]^{\frac{1}{2}} b_0 \cos \left(g_0 - \frac{2\pi k}{3} \right) \right\} \quad (6.17)$$

$$k = 1, 2, 3$$

respectively for a quadrupole surface with deformation b_0 and asymmetry γ_0 . Using $(b_0, g_0) = (.18, 27.46^\circ)$ we obtain

$$R_x = .995 R_0$$

$$R_y = .904 R_0$$

$$R_z = 1.101 R_0$$

On the basis of $\bar{s} = 12.442$, the predicted quadrupole moment of the first excited state is $Q(2_1) = -.324(\text{e} \cdot \text{barn})$. The measured value (58) in the same units is $-.49 \pm .06$. If the second order E2 operator is included in model calculations, $\bar{s}$ is raised to 12.747 and $Q(2_1)$ is then predicted to be $-.376(\text{e} \cdot \text{barn})$.

$$B. \quad {}^{166}\text{Er}, {}^{182}\text{W}, {}^{122}\text{Te}$$

When γ_0 is near 30° , the reduced energies of $K = 0, 2$ GS-band states serve to identify γ_0 , and to some extent C_γ , rather uniquely. This was the case in the application of $\bar{H}_{QP}$ to ${}^{106}\text{Pd}$. The situation is quite different when $\gamma_0 \approx 15^\circ$. Increasing C_γ then causes the energies

of $K \neq 0$ GS-band states to rise relative to those of $K = 0$ states. The same effect may be produced by holding C_γ fixed and decreasing γ_0 . [See Figure 5.44.] It consequently becomes difficult to determine a unique set $(\beta_0, \gamma_0, C_\gamma)$ from a knowledge of $m_\gamma = 0$ energies, particularly when $K > 2$ energies are unknown. The extent of the uncertainty is illustrated in Figures 6.7 and 6.8 for applications of the QP model to ^{166}Er and ^{182}W respectively. The DC model enjoys two of its more impressive successes in accounting for the low-energy structure of these two nuclei. Experimental energies have been taken from References (59) and (60) respectively. Their numerical values may be found in Tables E.6 and E.7, together with the corresponding DC and QP model energies. Experimental $B(E2)$ values taken from (61) have been used to compute the ratios which appear in the two figures.¹

For each of ^{166}Er and ^{182}W , two applications of the QP model are shown. These have been labeled QP#1 and QP#2; they are distinguished by high and low values of C_γ respectively. The GRID fitting procedures were invoked for each nucleus in turn, $0_2 = 0_\beta$ being assumed. Experimental levels appearing in Figures 6.7-6.8 and having $J \leq 7$ contributed to χ^2 [Equation (6.1)]. The dependence of χ^2 upon the $\bar{V}_{QP}$ parameters differed considerably from that encountered in the ^{106}Pd application

¹ In each of Figures 6.7-6.9, experimental and model values of $B(E2:J_i \rightarrow J_f)/B(E2:2_1 \rightarrow 0_1)$ are given. For the experimental portion of each figure, the ratios have been computed using the $B(E2:J_i \rightarrow J_f)$ values enclosed in parentheses. Units are those of $(e \cdot \text{barn})^2$ and experimental uncertainties are ~10%-20%.

Figure 6.7. ^{166}Er model and exp. spectra and B(E2) ratios (see caption of Figure 6.8)

Figure 6.8. ^{182}W spectra and $B(E2:J_i \rightarrow J_f)/B(E2:2_1 \rightarrow 0_1)$ ratios. The latter are given for the high spin to low spin transition ($J_i \geq J_f$). Exp. values (61) of $B(E2:J_i \rightarrow J_f)$ in (e·barn)² appear in parentheses

leading to Figure 6.2. A dominant absolute minimum was not observed in $\chi^2(\beta_0, \gamma_0, C_\gamma)$ for either ^{166}Er or ^{182}W . In the vicinity of the optimal β_0 [~ 4.5 for ^{166}Er , ~ 3.1 for ^{182}W], χ^2 , regarded as a function of (γ_0, C_γ) , was found to possess a long valley of relatively constant depth. Shallow minima within the bed of such a valley gave rise to the depicted QP model spectra. In the preparation of each figure, two local minima having vastly different values of C_γ were used, thus emphasizing the parameter ambiguity. The larger value of C_γ is seen to be associated with smaller optimal values of β_0 and γ_0 . The spread in γ_0 is particularly large for the model spectra representing ^{182}W .

Although QP#1 and QP#2 spectra are very similar for levels contributing to the fit, the spectra differ sharply in their γ -vibrational energies. This may be seen in Table 6.3. Energies of the GS-band $K = 4$

Table 6.3. Model energies (MeV) of selected states not appearing in Figures 6.7 and 6.8

J_i	^{166}Er		^{182}W	
	QP#1 (High C_γ)	QP#2 (Low C_γ)	QP#1 (High C_γ)	QP#2 (Low C_γ)
4_4	2.06	1.77	2.67	2.43
5_2	2.18	1.92	2.80	2.60
0_γ	3.43	2.11	3.06	2.41

states [$J_i = 4_4, 5_2$] are also higher for the high- C_γ Hamiltonians. As illustrated in Figures 6.7 and 6.8, the E2 transition schemes for fitted

levels are quite similar for the QP#1 and QP#2 model applications.¹ As might be expected, values for the high- C_γ fit are closer to those of the DC model, particularly for $\Delta K = 0$ transitions. $\Delta K \neq 0$ transitions, such as $2_2 \rightarrow 0_1$, are more sensitive to the value of γ_0 . For ^{166}Er and ^{182}W , these appear to be better predicted by the DC model than by either QP version. The former model also provides a better fit to the low-energy experimental spectra in each case, and is not plagued by parameter ambiguities. Hence the inclusion of γ vibrations does not further the present understanding of collective excitations in ^{166}Er and ^{182}W . However, the future identification of additional bands in these nuclei may merit renewed applications of the QP model.

When experimental candidates are available for both β and γ -vibrational levels, optimal $\bar{H}_{\text{QP}}$ parameters may be determined with little ambiguity. Such is the case for ^{122}Te , one of the nuclei to which the Gneuss-Greiner (GG) Hamiltonian was applied in (29). The small experimental value of

$$\frac{E(0_3) - E(0_2)}{E(0_2) - E(0_1)} = .43$$

prevents us from regarding both 0_2 and 0_3 as β vibrations, and hence precludes a fruitful application of the DC model. Indeed, GG model

¹ Interference effects between the 2_2 and 2_3 model states of ^{182}W are evident from the predicted strength of the $2_2 \rightarrow 0_2$ transition. $E(2_3) - E(2_2) \approx .12$ MeV for each of QP#1 and QP#2, but the low- C_γ version exhibits a greater mixing of the GS-band ($K = 2$) and β -band ($K = 0$) levels.

Figure 6.9. ¹²²Te model and experimental (29) spectra, $B(E2:J_i \rightarrow J_f)/B(E2:2_1 \rightarrow 0_1)$ ratios [$J_i \geq J_f$], and quadrupole moments. Exp. B(E2) values in (e.barn)² appear in parentheses

calculations find the ^{122}Te potential energy function [Figure 4.1] to be too shallow to localize γ . Consequently it does not prove profitable to regard γ as a fixed parameter. When all experimental levels appearing in Figure 6.9 are allowed to contribute to χ^2 , the optimal $\bar{H}_{QP}$ parameters are found to be $(\beta_0, \gamma_0, c_\gamma) = (1.37, .38^\circ, 1.00)$. $\bar{V}_{QP}(\beta', \gamma)$ thus resembles the GG potential surface in two particulars: the potential minimum lies near $\gamma_0 = 0^\circ$; and $\bar{V}_{QP}$ is not a steeply rising function of $(\gamma - \gamma_0)$. However, the two model spectra¹ exhibit some noteworthy differences. For example the GG model predicts a much larger value for the ratio $|Q(2_1)/Q(2_2)|$, and the two models do not agree on the energy ordering of GS-band $K = 2$ states. The splitting of the $N = \ell = 3$ [$J_i = 3_1, 4_2, 6_1$] states exhibited by the GG Hamiltonian cannot be achieved by $\bar{H}_{QP}$ for any set $(\beta_0, \gamma_0, c_\gamma)$. For the latter Hamiltonian, 4_2 rises above 3_1 whenever c_γ is increased from zero with (β_0, γ_0) fixed. The ordering of the corresponding experimental states could thus shed light on the necessity of replacing V_{QP} by a more elaborate function.

Within the interpretive framework of Chapter V, the 0_2 and 0_3 states in ^{122}Te may be thought of as β and γ -vibrational band heads respectively. $\bar{H}_{QP}$ is very near H_B^1 , however, and rotational and

¹Only GG model states considered during the test calculations of Chapter IV appear in Figure 6.9. For both the GG and QP models, quadrupole moment and $B(E2)$ calculations reflect the effect of the first-order $E2$ operator only. ^{122}Te experimental energies and $B(E2)$ values are those cited in (29). Model and experiment energies are listed in Table E.8.

Table 6.4. HQP parameters for ^{166}Er , ^{182}W and ^{122}Te applications of the QP Model

	^{166}Er (QP#1)	^{166}Er (QP#2)	^{182}W (QP#1)	^{182}W (QP#2)	^{122}Te
N_{max}	25	25	25	25	25
$\bar{s}$	.78	.78	.95	.95	1.05
β_0	4.38	4.55	3.09	3.15	1.37
γ_0	15.32°	14.93°	12.02°	5.36°	$.38^\circ$
C_γ	70.0	19.21	43.28	12.72	1.00
$\hbar\bar{\omega}$ (MeV)	1.3755	1.3884	.99307	.99870	.97106
b_{th}	3.995	4.098	2.362	2.352	.8336
D_1'	7.061	7.061	8.170	8.170	4.397
b_{ex}	1.1 ^a	1.1 ^a	.84 ^a	.84 ^a	.13 ^b
$\bar{s}$	13.456	13.629	13.700	13.671	11.135
b_0	.326	.334	.226	.230	.123
c_β (MeV)	255.5	257.9	186.4	186.7	120.4
c_γ (MeV)	96.3	26.7	43.0	12.7	.97
$B(10^{-42}\text{MeV-sec}^2)$	58.5	58.0	81.9	81.1	55.3
R_x/R_0	.95	.95	.96	.94	.96
R_y/R_0	.85	.85	.90	.92	.96
R_z/R_0	1.20	1.20	1.14	1.14	1.08

^aFrom Reference (61).^bFrom Reference (29).

vibrational excitations should not be regarded as cleanly uncoupled. When Equations (6.4)-(6.8) are used to recover the parameters of H_{QP} [Table 6.4], b_0 is found to be much smaller for ^{122}Te than for the other nuclei considered in this section. ^{166}Er , which is furthest from doubly-magic, has the largest model value of the deformation parameter. It also has the largest value of c_β . From Table 4.1 and Equation (4.5), the mass parameter B may be seen to range [in units of $10^{-42} \text{ MeV} \cdot \text{sec}^2$] from 32.1 [BA-128] to 140.3 [XE-134] for the isotopes treated by Habs et al. (29, 30). The values of B in Table 6.4 are well within these limits. For ^{122}Te , the QP and GG model values of B differ by less than 2%.

It is noteworthy that optimal values of B greatly exceed the classical estimates. For an irrotational droplet of radius R_0 and mass density ρ_0 , undergoing quadrupole surface oscillations, we may deduce (5)

$$B = \frac{1}{2} \rho_0 R_0^5 \quad (6.18)$$

If we assume

$$R_0 = 1.2A^{1/3} \text{ Fermi}$$

$$\text{Average (bound) nucleon mass} = (939 - 8) \text{ MeV}/c^2$$

we may write Equation (6.18) as

$$B = .001778A^{5/3} [10^{-42} \text{ MeV} \cdot \text{sec}^2] \quad (6.19)$$

For ^{106}Pd , ^{122}Te , and ^{182}W , Equation (6.19) estimates the classical mass parameters as 4.2, 5.3 and 10.4 respectively, in units of $[10^{-42} \text{ MeV} \cdot \text{sec}^2]$. Optimal values are 34.3, 55.3, and 81.9.

c. $^{186, 188, 190, 192}\text{Os}$

The experimental low-energy spectra of four even-A osmium isotopes are depicted in Figure 6.10. Only positive parity levels are shown and several such states above ~ 1.5 MeV have been omitted. The experimental energies, taken from (62) and the works cited therein, have also been listed in Tables E.9-E.12. In each of the four nuclei, two $J = 0$ states appear below ~ 1.5 MeV which we may hope to associate with shape-vibrational excitations. Furthermore candidates for the $K = 0, 2$ and 4 rotational sequences of the GS band may be readily identified. These have been horizontally segregated in Figure 6.10. Two trends become evident from a cursory examination of the GS-band energies. As A increases:

- 1) the reduced energies of the $K = 0$ states $J_i = 4_1, 6_1, 8_1$ fall, as does that of 0_2 ; and
- 2) the energies of the $K = 2$ and $K = 4$ sequences shift downward with respect to those of the $K = 0$ states.

The first trend may indicate a softening of the potential minimum, particularly if 0_2 is β -vibrational. Within the framework of the rigid quadrupole rotor, the second indicates that γ_0 is increasing with A .

The size of the γ_0 variation may be estimated by imposing a sharp minimum in $\bar{V}_{QP}$ [i.e., fixing β_0 and C_γ at large values] and varying γ_0 to best fit the $K = 0, 2$ spectrum of each isotope. The results of such a series of calculations are displayed in Figure 6.11. γ_0 and $\hbar\omega$ were

Figure 6.10. Experimental even-parity (collective?) states in $^{186,188,190,192}\text{Os}$ [from Reference (62)]

K=0,2 levels in the even osmium isotopes.
 In $\bar{H}_{QP}$ calculations $(\beta_0, C\gamma) = (4, 40)$ was fixed
 and $(\gamma_0, \hbar\bar{\omega})$ adjusted for best fit to exp. levels shown.
 Final diagonalizations used $N_{MAX}=25$, $\xi=.8$.
 B(E2) transition rates are in units of $B(E2: 2_1 \rightarrow 0_1) \equiv b$.

Figure 6.11. Application of a "quasi-rigid" version of $\bar{H}_{QP}$ to GS-band K = 0,2 levels of osmium nuclei

determined by using the GRID fitting procedure with (β_0, C_γ) fixed at (4, 40) in each instance. As expected, the optimal value of γ_0 increases with A in this "rigid" approximation. The addition of each pair of neutrons adds $\sim 2^\circ$ to the asymmetry parameter. The quality of the fit to the $K = 0$ ($J \leq 6$) and $K = 2$ ($J \leq 5$) levels is best for ^{186}Os and deteriorates as A rises. The theoretical 6_1 energy falls substantially below its experimental counterpart, and the theoretical $K = 2$ energies begin to pair in a manner that is not experimentally observed. A major difficulty of the "rigid" approximation concerns the energy of the $J = K = 4$ level which is tabulated at the bottom of Figure 6.11. This state did not contribute to the fitting process and its predicted energy is $\sim 50\%$ too high in each case. For the transitions shown in the figure, (first order) model $B(E2)$ values are in reasonable agreement with experiment.¹ The dimensionless quadrupole moment, $Q(2_1)/[B(E2:2_1 \rightarrow 0_1)]^{1/2}$, drops more rapidly with increasing A than the model predicts. If the experimental values are accurate, they could be reproduced in ^{190}Os and ^{192}Os by enlarging γ_0 slightly. Recall that $Q(J_i)$ vanishes in first order when $\gamma_0 = 30^\circ$ in the QP Hamiltonian.

In the remainder of this section we explore the consequences of relaxing the constraints upon β_0 and C_γ . Assuming the experimental 0_2 and 0_3 states to be shape vibrational, sufficient energy information

¹ Experimental $B(E2)$'s and quadrupole moments for the Os isotopes alluded to in this work are generally those cited in (63). The only exceptions are for $6_1 \rightarrow 4_1$ transition rates which have been taken from (61). Quoted experimental errors are $\sim 10\%$ for $B(E2)$ values and 20-40% for quadrupole moments.

exists to determine optimal QP model parameters. We ask to what extent the model can account for the energies of the $K = 0, 2, 4$ GS-band sequences, and those of the states 0_2 and 0_3 . In the QP model calculations performed to answer this question, the four osmium nuclei were treated similarly. For each, only the experimental energies of the states¹

$$J_i = \begin{cases} 0_1, 2_1, 4_1 & \text{GS band, } K = 0 \\ 2_2, 3_1, 4_2, 5_1 & K = 2 \\ 4_3, 5_2 & K = 4 \\ 0_2, 2_3, 0_3 & \beta \text{ and } \gamma \text{ bands, } K = 0 \end{cases}$$

contributed to the fitting process. The band assignments assumed for these levels are as indicated. For each nucleus, three separate fitting procedures were pursued. In the first, designated here as $(\beta\gamma)$, 0_2 and 2_3 were assumed to belong to the first β band while 0_3 was taken as the lowest γ vibration. The band assignments of these three states were interchanged for the second fitting procedure, $(\gamma\beta)$. In the course of $(\beta\gamma)$ and $(\gamma\beta)$ calculations, each of $\{\beta_0, \gamma_0, C_\gamma\}$ was varied in the efforts to reproduce experimental spectra. However, in the third procedure, $(\gamma 0)$, γ_0 was fixed at 0° in the spirit of the rotation-vibration model of Faessler et al. (11). During the $(\gamma 0)$ model applications, various band assignments were attempted for the states

¹ Here the subscript of J_i refers to the i^{th} occurrence of J in the experimental spectrum of Figure 6.10.

$\{0_2, 2_3, 0_3\}$. Whenever the GRID fitting process indicated that the optimal value of C_Y was ≈ 5 , the interpolation method of calculating model energies was replaced by 15-phonon diagonalization and the fit was redone. This proved to be necessary for the $(\gamma\beta)$ and $(\gamma 0)$ calculations. [At small values of C_Y , the accuracy of interpolated γ -vibrational energies was doubted, particularly when γ_0 was also small]. At the conclusion of every fitting process, a final diagonalization of the appropriate $\bar{H}_{QP}$ was performed in a 25-phonon basis. Optimally-scaled eigenvalues resulting from these diagonalizations are graphically presented in Figures 6.12-6.15. In each figure experimental levels are also depicted, as are theoretical levels resulting from an application of the DC model. Numerical values of model and experimental energies may be found in Tables E.9-E.12.

The DC model effectively offers a partial lifting of the "rigidity" constraints imposed during the production of Figure 6.11. It thus provides a bridge between the rigid rotor and the more sophisticated QP model. DC model calculations for the osmium isotopes involved the variation of three parameters $\{\mu, \gamma_0, \hbar\omega\}$ so as to obtain a best fit to the experimental energies¹ of

$$J_i = \begin{cases} 0_1, 2_1, 4_1, 6_1 & \text{GS band} \\ 2_2, 3_1, 4_2, 5_1 & \\ 0_2, 2_3 & \text{B band} \end{cases}$$

¹The states $4_2, 5_1$ and 6_1 did not contribute to the ^{186}Os DC model fit.

Figure 6.13. ^{188}Os experimental and model [$J \leq 10$, $E \leq 2 \text{ MeV}$] energies

Davydov-Chaban
Model
 $\gamma = 20.723$
 $1/\mu = 2.584$
 $\hbar\omega = .917265 \text{ MeV}$

^{190}Os
Experiment

$\bar{H}_{QP}(\beta\gamma)$
 $\beta_0 = 2.59$
 $\gamma_0 = 24.6^\circ$

$C_\gamma = 14.6$

$\hbar\bar{\omega} = .803997$

$\tilde{s} = .95$

$\bar{H}_{QP}(\gamma\beta)$
 $\beta_0 = 4.02$
 $\gamma_0 = 20.5^\circ$

$C_\gamma = 1.12$

$\hbar\bar{\omega} = 1.44873$

$\tilde{s} = .80$

$\bar{H}_{QP}(\gamma 0)$
 $\beta_0 = 4.01$
 $\gamma_0 = 0^\circ$

$C_\gamma = .436$

$\hbar\bar{\omega} = 1.43475$

$\tilde{s} = .80$

Figure 6.14. ^{190}Os experimental and model [$J \leq 10$, $E \lesssim 2 \text{ MeV}$] energies

Figure 6.15. ^{192}Os experimental and model [$J \leq 10$, $E \lesssim 2 \text{ MeV}$] energies

The assignment of 0_2 and 2_3 to the first β band parallels that of the $(\beta\gamma)$ version of the QP model applications. As before, DC model calculations found the optimal γ_0 to increase with increasing A [Table 6.5]. Both $1/\mu$ and the quality of the fit were found to fall as A increased.

Table 6.5. Optimal model value of γ_0 . ["Rigid" refers to QP model with $(\beta_0, c_\gamma) = (4, 40)$]

Model	186_{Os}	188_{Os}	190_{Os}	192_{Os}
"rigid"	19.32°	21.78°	24.17°	25.90°
DC	15.48°	18.18°	20.72°	23.62°
QP($\beta\gamma$)	14.9°	21.3°	24.6°	30°

Major differences between model and experimental spectra are evident in Figures 6.12-6.15. These differences may be conveniently discussed in four parts by following the partitioning scheme used in the figures [GS-band $K = 0$, GS-band $K = 2$, GS-band $K = 4$, other bands]. We consider each in turn. The $(\beta\gamma)$ and $(\gamma\beta)$ results will be compared with those of the DC model and experiment. Table 6.6 facilitates the discussion by providing the values of key energy ratios. The $(\gamma 0)$ applications of the QP model will be considered separately.

GS band $K = 0$ levels. Model 2_1 energies are quite close to the experimental values and exact agreement could be imposed by slight modifications of the energy scale factors. The energies of even-spin yrast levels of higher J , however, differ significantly from the experimental values. In the case of the energy ratio

Table 6.6. Comparison of selected ratios of relative energies

Energy Ratio ^a	Model	$^{186}_{0s}$	$^{188}_{0s}$	$^{190}_{0s}$	$^{192}_{0s}$
$\frac{8_1}{2_1}$	Exp.	10.37	9.77	8.91	8.29
	DC	9.05	8.42	7.20	6.72
	QP($\beta\gamma$)	8.00	7.19	5.99	5.53
(K=0)	QP($\gamma\beta$)	8.02	7.30	6.58	6.07
$\frac{3_1-2_2}{4_2-3_1}$	Exp.	.88	.90	.99	.92
	DC	.73	.68	.64	.56
	QP($\beta\gamma$)	.99	.95	.89	1.14
(K=2)	QP($\gamma\beta$)	1.94	1.88	4.41	3.05
$\frac{4_3}{2_1}$ (K=4)	Exp.	9.87	8.26	6.22	5.19
	DC	17.80	13.09	9.20	7.29
(K=0)	QP($\beta\gamma$)	11.22	8.36	6.30	5.31
	QP($\gamma\beta$)	9.60	7.99	6.60	5.95
$\frac{0_3}{0_2}$	Exp.	1.37	1.36	1.70	1.26
	DC	2.01	2.01	2.04	2.04
	QP($\beta\gamma$)	1.57	1.39	1.71	1.35
	QP($\gamma\beta$)	1.35	1.32	1.62	1.23

^aThe state label J_i refers to the i^{th} state of spin J in the experimental spectrum (ordered by increasing energy). The K-sequence is indicated for members of the GS-band. See Figures 6.12-6.15.

$$\frac{8_1}{2_1} \equiv \frac{E(8_1) - E(0_1)}{E(2_1) - E(0_1)}$$

displayed in Table 6.6, the DC and QP model values average 16% and 24% below the experimental ratios respectively. The difficulty lies not in an inherent inability of the models to reproduce the experimental spacings of the $0_1, 2_1, 4_1, 6_1, 8_1$ sequence, but rather in the need to simultaneously reflect other features of the experimental spectra. The apparent edge of the DC model over the $(\beta\gamma)$ and $(\gamma\beta)$ versions of the QP model would probably disappear if the $J = K = 4$ state were included in the DC fitting process.

GS band $K = 2$ levels. Model levels within this sequence generally exhibit an energy pairing of adjacent even and odd spin states. This pairing, which is not manifested experimentally, may be of either of two types. The pairing types can be distinguished by the values of

$$r_J \equiv \frac{E(J) - E(J-1)}{E(J+1) - E(J)} \quad \begin{array}{l} J = 3, 5, 7, \dots \\ K = 2 \end{array} \quad (6.20)$$

The size of r_J relative to 1 determines whether the state of odd J is closer in energy to $J-1$ or to $J+1$:

$$r_J > 1 \text{ implies } J \text{ is closer to } J+1 \quad ;$$

$$r_J < 1 \text{ implies } J \text{ is closer to } J-1 \quad .$$

The $K = 2$ states of spin J and $J+1$ (J odd) develop from degenerate H'_B seed states having a common value of $[N, \lambda]$. The states remain degenerate for any γ -unstable generalized Bohr Hamiltonian. Consequently

we have

$$r_J = \infty \quad [\bar{H} = -\frac{1}{2}T + V(\beta'); \gamma\text{-unstable pairing}]$$

At the opposite extreme is the rigid rotor model which is characterized by $r_J < 1$ [Table 6.7]. For fixed J , r_J achieves its maximum value of

$$r_J = \frac{J}{J+1} \quad [\text{axially symmetric quadrupole rotor}] \quad (6.21)$$

at $\gamma_0 = 0^\circ$, and steadily decreases as γ_0 rises. Beyond $\gamma_0 = 15^\circ$, r_J drops rapidly, and the pairing of

$$(J-1, J) = (2, 3), (4, 5), \text{ and } (6, 7)$$

energies becomes visually obvious in Figure 5.5. Near $\gamma_0 = 30^\circ$, the $J-1$ state may actually rise above the J state in energy, giving rise to negative values of r_J . The DC model, which imposes γ stability, gives

Table 6.7. r_J as a function of γ_0 for a rigid quadrupole rotor

γ_0 :	3°	10°	20°	30°
r_3 :	.750	.742	.614	.375
r_5 :	.833	.802	.454	.083
r_7 :	.875	.796	.237	-.063
r_9 :	.900	.746	.048	-.167

rise to rotor-like pairing. This is particularly noticeable in the ^{190}Os and ^{192}Os applications where the optimal value of γ_0 is large.

Model and experimental values of r_3 are compared in Table 6.6 for the

osmium isotopes. The maximum rotor value, $r_3 = .75$, is exceeded by all but the DC model ratios. The QP model may exhibit either γ -stable or γ -unstable pairing depending upon the size of C_γ . In the $(\gamma\beta)$ applications, the small reduced energy of $0_2 = 0_\gamma$ requires C_γ to be very small; this results in abnormally large values of r_j . On the whole, the best rendering of GS-band $K = 2$ energies is provided by the $(\beta\gamma)$ applications of the QP model. C_γ is sufficiently large to produce the necessary splitting of the ℓ -multiplets [Figure 5.6], yet small enough to limit the extent of rotor-like pairing. Even so the model $K = 2$ energies are far from satisfactory.

GS band $K = 4$ levels. The reduced energy of the $J_i = 4_3$ state occurs consistently high in all model calculations [Table 6.6]. The error is especially large for the DC calculation, but it must be recalled that this state did not contribute to the DC fitting process. As A increases through the osmium isotopes, the reduced energies of all $J = 4$, GS-band states drop. A similar drop occurs when γ_0 is increased in the rigid rotor model; however, no value of γ_0 can account for the small experimental values of $4_2/2_1$ and $4_3/2_1$ in $^{190}, ^{192}\text{Os}$ [Table 6.8]. The ^{192}Os value of $4_3/4_1 = 1.84$ is difficult to achieve in the QP model for any set $(\beta_0, \gamma_0, C_\gamma)$. [The H_B value of $4_3/4_1 = 2$ may be lowered slightly by increasing C_γ near $(\beta_0, \gamma_0) = (0, 30^\circ)$. At $(\beta_0, \gamma_0, C_\gamma) = (0, 30^\circ, 40)$, for example, 20 and 25-phonon diagonalizations each yield $4_3/4_1 = 1.92$]. Although the experimental data is scarce, pairing difficulties also appear to plague the model calculations of $K = 4$ energies.

Table 6.8. Reduced energies of the GS band $J = 4$ states for the osmium isotopes (experiment), and for several limiting cases of $\bar{H}_{QP}$

Ratio:	$\frac{4_1}{2_1}$	$\frac{4_2}{2_1}$	$\frac{4_3}{2_1}$	$\frac{4_2}{4_1}$	$\frac{4_3}{4_1}$
^{186}Os (exp.)	3.17	7.82	9.87	2.47	3.12
^{188}Os (exp.)	3.08	6.23	8.26	2.02	2.68
^{190}Os (exp.)	2.93	5.11	6.22	1.74	2.12
^{192}Os (exp.)	2.82	4.41	5.19	1.57	1.84
H_{Bohr}	2.	3.	4.	1.5	2.
$\bar{H}_{QP} \left[\begin{array}{c} C_Y=0 \\ \beta_0=\infty \end{array} \right]$	2.5	4.5	7.	1.8	2.8
Rigid Rotor					
$\gamma_0=15^\circ$	3.27	9.27	26.73	2.83	8.17
20°	3.12	6.36	14.18	2.04	4.55
25°	2.84	5.51	8.69	1.94	3.06
30°	2.67	5.67	6.67	2.13	2.50

Table 6.9. Experimental and model values of r_5^1

	$^{186}_{Os}$	$^{188}_{Os}$	$^{190}_{Os}$	$^{192}_{Os}$
Exp.	.96	-	.73	-
DC	.85	.85	.85	.85
QP($\beta\gamma$)	1.17	1.31	1.38	2.32
QP($\gamma\beta$)	3.52	3.36	9.70	6.54

Table 6.10. r_5^1 for the rigid quadrupole rotor.

γ_0 :	3°	10°	20°	25°	30°
r_5^1 :	.830	.833	.825	.771	.583

The ratio

$$r_5^1 \equiv \frac{E(5) - E(4)}{E(6) - E(5)} \quad [K = 4 \text{ states}] \quad (6.22)$$

may be calculated experimentally only for the $A = 186$ and $A = 190$ isotopes [Table 6.9]. In each case it is less than 1. QP values are >1 due to the low strength of the optimal $C_\gamma(\gamma - \gamma_0)^2$ term. Although the DC model does poorly in locating the $J = K = 4$ states, its values of r_5^1 are not far from the experimental ones. For comparison, rigid rotor values are provided in Table 6.10.

Other bands. The need for a low-lying γ vibration is indicated by the inability of the DC calculations to produce a ratio of $0_3/0_2$ below 2 [Table 6.6]. The QP model has no difficulty in this regard. With

the exception of ^{188}Os , all model applications generally yield a $(2_3 - 0_2)$ energy spacing which is too large [Table 6.11].

Table 6.11. Experimental and model values of the energy ratio $(2_3 - 0_2)/(2_1 - 0_1)$.

	^{186}Os	^{188}Os	^{190}Os	^{192}Os
Exp.	1.07	1.42	1.09	.82
DC	1.24	1.24	1.26	1.26
QP($\beta\gamma$)	1.41	1.36	1.33	1.27
QP($\gamma\beta$)	2.14	1.94	2.00	1.71

Returning attention to Figures 6.12-6.15, the osmium model calculations may be summarized as follows. Neither the DC, QP($\beta\gamma$), or QP($\gamma\beta$) model adequately accounts for the experimental spectra. If the 0_3 and $K = 4$ energies are ignored, the DC model reasonably reproduces the remaining low-energy spectra. However this model leads to rigid-rotor-like, even-odd pairing of $K = 2$ states that is not evidenced experimentally. Even-odd pairing of GS band $K \neq 0$ energies may take either of two forms within the QP model: for large C_γ , the pairing approaches that of the rigid rotor; for small C_γ it resembles that of the γ -unstable vibrator. Attempts to interpret 0_2 as a γ vibration lead to $C_\gamma < 2.5$, and hence the latter effect dominates. The model energies of $K = 2$ and 4 states consequently bear little resemblance to experiment. One is thus led to interpret 0_3 as the γ vibration. The QP model with $C_\gamma \approx 10$ can produce 0_2 and 0_3 states near the experimentally observed energies.

In addition, GS band $K = 4$ energies can be substantially lowered below the DC values, and pairing difficulties can be reduced for the model states belonging to the $K = 2$ and 4 sequences of the GS band.

Within a given K sequence, the energy pairing of adjacent even and odd spin states does not occur in the rigid rotor model when γ_0 is small. The same result may be expected for the QP model if γ_0 is small and C_γ sufficiently large. With this in mind, the QP model was applied to the osmium nuclei with γ_0 fixed at 0° . The (γ_0) portions of Figures 6.12-6.15 display the results. When γ_0 is small, the energy of 0_γ rises very rapidly with increasing C_γ . Consequently, C_γ was found to be too small to produce a symmetric-rotor-like $K = 2$ sequence. This held true whether 0_γ was taken to be 0_2 or 0_3 . It was also discovered that the (γ_0) application could not produce the observed ordering of the 2_2 and 4_1 states in ^{192}Os .

The $(\beta\gamma)$ calculations thus appear to provide the best accounting of osmium energies available within the framework of the QP model. The H_{QP} parameters associated with the $(\beta\gamma)$ applications may be recovered by employing Equations (6.4)-(6.8). Equation (6.17) can then be used to determine BF-frame equilibrium radii $[R_x, R_y, R_z]$. Such calculations are summarized in Table 6.12. The model picture that emerges for the osmium isotopes is that of a nuclear droplet which, as A increases, becomes increasingly spherical and increasing soft to shape vibrations. That is, the addition of neutron pairs to ^{186}Os leads to decreasing deformation $[b_0]$, and increasing mass parameter $[B]$, as well as to the increasing asymmetry $[\gamma_0]$ previously noted.

Table 6.12. Basis and Hamiltonian parameters for the QP($\beta\gamma$) model applications

	$^{186}_{Os}$	$^{188}_{Os}$	$^{190}_{Os}$	$^{192}_{Os}$
$N_{\max}$ (J)	25	25	25	25
$\bar{s}$	.90	.87	.95	.95
β_o	3.08	3.20	2.59	2.81
γ_o	14.9°	21.3°	24.6°	30.0°
C_Y	8.38	9.72	14.6	9.06
$\hbar\bar{\omega}$ (MeV)	.9317	1.0226	.8040	.8540
b_{th}	2.047	2.135	1.589	1.829
D_1'	8.513	8.574	8.635	8.695
b_{ex}	.622	.550	.510	.442
$\bar{s}$	15.445	16.893	15.241	17.686
b_o	.199	.189	.170	.159
c_β (MeV)	222.3	291.8	186.8	267.1
c_Y (MeV)	7.81	9.94	11.74	7.74
$B(10^{-42} \text{ MeV-s}^2)$	110.9	120.9	125.2	158.7
R_x/R_o	.97	.98	.97	1.00
R_y/R_o	.91	.91	.93	.91
R_z/R_o	1.12	1.11	1.10	1.09

One is left with the impression that the QP Hamiltonian provides all of the ingredients [rotations of a quadrupole droplet, β and γ shape vibrations] necessary for a full accounting of the experimental levels appearing in Figures 6.12-6.15. However adjustments to the kinetic or potential energy operator are evidently required if the experimental spectra are to be accurately reproduced. The work of R. Sedlmayr et al. (63) indicates that the problem does not lie solely in the QP form of $V(\beta, \gamma)$. In their investigation of the even-even osmium isotopes, these authors employed the GG Hamiltonian of Equation (4.3). [Recall that H_{GG} contains the same kinetic term as H_{QP} , but possesses a more elaborate potential energy function.] Optimal GG model parameters were determined by fitting the low-energy experimental spectra of $^{184}, ^{186}, ^{188}, ^{190}, ^{192}\text{Os}$. Unfortunately, the resulting model energies were not tabulated in (63). However, from figures contained in that work, one gathers that the GG-model fits are similar in quality to the QP($\beta\gamma$) ones and exhibit the same shortcomings. GG-model $B(E2)$ values and quadrupole moments were tabulated and these are compared with DC and QP model values in Tables E.13-E.16. As in the present work, Sedlmayr et al. found increasing asymmetry and decreasing deformation for the heavier osmium isotopes. These trends also emerge in the work of Kumar and Baranger (64) when collective (quadrupole) Hamiltonians appropriate to the osmium nuclei are deduced from microscopic calculations.

We are thus led to expect that the most profitable modifications of H_{QP} will involve alterations of the kinetic energy operator, $T(\beta, \gamma, \theta_i)$. This is not unanticipated as T was originally deduced (4) by considering

small amplitude oscillations about spherical equilibrium. In the present work T has been retained even when a sharp minimum in $V_{QP}(\beta, \gamma)$ forces a decidedly non-spherical equilibrium shape. Under such circumstances, higher order terms in the kinetic energy operator should probably be incorporated into the model. As may be seen from the rigid rotor limit, small changes in the Bohr moments of inertia, particularly near axial symmetry, can induce a large change in the resulting spectra. In light of the odd-even pairing difficulties encountered in the QP model applications, modifications to the dynamical moments of inertia would not be unwelcome. It is comforting to note that such modifications of the quadrupole Hamiltonian would not seriously inhibit our ability to solve the associated Schroedinger Equation. The intrinsic-coordinate eigenfunctions, ψ_α , and the expansion techniques developed and refined in this thesis could continue to be of service.

VII. APPENDIX A: SYMMETRIES IN THE $(\beta, \gamma, \theta_i)$ REPRESENTATION

A. Collective Coordinates

The collective coordinates $(\beta, \gamma, \theta_i)$ were defined in Chapter II. Let us briefly review the defining procedure outlined there. We assume that any precise measurement of the entire nuclear boundary by a laboratory [LAB] observer results in a surface of the form

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\mu=-2}^2 \alpha_{\mu} Y_{2\mu}^*(\theta, \phi) \right] \quad . \quad (A.1)$$

Physically the radius $R(\theta, \phi)$ [from the center of mass to the boundary, along the ray specified by the LAB polar angles θ and ϕ] must be real. Consequently the generalized coordinates α_{μ} must satisfy

$$\alpha_{\mu}^* = (-1)^{\mu} \alpha_{\mu} \quad . \quad (A.2)$$

The distinct [LAB] quadrupole surfaces are in one-to-one correspondence with the distinct sets $\{\alpha_{\mu}: \mu = -2, -1, \dots, 2\}$ satisfying Equation (A.2). The Bohr coordinates are introduced by specifying a rotation that takes the LAB reference axes into coincidence with a set of principal axes of the quadrupole droplet. In such a principal-axis frame [BF frame], the nuclear surface can be expressed as

$$R(\theta', \phi') = R_0 \left[1 + \sum_{\mu} a_{\mu} Y_{2\mu}^*(\theta', \phi') \right] \quad , \quad (A.3)$$

where the a_{μ} are real and obey

$$a_1 = a_{-1} = 0 \quad ; \quad a_2 = a_{-2} \quad . \quad (A.4)$$

The LAB and BF surface coordinates are related by

$$a_v = \sum_{\mu} D_{\mu v}^2(\theta_i) \alpha_{\mu} \quad , \quad (\text{A.5})$$

where θ_i are the LAB Euler angles specifying the LAB→BF rotation. The nuclear surface as seen by a BF observer is completely specified by two real coordinates, a_0 and a_2 . The shape parameters β and γ may be equivalently used for this purpose:

$$\begin{aligned} a_0 &= \beta \cos \gamma & 0 \leq \beta < \infty \\ a_2 &= \frac{\beta}{\sqrt{2}} \sin \gamma & 0 \leq \gamma < 2\pi \end{aligned} \quad (\text{A.6})$$

The meaning of the two shape parameters is illustrated graphically by Figures A.1 and A.2. β is seen to measure the overall deviation from sphericity, while γ determines the degree of rotational asymmetry about the BF z-axis.

There are 24 distinct ways of selecting right-handed sets of principal axes for the droplet. In any one of these possible BF frames, Equations (A.3) and (A.4) hold. Consequently any one of 24 sets $\{\beta, \gamma, \theta_i\}$ can be used to specify the surface determined by a given set $\{\alpha_{\mu}\}$. This under-specification of the Bohr coordinates leads to several symmetry relations for the eigenfunctions $\psi_{N\ell v J M}^S(\beta, \gamma, \theta_i)$. In Appendix B of Reference (22), symmetry relations were deduced by first enumerating the 24 rotations which connect possible BF frames. This led to three independent symmetries of the $\psi_{N\ell v J M}^S$. In this appendix, a different approach is used and a fourth symmetry is discovered.

Figure A.1. Effect of increasing β . In this series of drawings γ is fixed at 20° and β takes on the values 0, 0.3, 0.6, 0.8, and 1.0, respectively, from left to right. In each case the surface is viewed from the point $(x,y,z) = (1,2,2)$ in the body-fixed (BF) frame, and the z axis is upward

Figure A.2. Effect of increasing γ . Here β is fixed at 0.8 and, from left to right, γ runs through the values 0° , 15° , 30° , 45° , and 60° . Again the viewing point is $(x, y, z) = (1, 2, 2)$. Notice that the $\gamma = 0^\circ$ surface has axial symmetry about the z direction

B. A Symmetry of $\psi_{N\ell\nu JM}^S(\alpha)$

In the creation/destruction operator representation [Figure 2.1], eigenstates of H_B may be constructed by operating on the vacuum state $|0\rangle$ with a series of creation operators. The general eigenstate $|N\ell\nu JM\rangle$ of Equation (2.21) belongs to the $[N]$ symmetric IR of $U(5)$, and may consequently be written as

$$|N\ell\nu JM\rangle = \sum_{\nu} A(\nu) [b_2^+]^{\nu_2} [b_1^+]^{\nu_1} \dots [b_{-2}^+]^{\nu_{-2}} |0\rangle, \quad (A.7)$$

where the $A(\nu)$ are constants, and the exponents ν_i satisfy

$$\sum_{i=-2}^2 \nu_i = N. \quad (A.8)$$

Recalling Equation (2.24) and Figure 2.1, we find that we may write Equation (A.7) in the α -coordinate representation by making the replacements

$$|0\rangle \rightarrow \langle\alpha|0\rangle = \exp -\frac{1}{2} \sum_{\mu} (-1)^{\mu} \alpha_{\mu}^{\dagger} \alpha_{-\mu}^{\dagger}, \quad (A.9)$$

$$b_{\mu}^{\dagger} \rightarrow \frac{1}{\sqrt{2}} \left[\alpha_{\mu}^{\dagger} - (-1)^{\mu} \frac{\partial}{\partial \alpha_{-\mu}^{\dagger}} \right],$$

$$\alpha_{\mu}^{\dagger} \equiv \left[\frac{BC}{\hbar^2} \right]^{\frac{1}{4}} \alpha_{\mu}.$$

This results in¹

¹ H_B is assumed to be given by Equations (2.7)-(2.10); thus the upper label on ψ is $s = [BC/\hbar^2]^{\frac{1}{4}}$.

$$\begin{aligned}
\psi_{N\ell\nu JM}^S(\underline{\alpha}) &= \langle \underline{\alpha} | N\ell\nu JM \rangle \\
&= 2^{-N/2} \sum_{\underline{\nu}} A(\underline{\nu}) \left\{ \left[\alpha'_2 - \frac{\partial}{\partial \alpha'_{-2}} \right]^{v_2} \left[\alpha'_1 + \frac{\partial}{\partial \alpha'_{-1}} \right]^{v_1} \dots \right. \\
&\quad \left. \left[\alpha'_{-2} - \frac{\partial}{\partial \alpha'_2} \right]^{v_{-2}} \right\} \langle \underline{\alpha} | 0 \rangle .
\end{aligned} \tag{A.10}$$

Under the inversion $\underline{\alpha} \rightarrow -\underline{\alpha}$, $\langle \underline{\alpha} | 0 \rangle$ is unaltered, and the expression in braces in the above equation is unchanged except for multiplication by the phase factor

$$(-1)^{\sum v_i} = (-1)^N = (-1)^\ell .$$

The last equality follows from the $U(5) \supset R(5)$ branching rule, Equation (2.33). Hence we conclude

$$\psi_{N\ell\nu JM}^S(-\underline{\alpha}) = (-1)^\ell \psi_{N\ell\nu JM}^S(\underline{\alpha}) . \tag{A.11}$$

C. Symmetries of $\psi_{N\ell\nu JM}^S(\beta, \gamma, \theta_i)$

Transformations of the coordinates $(\beta, \gamma, \theta_i)$ which leave the $\alpha_\mu(\beta, \gamma, \theta_i)$ either unchanged or multiplied by (-1) will lead to symmetry relations of the $\psi_{N\ell\nu JM}^S(\beta, \gamma, \theta_i)$. These symmetries are based on the identities

$$\psi_{N\ell\nu JM}^S(\underline{\alpha}) = \psi_{N\ell\nu JM}^S(\underline{\alpha}) \quad [\text{Type 1}] \tag{A.12a}$$

$$\psi_{N\ell\nu JM}^S(-\underline{\alpha}) = (-1)^\ell \psi_{N\ell\nu JM}^S(\underline{\alpha}) \quad [\text{Type 2}] . \tag{A.12b}$$

Suppose that $(\beta, \gamma, \theta_i)$ and $(\bar{\beta}, \bar{\gamma}, \bar{\theta}_i)$ are two sets of Bohr coordinates, and that α and $\bar{\alpha}$ are their associated surface expansion coefficients. The latter are uniquely determined from the former by Equations (A.6) and

$$\alpha_\mu = \sum_{\nu} D_{\mu\nu}^{2*}(\theta_i) a_\nu \quad . \quad (\text{A.13})$$

From Equations (A.12) we then have

$$\alpha = \bar{\alpha} \text{ implies } \psi_{N\ell\nu JM}^S(\beta, \gamma, \theta_i) = \psi_{N\ell\nu JM}^S(\bar{\beta}, \bar{\gamma}, \bar{\theta}_i) \quad [\text{Type 1}] \quad (\text{A.14a})$$

$$\alpha = -\bar{\alpha} \text{ implies } \psi_{N\ell\nu JM}^S(\beta, \gamma, \theta_i) = (-1)^\ell \psi_{N\ell\nu JM}^S(\bar{\beta}, \bar{\gamma}, \bar{\theta}_i) \quad [\text{Type 2}]. \quad (\text{A.14b})$$

It now remains to discover coordinate transformations

$$\bar{\beta} = \bar{\beta}(\beta, \gamma, \theta_i) \quad , \quad \bar{\gamma} = \bar{\gamma}(\beta, \gamma, \theta_i) \quad , \quad \bar{\theta}_i = \bar{\theta}_i(\beta, \gamma, \theta_i) \quad (\text{A.15})$$

belonging to each of the two types. We consider only those coordinate transformations which satisfy $\alpha = \bar{\alpha}$ or $\alpha = -\bar{\alpha}$ for all values of $(\beta, \gamma, \theta_i)$. Initially, it proves convenient to employ the equivalent collective coordinates (a_0, a_2, θ_i) and $(\bar{a}_0, \bar{a}_2, \bar{\theta}_i)$ in place of $(\beta, \gamma, \theta_i)$ and $(\bar{\beta}, \bar{\gamma}, \bar{\theta}_i)$ respectively. We begin with

$$\alpha_\mu = e^{i\eta} \bar{\alpha}_\mu \quad \eta = \begin{cases} 0 & [\text{Type 1}] \\ \pi & [\text{Type 2}] \end{cases} \quad . \quad (\text{A.16})$$

By virtue of Equation (A.13) this may be rewritten as

$$\sum_{\nu} D_{\mu\nu}^{2*}(\theta_i) a_\nu = e^{i\eta} \sum_{\nu} D_{\mu\nu}^{2*}(\bar{\theta}_i) \bar{a}_\nu \quad , \quad (\text{A.17})$$

where the a_v and $\bar{a}_v$ satisfy Equations (A.4) independently. To proceed further we must assume a relationship between the $\underline{\theta}$ and the $\bar{\underline{\theta}}$. For example¹

$$\bar{\underline{\theta}} = \underline{\theta} \cdot \underline{\phi} \quad , \quad (\text{A.18})$$

where $\underline{\phi} = (\phi_1, \phi_2, \phi_3)$ is constant and the product is R(3) group multiplication. That is, $\bar{\underline{\theta}}$ specifies the active rotation, $R(\bar{\underline{\theta}})$, which is equivalent to the successive application of $R(\underline{\phi})$ followed by $R(\underline{\theta})$.

Equation (A.18) has an immediate interpretation. When

$\underline{\theta}$ specifies the LAB $\rightarrow$ BF rotation as parameterized by LAB,

$\bar{\underline{\theta}}$ specifies the LAB $\rightarrow \overline{\text{BF}}$ rotation as parameterized by LAB,

and $\underline{\phi}$ specifies the BF $\rightarrow \overline{\text{BF}}$ rotation as parameterized by BF,

Equation (A.18) can be shown to hold [see Appendix F]. Furthermore, we have

$$D_{\mu\nu}^{2*}(\bar{\theta}_i) = \sum_{\epsilon} D_{\mu\epsilon}^{2*}(\theta_i) D_{\epsilon\nu}^{2*}(\phi_i) \quad , \quad (\text{A.19})$$

since the rotation matrices realize the group multiplication. Substituting Equation (A.19) into Equation (A.17), multiplying by $D_{\mu\nu}^2(\theta_i)$, and integrating over the space of the Euler angles (θ_i) leads to

$$a_{\nu'} = e^{i\eta} \sum_{\nu} D_{\nu'\nu}^{2*}(\phi_i) \bar{a}_{\nu} \quad . \quad (\text{A.20})$$

¹The alternate assumption $\bar{\underline{\theta}} = \underline{\phi} \cdot \underline{\theta}$ leads to $D_{\mu\mu'}^2(\phi_i) \propto \delta_{\mu\mu'}$, and consequently results in no transformations that cannot be found by pursuing Equation (A.18).

Inverting and employing $a_{-\mu} = (-1)^\mu a_\mu$ then yields

$$\bar{a}_\mu = e^{-i\eta} \sum_{\nu \geq 0} \frac{[D_{\nu\mu}^2(\phi_i) + (-1)^\nu D_{-\nu\mu}^2(\phi_i)]}{(1 + \delta_{\nu,0})} a_\nu \quad . \quad (\text{A.21})$$

When $\mu = \pm 1$ in Equation (A.21), we may use $\bar{a}_{\pm 1} = a_{\pm 1} = 0$ and the assumed arbitrariness of a_0 and a_2 to deduce

$$\boxed{D_{\nu,\pm 1}^2(\phi_i) + D_{-\nu,\pm 1}^2(\phi_i) = 0 \quad ; \quad \nu = 0, 2} \quad . \quad (\text{A.22})$$

A weaker but more general condition may be deduced by substituting Equation (A.21) into each side of $\bar{a}_{-\mu} = (-1)^\mu \bar{a}_\mu$, and then invoking the arbitrariness of a_0 and a_2 :

$$\boxed{D_{\nu,\mu}^2(\phi_i) + D_{-\nu,\mu}^2(\phi_i) = (-1)^\mu [D_{\nu,-\mu}^2(\phi_i) + D_{-\nu,-\mu}^2(\phi_i)] ; \begin{matrix} \nu = 0, 2 \\ \text{all } \mu \end{matrix}} \quad . (\text{A.23})$$

Notice that the boxed equations, which determine the possible connections between $\underline{\theta}$ and $\bar{\underline{\theta}}$, are independent of $e^{i\eta}$ and hence are independent of transformation type.

Due to the rotation matrix symmetry $D_{m',m}^{J*}(\phi_i) = (-1)^{m'-m} D_{-m',-m}^J(\phi_i)$, the two boxed equations yield only four independent conditions on ϕ .

These may be taken to be

$$D_{0,1}^2(\phi_i) = 0 \quad , \quad (\text{A.24a})$$

$$D_{2,1}^2(\phi_i) + D_{-2,1}^2(\phi_i) = 0 \quad , \quad (\text{A.24b})$$

$$D_{0,2}^2(\phi_i) = D_{0,-2}^2(\phi_i) \quad , \quad \text{and} \quad (\text{A.24c})$$

$$D_{2,2}^2(\phi_i) + D_{-2,2}^2(\phi_i) = D_{2,-2}^2(\phi_i) + D_{-2,-2}^2(\phi_i) \quad . \quad (\text{A.24d})$$

At this point we may employ the factored form of the rotation matrices

$$D_{m',m}^J(\phi_i) = e^{-im'\phi_1} d_{m',m}^J(\phi_2) e^{-im\phi_3} \quad (\text{A.25})$$

and insert explicit forms for the $d_{m',m}^2(\phi_2)$. For example, Equation (A.24a) becomes [see Figure F.1]

$$e^{-i\phi_3} d_{01}^2(\phi_2) = e^{-i\phi_3} \left[\frac{\sqrt{6}}{2} \sin \phi_2 \cos \phi_2 \right] = 0 \quad ,$$

implying that $\phi_2 = 0, \frac{\pi}{2}$, or π . In a straightforward manner, 24 distinct rotations ϕ may be found which are simultaneous solutions of Equations (A.24). These have been listed in Table A.1. In every case the $\overline{BF}$ axes defined by

$$R(\phi): BF \rightarrow \overline{BF}$$

may be obtained by a relabeling of the BF axes. For each solution ϕ , Table A.1 specifies the relationship between the BF and $\overline{BF}$ coordinates of an arbitrary point $[(x, y, z) \text{ and } (\bar{x}, \bar{y}, \bar{z}) \text{ respectively}]$.

The rotation ϕ relates $\bar{u}$ to u through Equation (A.18). The corresponding relationship between $(\bar{\beta}, \bar{\gamma})$ and (β, γ) is deduced from Equation (A.21) which may be written more explicitly as

$$e^{i\eta} a_0^- = \left[\frac{3}{2} \cos^2 \phi_2 - \frac{1}{2} \right] a_0 + \left[\frac{\sqrt{6}}{4} \sin^2 \phi_2 (e^{-2i\phi_1} + e^{2i\phi_1}) \right] a_2, (\text{A.26a})$$

and

$$e^{i\eta^-} a_2 = \left[\frac{\sqrt{6}}{4} \sin^2 \phi_2 e^{-2i\phi_3} \right] a_0 + \frac{1}{4} \left[(1 + \cos \phi_2)^2 e^{-2i(\phi_1 + \phi_3)} + (1 - \cos \phi_2)^2 e^{2i(\phi_1 - \phi_3)} \right] a_2 \quad . \quad (\text{A.26b})$$

In the case $\phi = (0, \frac{1}{2}\pi, \frac{1}{2}\pi)$, for example, the above two equations become

$$e^{i\eta^-} a_0 = -\frac{1}{2} a_0 + \frac{\sqrt{6}}{2} a_2 \quad \text{and}$$

$$e^{i\eta^-} a_2 = \left(\frac{-\sqrt{6}}{4} \right) a_0 - \frac{1}{2} a_2 \quad .$$

In terms of the shape parameters we have

$$e^{i\eta^-} \cos \bar{\gamma} = -\frac{1}{2} \beta \cos \gamma + \frac{\sqrt{3}}{2} \beta \sin \gamma = \beta \cos \left[\gamma - \frac{2\pi}{3} \right] \quad \text{and}$$

$$e^{i\eta^-} \sin \bar{\gamma} = -\frac{\sqrt{3}}{2} \beta \cos \gamma - \frac{1}{2} \beta \sin \gamma = \beta \sin \left[\gamma - \frac{2\pi}{3} \right] \quad .$$

For the type 1 transformation [$e^{i\eta} = +1$], we thus conclude

$$\bar{\beta} = \beta \quad , \quad \bar{\gamma} = \gamma - \frac{2\pi}{3} \quad [\text{Type 1} \quad ; \quad \phi = (0, \frac{1}{2}\pi, \frac{1}{2}\pi)] \quad .$$

To find the associated type 2 transformation, it is helpful to first recall the trigonometric identities $\sin(a + \pi) = -\sin(a)$ and $\cos(a + \pi) = -\cos(a)$. We may then write immediately

$$\bar{\beta} = \beta \quad , \quad \bar{\gamma} = \gamma - \frac{2\pi}{3} + \pi \quad [\text{Type 2} \quad ; \quad \phi = (0, \frac{1}{2}\pi, \frac{1}{2}\pi)] \quad .$$

For each of the 24 rotations ϕ , there is one type 1 and one type 2 Bohr-coordinate transformation for which Equation (A.16) holds. For the type 1 transformations [Table A.1]

$$\bar{\beta} = \beta \quad , \quad \text{and}$$

Table A.1. Enumeration of the 24 distinct type I coordinate transformations. In all cases $\bar{\beta} = \beta$. As the fourth column indicates, every transformation may be generated by the successive application of three basic transformations (marked by *). The group of 24 transformations is isomorphic with the octahedral group. The last column relates the cartesian coordinates of two frames, BF and $\overline{\text{BF}}$, connected by ϕ : $\text{BF} \rightarrow \overline{\text{BF}}$.

	(ϕ_1, ϕ_2, ϕ_3) $\text{BF} \rightarrow \overline{\text{BF}}$	$\bar{\gamma}$	Expression in terms of generators	$(\bar{x}, \bar{y}, \bar{z})$
1	(0, 0, 0)	γ	$R_1^2 = R_2^4 = R_3^3$	(x, y, z)
2	$(-\frac{1}{2}\pi, \frac{1}{2}\pi, \frac{1}{2}\pi)$	$-\gamma - 2\pi/3$	$R_1 R_2 R_3^2$	(x, z, -y)
3*	$(-\frac{1}{2}\pi, \pi, \frac{1}{2}\pi)$	γ	R_1	(x, -y, -z)
4	$(\frac{1}{2}\pi, \frac{1}{2}\pi, -\frac{1}{2}\pi)$	$-\gamma - 2\pi/3$	$R_2 R_3^2$	(x, -z, y)
5	(0, π , 0)	γ	$R_1 R_2^2$	(-x, y, -z)
6	$(\frac{1}{2}\pi, \frac{1}{2}\pi, \frac{1}{2}\pi)$	$-\gamma - 2\pi/3$	$R_2^3 R_3^2$	(-x, z, y)
7	(π , 0, 0)	γ	R_2^2	(-x, -y, z)
8	$(-\frac{1}{2}\pi, \frac{1}{2}\pi, -\frac{1}{2}\pi)$	$-\gamma - 2\pi/3$	$R_1 R_2^3 R_3^2$	(-x, -z, -y)
9	$(-\frac{1}{2}\pi, \pi, 0)$	$-\gamma$	$R_1 R_2$	(y, x, -z)
10*	(0, $\frac{1}{2}\pi$, $\frac{1}{2}\pi$)	$\gamma - 2\pi/3$	R_3	(y, z, x)
11*	$(\frac{1}{2}\pi, 0, 0)$	$-\gamma$	R_2	(y, -x, z)
12	(π , $\frac{1}{2}\pi$, $-\frac{1}{2}\pi$)	$\gamma - 2\pi/3$	$R_1 R_3$	(y, -z, -x)
13	(0, 0, $-\frac{1}{2}\pi$)	$-\gamma$	R_2^3	(-y, x, z)
14	(π , $\frac{1}{2}\pi$, $\frac{1}{2}\pi$)	$\gamma - 2\pi/3$	$R_1 R_2^2 R_3$	(-y, z, -x)
15	$(\frac{1}{2}\pi, \pi, 0)$	$-\gamma$	$R_1 R_2^3$	(-y, -x, -z)
16	(0, $\frac{1}{2}\pi$, $-\frac{1}{2}\pi$)	$\gamma - 2\pi/3$	$R_2^2 R_3$	(-y, -z, x)
17	$(\frac{1}{2}\pi, \frac{1}{2}\pi, \pi)$	$\gamma + 2\pi/3$	R_3^2	(z, x, y)
18	(π , $\frac{1}{2}\pi$, π)	$-\gamma + 2\pi/3$	$R_1 R_2 R_3$	(z, y, -x)
19	$(-\frac{1}{2}\pi, \frac{1}{2}\pi, \pi)$	$\gamma + 2\pi/3$	$R_1 R_3^2$	(z, -x, -y)
20	(0, $\frac{1}{2}\pi$, π)	$-\gamma + 2\pi/3$	$R_2 R_3$	(z, -y, x)
21	$(-\frac{1}{2}\pi, \frac{1}{2}\pi, 0)$	$\gamma + 2\pi/3$	$R_1 R_2^2 R_3^2$	(-z, x, -y)
22	(0, $\frac{1}{2}\pi$, 0)	$-\gamma + 2\pi/3$	$R_2^3 R_3$	(-z, y, x)
23	$(\frac{1}{2}\pi, \frac{1}{2}\pi, 0)$	$\gamma + 2\pi/3$	$R_2^2 R_3^2$	(-z, -x, y)
24	(π , $\frac{1}{2}\pi$, 0)	$-\gamma + 2\pi/3$	$R_1 R_2^3 R_3$	(-z, -y, -x)

$$\bar{\gamma} = \text{one of } \{\pm\gamma, \pm\gamma \pm \frac{2\pi}{3}\} .$$

Corresponding to each type 1 transformation there exists a type 2 transformation given by

$$\begin{aligned}\phi_{\text{type 2}} &= \phi_{\text{type 1}} \\ \bar{\beta}_{\text{type 2}} &= \bar{\beta}_{\text{type 1}} \\ \bar{\gamma}_{\text{type 2}} &= \bar{\gamma}_{\text{type 1}} + \pi\end{aligned} \quad . \quad (\text{A.27})$$

All type 1 transformations may be generated by the successive application of three basic ones:

$$R_1: \quad \phi = (-\frac{1}{2}\pi, \pi, \frac{1}{2}\pi) \quad \bar{\beta} = \beta \quad \bar{\gamma} = \gamma \quad , \quad (\text{A.28a})$$

[Rotation through π
about BF x-axis]

$$R_2: \quad \phi = (\frac{1}{2}\pi, 0, 0) \quad \bar{\beta} = \beta \quad \bar{\gamma} = -\gamma \quad , \quad (\text{A.28b})$$

[Rotation through $\frac{1}{2}\pi$
about BF z-axis]

$$R_3: \quad \phi = (0, \frac{1}{2}\pi, \frac{1}{2}\pi) \quad \bar{\beta} = \beta \quad \bar{\gamma} = \gamma - \frac{2\pi}{3} \quad . \quad (\text{A.28c})$$

[Rotation through $\frac{2\pi}{3}$
about BF $(\hat{x}+\hat{y}+\hat{z})$ direction]

All type 2 transformations may be generated by combining these three with

$$R_4: \quad \phi = (0, 0, 0) \quad \bar{\beta} = \beta \quad \bar{\gamma} = \gamma + \pi \quad . \quad (\text{A.28d})$$

Each of the R_i leads to an independent symmetry of the Bohr eigenfunctions. If we write $\psi_{N\ell v J M}^S$ in the factored form of Equation (2.25)

$$\psi_{N\ell v J M}^S(\beta, \gamma, \theta_i) = F_{N\ell}(\beta) \phi_{\ell v J M}(\gamma, \theta_i) \quad , \quad F_{N\ell}(\beta) = s^{5/2} f_{N\ell}(s\beta) \quad , (\text{A.29})$$

and expand the angular factor in rotation matrices¹

$$\Phi_{\ell\nu JM}(\gamma, \theta_i) = \sum_{J', M', K} g_{\ell\nu J' M' K}^{\eta}(\gamma) D_{M' K}^{J' \star}(\theta_i) = \sum_{K=-J}^J g_{\ell\nu JK}^{\eta}(\gamma) D_{MK}^{J \star}(\theta_i), \quad (\text{A.30})$$

the symmetries of ψ may be expressed as symmetries of g^{η} . Equations (A.14), (A.19), (A.29), (A.30), and $\bar{\beta} = \beta$ give rise to

$$g_{\ell\nu JK}^{\eta}(\gamma) = \left[\sum_{K'=-J}^J g_{\ell\nu JK'}^{\eta}(\bar{\gamma}) D_{KK'}^{J \star}(\phi_i) \right] \times \begin{cases} 1 & (\text{type 1}) \\ (-1)^{\ell} & (\text{type 2}) \end{cases}. \quad (\text{A.31})$$

Evaluating the right hand side of the above equation for each of the four basic symmetries yields

$$R_1: g_{\ell\nu JK}^{\eta}(\gamma) = (-1)^J g_{\ell\nu J, -K}(\gamma), \quad (\text{A.32a})$$

$$R_2: = e^{iK\pi/2} g_{\ell\nu JK}(-\gamma), \quad (\text{A.32b})$$

$$R_3: = \sum_{K'} g_{\ell\nu JK'}^{\eta}(\gamma - \frac{2\pi}{3}) D_{KK'}^{J \star}(0, \frac{1}{2}\pi, \frac{1}{2}\pi), \quad (\text{A.32c})$$

$$R_4: = (-1)^{\ell} g_{\ell\nu JK}(\gamma + \pi). \quad (\text{A.32d})$$

The first two properties may be used to rewrite the last sum in Equation (A.30)

$$\Phi_{\ell\nu JM}(\gamma, \theta_i) = \sum_{\substack{K \geq 0 \\ \text{even}}}^J g_{\ell\nu JK}^{\eta}(\gamma) \frac{D_{MK}^{J \star}(\theta_i) + (-1)^J D_{M, -K}^{J \star}(\theta_i)}{(1 + \delta_{K, 0})}. \quad (\text{A.33})$$

¹From the assumed angular momentum character (JM) of $\psi_{N\ell\nu JM}$, it is easily shown that only $(J'M') = (JM)$ contributes to the sum in Equation (A.30), and that the g coefficient must be independent of M .

Figure A.3. Illustration of surface symmetries. From left to right, the top row of drawings depicts the surfaces (β, γ) , $(\beta, -\gamma)$, and $(\beta, \gamma - 120^\circ)$ as seen from the BF point $(x, y, z) = (1, 2, 2)$. Here $\beta = 0.9$ and $\gamma = 20^\circ$. The prime meridian and semiequator have been drawn as double lines to aid orientation. Directly below each drawing is a second view of the same surface from a rotated vantage point (x', y', z') . The new vantage point is determined by $\underline{x}' = R_i^{-1} \underline{x}$ where the R_i ($i=1, 2, 3$) are the rotational parts of Equations (A.28). From left to right R_1 , R_2 , and R_3 have been applied to obtain $(x', y', z') = (x, -y, -z)$, $(y, -x, z)$, and (y, z, x) , respectively. The three surface views of the bottom row can be seen to be identical to the initial view at top left. Thus the surfaces of the top row are not distinct in the sense that they may be rotated into one another. Furthermore, the rotation R_1 takes the top left surface into itself

Equation (A.32a) indicates that $K = 0$ does not contribute to the above sum when J is odd.

Type I transformational symmetries arise from our ability to parameterize a given quadrupole surface with different sets of Bohr coordinates. BF frame surfaces [Equation (A.3)] determined by (β, γ) , $(\beta, -\gamma)$, and $(\beta, \gamma - \frac{2\pi}{3})$ are consequently equivalent in the sense that they may be rotated into one another. This is illustrated in Figure A.3. If $V(\beta, \gamma)$ is the collective potential energy function for a homogeneous nuclear droplet, we expect

$$V(\beta, \gamma) = V(\bar{\beta}, \bar{\gamma}) \quad (\text{A.34})$$

for type I transformations, or more specifically

$$V(\beta, \gamma) = V(\beta, -\gamma) = V(\beta, \gamma - \frac{2\pi}{3}) \quad \left[\begin{array}{c} \text{quadrupole} \\ \text{surface} \\ \text{symmetries} \end{array} \right] . \quad (\text{A.35})$$

When $V(\beta, \gamma)$ is specified on $0 \leq \beta \leq \infty$, $0 \leq \gamma \leq \pi/3$, Equation (A.35) serves to define it elsewhere. The R_4 operation $\gamma \rightarrow \bar{\gamma} = \gamma + \pi$ reflects the nuclear surface through a sphere of radius R_0 . We have no a priori expectation that such an operation should leave the potential energy unchanged.

D. Symmetries of the γ Probability Density

The γ -coordinate probability density [see Equation (2.42)] of the normalized Bohr eigenfunction $\psi_{N\ell vJM}(\beta, \gamma, \theta_i)$ is given by

$$P(\gamma) = \frac{|\sin 3\gamma|}{8\pi^2} \int_0^\infty \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} \psi_{N\ell\nu JM}^* \psi_{N\ell\nu JM} \beta^4 \sin \theta_2 d\beta d\theta_1 d\theta_2 d\theta_3. \quad (A.36)$$

$\beta \quad \theta$

In this section we show that $P(\gamma) = P(\bar{\gamma})$, where $\bar{\gamma}$ is any of the possibilities arising in the type 1 or type 2 coordinate transformations. If Equations (A.29) and (A.30) are substituted into Equation (A.36), and the integrations are performed, we find

$$P(\gamma) = \frac{|\sin 3\gamma|}{(2J+1)} \sum_{K=-J}^J g_{\ell\nu JK}^{\eta*}(\gamma) g_{\ell\nu JK}^{\eta}(\gamma). \quad (A.37)$$

$g_{\ell\nu JK}^{\eta}$ is a real-valued function, and the complex conjugation is retained here for later convenience. Equation (A.31) is now used in the above equation:

$$\begin{aligned} P(\gamma) &= \frac{|\sin 3\gamma|}{2J+1} \sum_K \left[\sum_{K'} g_{\ell\nu JK'}^{\eta*}(\bar{\gamma}) D_{KK'}^J(\phi_i) \right] \begin{Bmatrix} 1 \\ (-1)^\ell \end{Bmatrix} \\ &\quad \left[\sum_{K''} g_{\ell\nu JK''}^{\eta}(\bar{\gamma}) D_{KK''}^{J*}(\phi_i) \right] \begin{Bmatrix} 1 \\ (-1)^\ell \end{Bmatrix} \\ &= \frac{|\sin 3\gamma|}{2J+1} \sum_{K'K''} g_{\ell\nu JK'}^{\eta*}(\bar{\gamma}) g_{\ell\nu JK''}^{\eta}(\bar{\gamma}) \underbrace{\left[\sum_K D_{KK'}^J(\phi_i) D_{KK''}^{J*}(\phi_i) \right]}_{\delta_{K',K''}} \\ &= \frac{|\sin 3\gamma|}{|\sin 3\bar{\gamma}|} P(\bar{\gamma}) \\ &= P(\bar{\gamma}) \end{aligned} \quad (A.38)$$

The last equality may be verified by evaluating $|\sin 3\gamma|/|\sin 3\bar{\gamma}|$ for

each possible type 1 or type 2 transformation. The independent symmetries of $P(\gamma)$ may be found by considering Equation (A.38) for each of the R_i :

$$P(\gamma) = P(-\gamma) = P(\gamma - \frac{2\pi}{3}) = P(\gamma + \pi) \quad . \quad (A.39)$$

The specification of $P(\gamma)$ on $0 \leq \gamma \leq \pi/6$ thus serves to define $P(\gamma)$ everywhere on $0 \leq \gamma \leq 2\pi$.

E. Effects of Reflecting $V(\beta, \gamma)$ About $\gamma = 30^\circ$

Let

$$H = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \quad (A.40a)$$

be a generalized Bohr Hamiltonian. $V(\beta, \gamma)$ is assumed to possess the quadrupole surface symmetries [Equation (A.35)] but is otherwise arbitrary. We can define a related Hamiltonian by retaining the kinetic term of H and replacing $V(\beta, \gamma)$ by its reflection about $\gamma = 30^\circ$:

$$H' = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + V'(\beta, \gamma) \quad (A.40b)$$

$$V'(\beta, \gamma) \equiv V(\beta, \frac{\pi}{3} - \gamma) \quad .$$

It may be easily shown that $V'(\beta, \gamma)$ so defined must also obey the quadrupole surface symmetries, and that

$$V'(\beta, \gamma) \equiv V(\beta, \gamma + \pi)$$

is an equivalent definition of V' . We now show that for every eigenfunction ϕ of H , there is an associated eigenfunction ϕ' of H' with the

same energy E . In the Schrodinger equation for H ,

$$H\phi(\beta, \gamma, \theta_i) = E\phi(\beta, \gamma, \theta_i) \quad , \quad (A.41a)$$

we make the change of variable $\gamma' = \gamma - \pi$. From the form of T [Equation (2.11)] and

$$\sin(\gamma - a) = \sin(\gamma' + \pi - a) = -\sin(\gamma' - a)$$

$$\sin(3\gamma) = \sin(3\gamma' + 3\pi) = -\sin(3\gamma')$$

$$\frac{\partial}{\partial \gamma} = \frac{\partial}{\partial \gamma'}$$

we deduce that the change of variable results in

$$\left[\frac{-\hbar^2}{2B} T(\beta, \gamma', \theta_i) + V(\beta, \gamma' + \pi) \right] \phi(\beta, \gamma' + \pi, \theta_i) = E\phi(\beta, \gamma' + \pi, \theta_i) \quad . \quad (A.41b)$$

Deleting the prime on the (dummy) variable γ' then yields

$$H'\phi(\beta, \gamma + \pi, \theta_i) = E\phi(\beta, \gamma + \pi, \theta_i) \quad .$$

Consequently, if $\phi(\beta, \gamma, \theta_i)$ is an eigenfunction of H with eigenvalue E , then

$$\phi'(\beta, \gamma, \theta_i) = \phi(\beta, \gamma + \pi, \theta_i) \quad (A.42)$$

is an eigenfunction of H' with eigenvalue E . Furthermore if ϕ has the expansion

$$\phi(\beta, \gamma, \theta_i) = \sum_{\alpha} a_{\alpha} \psi_{\alpha}^S(\beta, \gamma, \theta_i) \quad , \quad \alpha = (N_{\alpha}, \ell_{\alpha}, \nu_{\alpha}, J_{\alpha}, M_{\alpha}) \quad , \quad (A.43a)$$

then, from symmetry R_4 , ϕ' has the expansion

$$\begin{aligned}
\phi'(\beta, \gamma, \theta_i) &= \sum_{\alpha} a_{\alpha} \psi_{\alpha}^S(\beta, \gamma + \pi, \theta_i) \\
&= \sum_{\alpha} a_{\alpha} (-1)^{\ell_{\alpha}} \psi_{\alpha}^S(\beta, \gamma, \theta_i) \quad .
\end{aligned} \tag{A.43b}$$

We now consider the effect of the potential energy reflection upon quadrupole moments and B(E2) transition rates. Let ϕ_1 and ϕ_2 be any two eigenfunctions of H, and let ϕ'_1 and ϕ'_2 be the corresponding eigenfunctions of H' obtained from Equation (A.42). From Equations (3.45), (3.48) and (3.49), quadrupole moments and transition rates are, in first order, proportional to reduced matrix elements of α_{μ} :

$$\begin{aligned}
Q(\phi_1) &\propto \langle \phi_1 || \alpha || \phi_1 \rangle \\
B(E2: \phi_1 \rightarrow \phi_2) &\propto |\langle \phi_2 || \alpha || \phi_1 \rangle|^2 \quad . \quad \text{[first order]} \tag{A.44}
\end{aligned}$$

Regarding α_{μ} as a function of the Bohr coordinates, we may note that

$$\begin{aligned}
\beta \cos(\gamma + \pi) &= -\beta \cos \gamma = -a_0 \\
\frac{\beta}{\sqrt{2}} \sin(\gamma + \pi) &= \frac{-\beta}{\sqrt{2}} \sin \gamma = -a_2
\end{aligned}$$

and use Equations (A.6) and (A.13) to conclude

$$\alpha_{\mu}(\beta, \gamma + \pi, \theta_i) = -\alpha_{\mu}(\beta, \gamma, \theta_i) \quad . \tag{A.45}$$

We will also require $|\sin 3(\gamma + \pi)| = |\sin 3\gamma|$ which ensures that the volume element of Equation (2.14) satisfies

$$d\Omega(\beta, \gamma + \pi, \theta_i) = d\Omega(\beta, \gamma, \theta_i) \quad . \tag{A.46}$$

Consider now the matrix element

$$\begin{aligned}
\langle \phi_2' | \alpha_\mu | \phi_1' \rangle &= \int_{\Omega(\beta, \gamma, \theta_i)} \phi_2'^* (\beta, \gamma, \theta_i) \alpha_\mu (\beta, \gamma, \theta_i) \phi_1' (\beta, \gamma, \theta_i) d\Omega(\beta, \gamma, \theta_i) \\
&= \int_{\Omega(\beta, \gamma, \theta_i)} \phi_2'^* (\beta, \gamma + \pi, \theta_i) \alpha_\mu (\beta, \gamma, \theta_i) \phi_1' (\beta, \gamma + \pi, \theta_i) d\Omega(\beta, \gamma, \theta_i) .
\end{aligned}$$

Making the change of variable $\gamma' = \gamma + \pi$ and using Equations (A.45) and (A.46) yields

$$\begin{aligned}
\langle \phi_2' | \alpha_\mu | \phi_1' \rangle &= \int_{\Omega(\beta, \gamma', \theta_i)} \phi_2'^* (\beta, \gamma', \theta_i) [-\alpha_\mu (\beta, \gamma', \theta_i)] \phi_1' (\beta, \gamma', \theta_i) d\Omega(\beta, \gamma', \theta_i) \\
&= -\langle \phi_2 | \alpha_\mu | \phi_1 \rangle .
\end{aligned} \tag{A.47}$$

Consequently, in first order,

$$Q(\phi_1') = -Q(\phi_1) \tag{A.48a}$$

$$B(E2: \phi_1' \rightarrow \phi_2') = B(E2: \phi_1 \rightarrow \phi_2) . \tag{A.48b}$$

Equations (A.48) are used in Chapter V to limit the investigated range of γ_0 in $\bar{H}_{QP}$.

We may define the operator W by its effect upon an arbitrary function of the Bohr coordinates:

$$W[h(\beta, \gamma, \theta_i)] = h(\beta, \gamma + \pi, \theta_i) . \tag{A.49}$$

If $V(\beta, \gamma)$ is left unaltered by a reflection about $\gamma = 30^\circ$, then

$$V'(\beta, \gamma) \equiv V(\beta, \gamma + \pi) = V(\beta, \gamma) \tag{A.50}$$

and consequently

$$W[V(\beta, \gamma)] = V(\beta, \gamma) .$$

Under such circumstances the Hamiltonian of Equation (A.40a) commutes with W and simultaneous eigenfunctions of the two operators may be found. If h is an eigenfunction of W with eigenvalue w , we may use the fact that W^2 is the identity operator to deduce that

$$Wh = wh; W^2 = 1 \quad \text{imply} \quad w = \pm 1 \quad . \quad (\text{A.51})$$

For example when $V(\beta, \gamma) = \frac{1}{2}C\beta^2$,

$$[H_B, W] = 0$$

and simultaneous eigenfunctions of H_B and W may be found. These are simply the $\psi_{N\ell vJM}^S$:

$$W \psi_{N\ell vJM}^S(\beta, \gamma, \theta_i) = \psi_{N\ell vJM}^S(\beta, \gamma + \pi, \theta_i) = (-1)^\ell \psi_{N\ell vJM}^S(\beta, \gamma, \theta_i) \quad , \quad (\text{A.52})$$

and the eigenvalue of W , $w = (-1)^\ell$, may be aptly named the " ℓ -parity". The eigenstate of H in Equation (A.43a) will be an eigenstate of W if a_α vanishes for all odd or all even values of ℓ_α . For such a state of definite ℓ -parity

$$\phi'(\beta, \gamma, \theta_i) \equiv \phi(\beta, \gamma + \pi, \theta_i) = \pm \phi(\beta, \gamma, \theta_i) \quad ,$$

and we may deduce from Equations (A.47) and (A.48) that

$$Q(\phi) = 0 \quad (\text{A.53a})$$

in first order. One may also easily show that

$$B(E2: \phi_1 \rightarrow \phi_2) = 0 \quad (\text{A.53b})$$

in first order if ϕ_1 and ϕ_2 are eigenstates of W with the same ℓ -parity.

The generalized Bohr Hamiltonians treated in this thesis have the property of reducing to H_B in some limit. We may write

$$H\phi_{Jmq} = E_q \phi_{Jmq} \quad (A.54a)$$

$$H = H_B + U(\beta, \gamma) \quad (A.54b)$$

where $U(\beta, \gamma) = 0$ for some set of Hamiltonian parameters. Occasionally $U(\beta, \gamma)$ possesses a symmetry which can be used to partition the eigenfunctions ψ_i^S of H_B into two classes, C_1 and C_2 . That is

$$\langle \psi_i^S | \frac{U(\beta, \gamma)}{H} | \psi_j^S \rangle = 0 \quad \text{if} \quad \left\{ \begin{array}{l} \psi_i^S \text{ belongs to } C_1 \\ \text{and} \\ \psi_j^S \text{ belongs to } C_2 \end{array} \right\} \quad (A.55a)$$

where

$$\begin{aligned} C_1 \cup C_2 &= \text{set of all basis functions, } \psi_k^S, \\ C_1 \cap C_2 &= \text{empty set} \end{aligned} \quad (A.55b)$$

For example if $U(\beta, \gamma)$ is unaltered by $\gamma \rightarrow \gamma + \pi$, C_1 and C_2 may be taken to be the sets of Bohr eigenfunctions with even and odd ℓ -parity respectively. Equations (A.55) will then hold. Another example frequently encountered in this work is

$$U(\beta, \gamma) = U(\beta)$$

for which we may choose

$$C_1 = \text{set of all } \psi_i^S \text{ with } \ell_i = \ell$$

$$C_2 = \text{set of all } \psi_i^S \text{ with } \ell_i \neq \ell$$

Consider now the eigenstate ϕ_{JMq} of Equation (A.54a) in the event that Equations (A.55) hold. In terms of the orthonormal ψ_i^s we have the expansion

$$\phi_{JMq} = \sum_i a_i^q \psi_i^s \quad i = (N_i, \ell_i, t_i, JM) \quad (A.56)$$

We may show:

$$\begin{aligned} &\text{if there is no eigenfunction } \phi_{JMq_1} \text{ of } H \text{ degenerate} \\ &\text{with } \phi_{JMq}, \text{ then only } \psi_i^s \text{ belonging to a single class} \\ &[\text{i.e., } C_1 \text{ or } C_2] \text{ have non-zero coefficients in the} \\ &\text{sum of Equation (A.56).} \end{aligned} \quad (A.57)$$

Consequently ϕ_{JMq} possesses the class property. This is typically the case for $\bar{H}_{QP}$ eigenfunctions [when Equations (A.55) hold]. For example when $C_Y = 0$ and $\beta_0 \neq 0$, ϕ_{JMq} of $\bar{H}_{QP}$ is generally not degenerate with a linearly independent ϕ_{JMq_1} . Consequently ϕ_{JMq} possesses ℓ as a good quantum number, and only states with $\ell_i = \ell$ occur on the right hand side of Equation (A.56).¹ Similarly when $C_Y \neq 0$ and $\gamma_0 = 30^\circ$, we have

$$\bar{V}_{QP}(\beta, \gamma + \pi) = \bar{V}_{QP}(\beta, \gamma)$$

and, in the absence of degeneracy, ϕ_{JMq} will be a state of good ℓ -parity. When ϕ_{JMq_1} [degenerate with ϕ_{JMq}] exists, the solution of Equations (A.54), obtained by diagonalizing the matrix $[H]$, is not guaranteed to

¹ Because $\langle \psi_i^s | \psi_j^{s'} \rangle \propto \delta_{\ell_i, \ell_j}$ for any s and s' , the value of s in Equation (A.56) is immaterial. If, for example, only states with $\ell_i = 8$ occur in Equation (A.56) then only $\ell_i = 8$ will occur when the sum is expressed in the form $\sum_i a_i \psi_i^{s'}$.

belong to a single class. However, it is possible to find linear combinations of ϕ_{JMq} and $\phi_{JMq'}$ which possess the class properties.

We close the appendix with a brief proof of Assertion (A.57). Within the expansion technique, a solution to Equations (A.54) [such as Equation (A.56)] consists of a set of coefficients $\{a_i^q\}$ satisfying

$$\sum_j \langle \psi_i^s | H | \psi_j^s \rangle a_j^q = E_q a_i^q \quad (A.58)$$

The proof is by contradiction. Assume that Equation (A.56) satisfies Equation (A.54a) and that members of each class appear in the expansion. That is

$$\phi_{JMq} = \sum_{\psi_i^s \in C_1} b_i^q \psi_i^s + \sum_{\psi_j^s \in C_2} c_j^q \psi_j^s, \quad (A.59)$$

with at least one b_i^q and one c_j^q non-zero. Substituting Equation (A.59) into Equation (A.54a), multiplying by ψ_j^{s*} [a member of C_2], and integrating over $\Omega(\beta, \gamma, \theta_i)$, we obtain

$$\sum_{\psi_j^s \in C_2} \langle \psi_j^s | H | \psi_j^s \rangle c_j^q = E_q c_j^q, \quad (A.60)$$

where Equation (A.55a) has been used. Consulting Equations (A.55a) and (A.60) we find that

$$a_j^q = \begin{cases} c_j^q, & \psi_j^s \text{ in } C_2 \\ 0, & \psi_j^s \text{ in } C_1 \end{cases}$$

satisfies Equation (A.58), and hence

$$\phi_{JMq'} = \sum_{\psi_j^s \in C_2} c_j^q \psi_j^s$$

is a non-trivial solution with energy E_q that is linearly independent to ϕ_{JMq} . Thus if both classes appear in Equation (A.56) we may construct an eigenfunction degenerate with ϕ_{JMq} . Conversely if no such degeneracy occurs, only a single class can appear in Equation (A.56).

VIII. APPENDIX B: NORMALIZATION OF THE $\psi_{N\ell\nu JM}(\beta, \gamma, \theta_i)$

Exact eigenfunctions of the dimensionless Bohr Hamiltonian

$$H_B'(\beta', \gamma, \theta_i) = -\frac{1}{2}T(\beta', \gamma, \theta_i) + \frac{1}{2}\beta'^2, \quad (B.1)$$

as developed in Reference (22), have the factored form

$$\psi_{N\ell\nu JM}(\beta', \gamma, \theta_i) = f_{N\ell}(\beta') \phi_{\ell\nu JM}(\gamma, \theta_i). \quad (B.2)$$

The normalization of these eigenfunctions is discussed in this appendix, and computational techniques employed in the calculation of the A^η coefficients [Equation (2.30)] are described. For convenience, the prime on the radial variable, β' , is deleted in the following discussion.

We desire that normalized wavefunctions obey the condition

$$\langle N\ell\nu JM | N\ell\nu JM \rangle \equiv \int_{\Omega} \psi_{N\ell\nu JM}^* \psi_{N\ell\nu JM} d\Omega = 1 \quad (B.3)$$

where

$$d\Omega \equiv \beta^4 |\sin 3\gamma| d\beta d\gamma d\Omega(\theta_i) \quad (B.4)$$

$$d\Omega(\theta_i) \equiv \frac{\sin \theta_2 d\theta_1 d\theta_2 d\theta_3}{8\pi^2},$$

and the region of integration is

$$\Omega: \left. \begin{array}{l} 0 \leq \beta < \infty \\ 0 \leq \gamma \leq 2\pi \\ 0 \leq \theta_1 \leq 2\pi \\ 0 \leq \theta_2 \leq \pi \\ 0 \leq \theta_3 \leq 2\pi \end{array} \right\} \Omega(\theta_i)$$

Because of the factored form of ψ , we may insist upon two separate normalization conditions:

$$\langle N\ell | N\ell \rangle = 1 \quad (B.5a)$$

$$\langle \ell v J M | \ell v J M \rangle = 1 \quad , \quad (B.5b)$$

where the overlap factors are defined by

$$\langle N\ell | N'\ell' \rangle \equiv \int_0^\infty f_{N\ell}^*(\beta) f_{N'\ell'}(\beta) \beta^4 d\beta \quad , \quad (B.6)$$

$$\langle \ell v J M | \ell' v' J' M' \rangle \equiv \int_{\Omega(\theta_i)} \int_{\gamma=0}^{2\pi} \phi_{\ell v J M}^*(\gamma, \theta_i) \phi_{\ell' v' J' M'}(\gamma, \theta_i) |\sin 3\gamma| d\gamma d\Omega(\theta_i) \quad . \quad (B.7)$$

Expressions for $f_{N\ell}$ and $\phi_{\ell v J M}$, derived in (22), are stated by Equations (2.26)-(2.28). $f_{N\ell}$ is a rotational scalar, while $\phi_{\ell v J M}$ is an eigenstate of J^2 and J_z with eigenvalues $J(J+1)\hbar^2$ and $M\hbar$ respectively. The Wigner-Eckart theorem [Equation (F.79)] may be invoked to write

$$\begin{aligned} \langle \ell v J M | \ell' v' J' M' \rangle &= c(J' 0 J; M' 0 M) \langle \phi_{\ell v J} || 1 || \phi_{\ell' v' J'} \rangle \\ &= \delta_{JJ'} \delta_{MM'} \langle \phi_{\ell v J} || 1 || \phi_{\ell' v' J'} \rangle \quad . \end{aligned}$$

Consequently $\langle \ell v J M | \ell' v' J' M' \rangle$ is independent of the value of M so long as $-J \leq M \leq J$, and we may adopt the shortened notation

$$\langle \ell v J | \ell' v' J' \rangle \equiv \langle \ell v J, M=J | \ell' v' J' J \rangle \delta_{JJ'} \quad . \quad (B.8)$$

As discussed in Chapter II and in Reference (22), the eigenfunctions $\psi_{N\ell v J M}$ are orthogonal on the labels N and ℓ , as well as on J and M .

Thus

$$\begin{aligned}
\langle N\ell vJM | N'\ell'v'J'M' \rangle &= \langle N\ell | N'\ell' \rangle \langle \ell vJM | \ell'v'J'M' \rangle \\
&= \delta_{NN'} \delta_{\ell\ell'} \delta_{JJ'} \delta_{MM'} \langle \ell vJ | \ell v'J \rangle
\end{aligned} \tag{B.9}$$

when Equation (B.5a) is satisfied.

A. Normalization of $f_{N\ell}(\beta)$

The radial factor of $\psi_{N\ell vJM}$ [Equation (2.26)] may be rewritten by expressing the hypergeometric function as an associated [or "generalized"] Laguerre polynomial (53):

$$f_{N\ell}(\beta) = \eta_{N\ell} \beta^\ell e^{-\frac{1}{2}\beta^2} {}_1F_1(-n; \alpha; \beta^2) \tag{B.10a}$$

$$= \eta_{N\ell} \beta^\ell e^{-\frac{1}{2}\beta^2} \left[\frac{n!}{(\alpha, n)} L_n^{\alpha-1}(\beta^2) \right], \tag{B.10b}$$

$$n \equiv \frac{N-\ell}{2}, \quad \alpha \equiv \ell + 5/2,$$

$$(\alpha, n) \equiv (\alpha)(\alpha+1) \dots (\alpha+n-1).$$

The normalization constant $\eta_{N\ell}$ may be easily found by making use of the orthogonality property (53)

$$\int_0^\infty x^\epsilon e^{-x} L_n^\epsilon(x) L_m^\epsilon(x) dx = \delta_{mn} \frac{\Gamma(\epsilon+n+1)}{n!} \quad [\text{Re } \epsilon > 0].$$

Using Equations (B.5a), (B.6), and (B.10b), we have

$$1 = \eta_{N\ell}^2 \left[\frac{n!}{(\alpha, n)} \right]^2 \int_0^\infty \beta^{2\ell+4} e^{-\beta^2} L_n^{\alpha-1}(\beta^2) L_n^{\alpha-1}(\beta^2) d\beta$$

which, upon the change of variable $x = \beta^2$, becomes

$$\begin{aligned}
1 &= \eta_{N\ell}^2 \left[\frac{n!}{(\alpha, n)} \right]^2 \frac{1}{2} \int_0^\infty x^{\alpha-1} e^{-x} L_n^{\alpha-1}(x) L_n^{\alpha-1}(x) dx \\
&= \eta_{N\ell}^2 \left[\frac{n!}{(\alpha, n)} \right]^2 \frac{1}{2} \frac{\Gamma(\alpha + n)}{n!} .
\end{aligned}$$

Hence the required normalization constant is

$$\eta_{N\ell} = \left[\frac{2(\alpha, n)}{n! \Gamma(\alpha)} \right]^{\frac{1}{2}} . \quad (B.11)$$

B. Normalization of $\phi_{\ell\nu JM}(\gamma, \theta_i)$

The $R(5)$ factor of $\psi_{N\ell\nu JM}$ may be written, after the fashion of Equation (2.27), as

$$\phi_{\ell\nu JM}(\gamma, \theta_i) = \eta_{\ell\nu J} \sum_{\substack{K \geq 0 \\ \text{even}}}^J g_{\ell\nu JK}(\gamma) \frac{\langle \theta_i | J, M, |K\rangle}{(1 + \delta_{K,0})} . \quad (B.12)$$

Here

$$\langle \theta_i | J, M, |K\rangle \equiv D_{MK}^{J*}(\theta_i) + (-1)^J D_{M, -K}^{J*}(\theta_i) , \quad (B.13)$$

and $\eta_{\ell\nu J}$ is a normalization constant to be determined. The function $g_{\ell\nu JK}(\gamma)$ is that appearing in Reference (22):

$$g_{\ell\nu JK}(\gamma) = (\cos \gamma)^\ell \sum_{\sigma=0}^{\sigma_{\max}} A_\sigma(\ell\nu JK) (\tan \gamma)^{2\sigma + \frac{1}{2}K} . \quad (B.14)$$

The upper limit on the sum over σ depends upon K and ℓ as follows.

Define the integers m and p by

$$K = 4m + 2p \quad p = 0, 1 \quad m = 0, 1, 2, \dots .$$

Then

$$\sigma_{\max} = [\tfrac{1}{2}(\ell - p)]_{G1} - m \quad \left[\begin{array}{l} \text{if } n+1 > x \geq n \text{ with } n \\ \text{an integer, then } [x]_{G1} \equiv n \end{array} \right] .$$

A closed expression for the general coefficient $A_{\sigma}(\ell\nu JK)$ was determined in (22). It may be written as

$$A_{\sigma}(\ell\nu JK) = \left[\frac{6^{\ell}(J+K)! (J-K)!}{(J+\ell-3\nu)! (J-\ell+3\nu)! 12^{\frac{1}{2}K+2\sigma}} \right]^{\frac{1}{2}} \bar{A}_{\sigma}(\ell\nu JK) \quad (B.15)$$

where the barred coefficient, involving no square roots, is given by the nested sum

$$\begin{aligned} \bar{A}_{\sigma}(\ell\nu JK) &= (\ell-\nu)! \sum_e (-1)^e \binom{J-\ell+3\nu}{e} \binom{J+\ell-3\nu}{\ell-3\nu-K+e} \\ &\quad \sum_c (-1)^c 2^c \binom{\nu}{\frac{1}{2}K+2\sigma-c} \\ &\quad \sum_d (-1)^d \binom{\frac{1}{2}K+2\sigma-c}{\sigma-d} \frac{(2\nu+J+2c-3d-e)!}{(c-d)! d!} \\ &\quad \sum_f \frac{(-1)^f 2^f (\ell-\nu-c+3d+e+f)!}{(\ell-\nu-c-f)! f! (\ell+\nu+J+c+f+1)!} \end{aligned} \quad (B.16)$$

The summation indices e , c , d and f range over those values for which all factorials and combinational symbols in Equation (B.16) have non-negative arguments simultaneously:

$$\max\{0, 3\nu+K-\ell\} \leq e \leq \min\{J+K, J-\ell+3\nu\}$$

$$\max\{0, \tfrac{1}{2}K+2\sigma-\nu\} \leq c \leq \min\{\ell-\nu, \tfrac{1}{2}K+2\sigma\}$$

$$\max\{0, c-\sigma-\tfrac{1}{2}K\} \leq d \leq \min\{c, \sigma\}$$

$$0 \leq f \leq \ell-\nu-c$$

We now consider the calculation of the $\eta_{\ell\nu J}$, and hence of the normalized A-coefficients

$$A_{\sigma}^{\eta}(\ell\nu JK) \equiv \eta_{\ell\nu J} A_{\sigma}(\ell\nu JK) \quad (B.17)$$

An expression for $\eta_{\ell\nu J}$ may be obtained by substituting Equation (B.12) into the normalization condition, Equation (B.5b). However, as we also require values for the non-trivial $\langle \ell\nu J | \ell\nu' J' \rangle$, we begin with Equation (B.8) and develop an expression for the general R(5) overlap:

$$\begin{aligned} \langle \ell\nu JM | \ell'\nu' J' M' \rangle &= \eta_{\ell\nu J} \eta_{\ell'\nu' J'} \sum_{\substack{K' \geq 0 \\ \text{even}}}^{J'} \sum_{\substack{K \geq 0 \\ \text{even}}}^J \left[\int_0^{2\pi} g_{\ell\nu JK}^*(\gamma) g_{\ell'\nu' J' K'}(\gamma) \right. \\ &\quad \left. \times |\sin 3\gamma| d\gamma \right] \frac{\langle J, M, |K| | J', M', |K'| \rangle}{(1 + \delta_{K,0})(1 + \delta_{K',0})} \quad (B.18) \end{aligned}$$

The integral over the Euler angles may be evaluated by using the orthogonality property of the rotation matrices on the unit sphere [Equation (F.47)],

$$\begin{aligned} \langle J, M, |K| | J', M', |K'| \rangle &\equiv \int_{\Omega(\theta_i)} \langle \theta_i | J, M, |K| \rangle^* \langle \theta_i | J' M' | K' \rangle d\Omega(\theta_i) \\ &= \frac{2(1 + (-1)^J \delta_{K,0})}{2J + 1} \delta_{JJ'} \delta_{MM'} \delta_{KK'} \quad (B.19) \end{aligned}$$

Using this result in Equation (B.18), and expanding the γ integrand with Equation (B.14) leads to

$$\begin{aligned} \langle \ell\nu JM | \ell'\nu' J' M' \rangle &= \delta_{JJ'} \delta_{MM'} \eta_{\ell\nu J} \eta_{\ell'\nu' J'} \overline{\langle \ell\nu J | \ell'\nu' J' \rangle} \\ &\quad \times \frac{2}{2J+1} \left[\frac{6^{\ell+\ell'}}{(J+\ell-3\nu)! (J-\ell+3\nu)! (J+\ell'-3\nu')! (J-\ell'+3\nu')!} \right]^{\frac{1}{2}}, \quad (B.20a) \end{aligned}$$

where the barred overlap involves no square roots,

$$\begin{aligned} \overline{\langle \ell \nu J | \ell' \nu' J \rangle} &\equiv \sum_{\substack{K \geq 0 \\ \text{even}}}^J \frac{(1 + (-1)^J \delta_{K,0})}{(1 + \delta_{K,0})^2} (J+K)! (J-K)! 12^{-\frac{1}{2}K} \\ &\times \sum_{\sigma=0}^{\sigma_{\max}} 12^{-\sigma} \bar{A}_{\sigma}(\ell \nu J K) \sum_{\sigma'=0}^{\sigma'_{\max}} 12^{-\sigma'} \bar{A}_{\sigma'}(\ell' \nu' J K) \\ &\times \mathcal{J}(\ell + \ell' - K - 2\sigma - 2\sigma', \tfrac{1}{2}K + \sigma + \sigma') \end{aligned} \quad (\text{B.20b})$$

The integral remaining in Equation (B.20b) is of the form

$$\mathcal{J}(s, q) \equiv \int_0^{2\pi} (\cos \gamma)^s (\sin \gamma)^{2q} |\sin 3\gamma| d\gamma \quad (\text{B.21a})$$

where s and q are non-negative integers. When s is odd, the integrand is even about $\gamma = \pi$ and odd about $\gamma = \frac{1}{2}\pi$; consequently $\mathcal{J}(s, q) = 0$. When s is even, $\mathcal{J}(s, q)$ may be evaluated by first using symmetry arguments to write

$$\int_0^{2\pi} = 4 \int_0^{\pi/3} + 2 \int_{\pi/3}^{2\pi/3},$$

and then making the change of variable $t = \cos \gamma$. Each integrand becomes a polynomial in t , and one finds

$$\mathcal{J}(s, q) = \begin{cases} 0 & (s \text{ odd}) \\ \sum_{m=0}^{q+1} (-1)^{m+1} \frac{(1+q+3m)}{(s+2m+1)(q+1)} \binom{q+1}{m} \frac{2^{s+2m} - 1}{2^{s+2m-2}} & (s \text{ even}) \end{cases} \quad (\text{B.21b})$$

Having developed the necessary formulae, we may now calculate the

A^η and the $\langle \ell v J | \ell v' J \rangle$ by the following procedure:

- 1) The $\bar{A}$ -coefficients are computed by performing the nested summations in Equation (B.16).
- 2) Necessary integrals $J(s, q)$ are computed from Equation (B.21b).
- 3) The barred overlaps $\overline{\langle \ell v J | \ell' v' J \rangle}$ are found from Equation (B.20b). [Those overlaps for which $\ell \neq \ell'$ should be computed as zero.]
- 4) The normalized A-coefficients are calculated from

$$A_{\sigma}^{\eta}(\ell v J K) = \left[\frac{\frac{1}{2}(2J+1)(J+K)!(J-K)!}{12^{\frac{1}{2}K+2\sigma} \overline{\langle \ell v J | \ell v J \rangle}} \right]^{\frac{1}{2}} \bar{A}_{\sigma}(\ell v J K) \quad (B.22)$$

which follows from Equations (B.5b), (B.12), (B.14), (B.17) and (B.20a).

- 5) Non-trivial overlaps between normalized wavefunctions are calculated from

$$\langle \ell v J | \ell v' J \rangle = \frac{\overline{\langle \ell v J | \ell v' J \rangle}}{[\overline{\langle \ell v J | \ell v J \rangle} \overline{\langle \ell v' J | \ell v' J \rangle}]^{\frac{1}{2}}} \quad (B.23)$$

In terms of the A^η , the properly normalized R(5) factor of $\psi_{N\ell v J M}$ is

$$\begin{aligned} \phi_{\ell v J M}(\gamma, \theta_i) &= \sum_{\substack{K \geq 0 \\ \text{even}}}^J g_{\ell v J K}^{\eta}(\gamma) \frac{\langle \theta_i | J, M, |K\rangle}{(1 + \delta_{K,0})} \\ &= \sum_{\substack{K=-J \\ \text{even}}}^J g_{\ell v J K}^{\eta}(\gamma) D_{MK}^{J*}(\theta_i) \quad , \end{aligned} \quad (B.24)$$

where

$$g_{\ell\nu JK}^{\eta}(\gamma) = \begin{cases} (\cos \gamma)^{\ell} \sum_{\sigma=0}^{\sigma_{\max}} A_{\sigma}^{\eta}(\ell\nu JK) (\tan \gamma)^{2\sigma+\frac{1}{2}K} & [K \geq 0] \\ (-1)^J g_{\ell\nu J, -K}^{\eta}(\gamma) & [K < 0] \end{cases} \quad (\text{B.25})$$

C. Computational Methods

As the A^{η} coefficients were to be calculated but a single time and stored for future use, it was essential that the calculations be done as accurately as possible. I insisted that the stored results be correct in the first ten significant figures. Since "double precision" computations on the available IBM 370/158 computer employ numbers having 16 decimal digits of precision [REAL*8], it seemed reasonable to expect that the A^{η} could be obtained to the desired accuracy with a rather straightforward REAL*8 FORTRAN code. This, however, turned out not to be the case.

Stanley A. Williams (65) suggested the alternate idea of calculating the $\bar{A}$ coefficients exactly using integer arithmetic. The rational fraction of two integers, m_1 and m_2 , could be represented by expressing it in terms of prime factors:

$$\frac{m_1}{m_2} = 2^{n_1} 3^{n_2} 5^{n_3} \dots 71^{n_{20}} \frac{n_{21}}{n_{22}} \quad (\text{B.26})$$

Here the "leftover" integers, n_{21} and n_{22} , have no prime factors smaller than 73. A standard FORTRAN integer [I*4] is limited in magnitude to $\sim 2 \times 10^{10}$, thus setting an internal upper limit on the size of the components, m_1 and m_2 , of a rational fraction. This limit was greatly

extended by expressing a given rational fraction as the sequence of 1*4 integers ($n_1, n_2, \dots, n_{22}$). Williams had also written a collection of FORTRAN subroutines to add, subtract, multiply and divide rational fractions represented in the form of Equation (B.26). Use was made of these routines in developing computer codes to calculate the $\bar{A}$ coefficients and the $\langle \ell v J | \ell v' J \rangle$ exactly as rational fractions. [Notice that integer arithmetic suffices for the first three of the five calculational steps outlined earlier.] These codes were of limited usefulness, however, as it was not difficult to have intermediate values of n_{21} overflowing [exceeding $\sim 2 \times 10^{10}$] in the add-or-subtract subroutine. In those cases where overflow did not occur, the exact value of $\bar{A}_\sigma(\ell v J K)$ could be compared with one calculated using REAL*8 arithmetic; it was found that the latter value was often accurate to less than ten significant figures, particularly when the value of σ was small. The difficulty was eventually traced to cancellations occurring in the nested sum of Equation (B.16). When sums of positive and negative terms were individually calculated, they were occasionally found to agree in magnitude to five or even 10 significant figures.

Because of the cancellation and overflow problems, it was clear that exact calculation of the $\bar{A}$ coefficients would be necessary, and that accomplishing this would require handling integers, n_{21} , which exceeded the usual FORTRAN size limits. Rational fractions were again represented in the manner of Equation (B.26); however, I allowed the leftover numerator to be an "extended integer" of 40 decimal digits. Each group of four adjacent digits was represented by a single 1*4

integer. Subroutines were written to add, subtract and multiply rational fractions whose n_{21} components were extended integers. This extension proved sufficient to avoid the overflow problems that had previously hampered attempts at exact calculation of the $\bar{A}$. At this point, three codes for calculating these coefficients were available:

- 1) ABAR8, which used REAL*8 arithmetic and occasionally produced inaccurate results because of cancellation effects;
- 2) ABAR, which used I*4 arithmetic and calculated the $\bar{A}$ exactly as rational fractions [when n_{21} did not overflow]; and
- 3) ABARX, which calculated the $\bar{A}$ exactly as rational fractions using extended integer arithmetic.

As expected, ABARX was slower and more costly to execute than ABAR; ABAR8 was considerably faster than either. During production runs for the calculation of the $\bar{A}$, the ABAR result was accepted if ABAR8 indicated that it was correct. Otherwise ABARX was used.

Extended integer arithmetic was also used to calculate the $\mathcal{J}(s, q)$ and the $\langle \ell v J | \ell' v' J \rangle$ as rational fractions. The $\bar{A}$ coefficients are ingredients in the calculation of the latter, and were subjected to extreme testing by verifying that

$$\langle \ell v J | \ell' v' J \rangle = 0 \quad \ell \neq \ell' .$$

Finally the A^η and $\langle \ell v J | \ell v' J \rangle$ ($v \neq v'$) were formed as REAL*8 numbers and stored on magnetic tape. The stored A^η were then subjected to a second level of testing: they were used in REAL*8 codes which calculated matrix elements of the unit operator.

The five-step calculational procedure of Section B was carried out in turn for each of the spins $J = 0, 2, 3, 4, \dots, 20$. The number of coefficients and non-trivial overlaps calculated for each J was limited by fixing the maximum value of ℓ considered [$\ell_{\max}$ in Table B.1]. As Table B.2 indicates, the number of $A_{\sigma}^{\eta}(\ell\nu JK)$ rises rapidly with increasing J and $\ell_{\max}$. For fixed ℓ and J , the $\phi_{\ell\nu JM}$ with J even require considerably more coefficients for their specification than do the $\phi_{\ell\nu, J\pm 1, M}$. Table B.3 contains a short list of the A^{η} for $J = 0$, and illustrates two general trends:

- 1) $A_{\sigma}^{\eta}(\ell\nu JK)$ tends to increase in magnitude as ℓ increases; and
- 2) For fixed $(\ell\nu JK)$, $A_{\sigma}^{\eta}(\ell\nu JK)$ rises and then falls as σ increases from 0 to $\sigma_{\max}$.

Table B.4 gives the number of distinct non-trivial overlaps $\langle \ell\nu J | \ell\nu' J \rangle$ which occur for several fixed values of ℓ and J . The multiplicity in the ν label [i.e., the number of distinct $\phi_{\ell\nu JJ}$ with fixed ℓ and J] is quite small for moderate values of ℓ and J . In the maximal basis calculations [Table B.1], the multiplicity was at worst four-fold. As an example, when $(\ell, J) = (24, 18)$, ν takes on the values 2, 3, 4 and 5. No more than two-fold multiplicity occurs for $J \leq 11$, and $J = 0, 2, 3, 4, 5$, and 7 are multiplicity free for all values of ℓ . All of the non-trivial overlaps for $J \leq 12$, $\ell \leq 12$ are listed in Table B.5.

Table B.1. Numbers of coefficients and overlaps calculated for each value of J

J	$l_{\max}$	Number of $\Phi_{l\nu JJ}$ ($l \leq l_{\max}$)	Number of $A_{\sigma}^{\eta}(l\nu JK)$ ($l \leq l_{\max}$; $K \geq 0$)	Number of $\langle l\nu J l\nu' J \rangle$ ($l \leq l_{\max}$; $\nu < \nu'$)
0	30	11	91	0
2	27	18	261	0
3	30	10	85	0
4	25	24	504	0
5	27	16	240	0
6	25	30	854	7
7	25	21	457	0
8	25	35	1266	13
9	25	26	766	6
10	25	39	1719	18
11	15	13	319	4
12	25	42	2191	27
13	15	13	393	5
14	25	44	2660	34
15	15	12	431	6
16	25	45	3098	39
17	15	9	360	3
18	25	45	3480	45
19	15	7	313	2
20	25	44	3778	48

Table B.2. Number of $A_0^n(l\nu JK)$ with fixed $J, K \geq 0$,
and $l \leq l_{\max}$

J	$l_{\max}$:	10	15	20	25	30
0		12	27	37	61	91
2		44	85	161	234	320
3		10	24	33	56	85
4		88	189	328	504	718
5		34	72	144	214	297
6		134	318	534	854	1248
7		63	157	288	457	663
8		173	420	814	1266	1814
9		86	256	460	766	1146
10		189	549	1059	1719	2529
11		91	319	690	1123	1650
12		170	656	1292	2191	3308
13		63	393	873	1503	2283
14		136	668	1564	2660	4008
15		49	431	1027	1885	2959
16		88	668	1715	3098	4820
17		28	360	1200	2244	3540
18		65	585	1785	3480	5610
19		0	313	1235	2552	4205
20		36	470	1843	3778	6199

Table B.3. All A_{σ}^{η} coefficients for $J = 0$ with $K \geq 0$ and $\ell \leq 20$. [.xxxD yy should be read as $(.xxx) \cdot 10^{yy}$]

ℓ	ν	J	K	σ	$A_{\sigma}^{\eta}(\ell\nu JK)$
0	0	0	0	0	0.500000000000000000D 00
3	1	0	0	0	0.8660254037844386D 00
3	1	0	0	1	-0.2598076211353316D 01
6	2	0	0	0	0.1118033988749895D 01
6	2	0	0	1	-0.1173935688187390D 02
6	2	0	0	2	0.1341640786499874D 02
6	2	0	0	3	-0.5590169943749474D 00
9	3	0	0	0	0.1322875655532295D 01
9	3	0	0	1	-0.2976470224947665D 02
9	3	0	0	2	0.1011999876482206D 03
9	3	0	0	3	-0.7341959888204238D 02
9	3	0	0	4	0.5952940449895329D 01
12	4	0	0	0	0.150000000000000000D 01
12	4	0	0	1	-0.585000000000000000D 02
12	4	0	0	2	0.396562500000000000D 03
12	4	0	0	3	-0.753750000000000000D 03
12	4	0	0	4	0.421875000000000000D 03
12	4	0	0	5	-0.472500000000000000D 02
12	4	0	0	6	0.562500000000000000D 00
15	5	0	0	0	0.1658312395177700D 01
15	5	0	0	1	-0.9949874371066200D 02
15	5	0	0	2	0.1122470202485906D 04
15	5	0	0	3	-0.4010006660589076D 04
15	5	0	0	4	0.5279652088147003D 04
15	5	0	0	5	-0.2511099544397832D 04
15	5	0	0	6	0.3389175957644424D 03
15	5	0	0	7	-0.9328007222874562D 01
18	6	0	0	0	0.1802775637731995D 01
18	6	0	0	1	-0.1541373170260855D 03
18	6	0	0	2	0.2606137531296315D 04
18	6	0	0	3	-0.1496585463010951D 05
18	6	0	0	4	0.3520820820490586D 05
18	6	0	0	5	-0.3592514954133640D 05
18	6	0	0	6	0.1531840994076348D 05
18	6	0	0	7	-0.2327270674834647D 04
18	6	0	0	8	0.1014061296224247D 03
18	6	0	0	9	-0.5633673867912484D 00

Table B.4. Number of $\langle \ell v J | \ell v' J \rangle$ with fixed J ,
 $v < v'$ and $\ell \leq \ell_{\max}$

J	$\ell_{\max}$:	10	15	20	25	30
0		0	0	0	0	0
2		0	0	0	0	0
3		0	0	0	0	0
4		0	0	0	0	0
5		0	0	0	0	0
6		2	4	5	7	9
7		0	0	0	0	0
8		3	6	10	13	16
9		1	3	4	6	8
10		3	8	13	18	23
11		1	4	8	11	14
12		2	11	18	27	36
13		0	5	10	15	20
14		1	10	23	34	45
15		0	6	13	22	31
16		0	9	24	39	54
17		0	3	16	27	38
18		0	6	24	45	66
19		0	2	15	30	45
20		0	3	24	48	72

Table B.5. All $\langle \ell v J | \ell v' J \rangle$ having $v < v'$, $J \leq 12$,
and $\ell \leq 12$

J	ℓ	v	v'	$\langle \ell v J \ell v' J \rangle$	
6	6	0	1	-.8017027062403220	D-01
6	9	1	2	-.9656020412619940	D-01
6	12	2	3	-.1037358222937086	D 00
8	7	0	1	-.1194030334785708	D 00
8	8	0	1	-.5434680820018298	D-02
8	10	1	2	-.1491232249988268	D 00
8	11	1	2	-.1148803011697616	D-01
9	9	0	1	.1873076010932257	D-01
9	12	1	2	.1908209754408954	D-01
10	8	0	1	-.1462145301373871	D 00
10	9	0	1	-.8349385342827916	D-02
10	10	0	1	.6620690490841561	D-02
10	11	1	2	-.1889635788785222	D 00
10	12	1	2	-.2041063417853270	D-01
11	10	0	1	.4091985510922771	D-01
11	11	0	1	.9299294355796804	D-02
12	9	0	1	-.1641782825881252	D 00
12	10	0	1	-.9642164667315264	D-02
12	11	0	1	.1334839510517106	D-01
12	12	0	1	.7578217969680127	D-02
12	12	0	2	.5286870228451461	D-02
12	12	1	2	-.2193057245440392	D 00

IX. APPENDIX C: CALCULATIONAL TECHNIQUES IN THE SOLUTION OF $H\phi = E\phi$

The calculational techniques used to obtain the eigenvalues and eigenfunctions of a generalized Bohr problem [Equations 3.9] are outlined in this appendix. Based on the methods of Chapter III, Section B, a seven step procedure is followed:

- 1) For each angular momentum J , a maximal expansion basis is selected. Its size is specified by the upper limit on the principal quantum number, $N_{\max}(J)$.
- 2) Matrix elements for potentials of the form

$$\begin{aligned} V_1 &= \beta^p f(\gamma) & p &= 0, 1, 2, \dots \\ \text{or } V_2 &= e^{-a\beta^2} \beta^p f(\gamma) & a &\geq 0 \end{aligned} \quad (C.1)$$

are computed between the [generally non-orthogonal] states ψ_α of the standard reduced Bohr problem. Radial and angular integrations are performed independently by making use of the closed expressions of Equations (2.25)-(2.30). The A^η coefficients and non-trivial overlaps $\langle \psi_\alpha | \psi_\beta \rangle$ are presumed to have been previously calculated by the methods of Appendix B.

- 3) Following Equation (3.26), the matrix $[U]$ is constructed. $[U]$ connects states of the original basis, ψ_α , with those of the orthonormal one, ψ_i [see Equation (3.22)].
- 4) $[U]$ is employed in the manner of Equation (3.30) to obtain matrix elements of the potential terms between the states ψ_i .
- 5) An expansion basis for treating the problem at hand is decided upon; its size and basis parameter $[\tilde{s}]$ are specified. [The size can be no larger than that of the maximal basis of step 1), for which standard reduced matrix elements $\langle i | V_k | j \rangle$ have been calculated.] Using Equation (3.32), matrix elements of

the Hamiltonian

$$[H]_{ij} = \langle \tilde{\psi}_i | H | \tilde{\psi}_j \rangle$$

are assembled from the $\langle i | V_k | j \rangle$. [For an example see Equation (3.34).]

- 6) Eigenvalues and eigenvectors of the matrix $[H]$ are determined by standard computational techniques. [The EISPACK (41) sub-routines TRED3, TRIDIB, TINVIT, and TRBAC3 are used].
- 7) The expansion coefficients for the eigenfunctions of H are back-transformed into their original $[\psi_\alpha]$ basis representation. This is done using Equation (3.29).

The bulk of this work is accomplished by two packages of computer codes: MEWORK which performs steps 2)-4); and THEORY which is responsible for the mechanics of steps 5)-7). Functional flowcharts of the two packages are provided in Figures C.1 and C.2.

In the following section, methods for calculating original-basis matrix elements are presented. The enumeration of basis states, and the details of transforming between the original and orthonormal bases are the topics of Section B. Section C then describes the initial testing of the MEWORK and THEORY packages. Some light is shed on the effect of mischoosing $\tilde{s}$, and attempts are made to reproduce calculations reported in the literature. In the final section we examine the manner in which the energy degeneracy of the Bohr Hamiltonian is broken for some simple choices of the potential energy function.

Figure C.1. Structure of the MEWORK package

Figure C.2. Structure of the THEORY package

A. Radial and Angular Matrix Elements

We consider now the calculation of matrix elements between the states ψ_α [$\alpha = (N_\alpha, \ell_\alpha, v_\alpha, J_\alpha, M_\alpha)$] which comprise a generally non-orthogonal set of solutions to the standard reduced Bohr problem [Equations (2.32)]. In particular we seek computationally useful expressions for

$$[V']_{\alpha\beta} \equiv \langle \psi_\alpha | h(\beta) f(\gamma) | \psi_\beta \rangle, \quad (C.2)$$

where the notation of Equation (3.7) has been adopted. The prime on V is to remind us that the matrix elements of $h(\beta)f(\gamma)$ are to be computed in the non-orthogonal basis. $f(\gamma)$ is assumed to be a bounded function obeying the potential energy symmetries [Equation (A.35)]

$$f(\gamma) = f(-\gamma) = f(\gamma - \frac{2\pi}{3}) \quad (C.3)$$

The radial factor $h(\beta)$ may take either of the two forms appearing in Equation (C.1):

$$h_1(\beta) = \beta^p \quad \text{or} \quad h_2(\beta) = e^{-a\beta^2} \beta^p; \quad (C.4)$$

$$p = 0, 1, 2, \dots, \quad a \geq 0.$$

Using the factored form of the Bohr eigenfunctions¹ [Equation (2.25)] we may write the desired matrix element as a product:

$$[V']_{\alpha\beta} = \langle N_\alpha \ell_\alpha | h(\beta) | N_\beta \ell_\beta \rangle \langle \ell_\alpha v_\alpha J_\alpha M_\alpha | f(\gamma) | \ell_\beta v_\beta J_\beta M_\beta \rangle, \quad (C.5)$$

¹The prime on the radial variable is not carried in this section. β is understood to be the β' of Figure 2.2.

with the definitions

$$\langle N\ell | h(\beta) | N'\ell' \rangle \equiv \int_0^\infty f_{N\ell}^*(\beta) h(\beta) f_{N'\ell'}(\beta) \beta^4 d\beta \quad , \quad (C.6)$$

$$\begin{aligned} \langle \ell v J M | f(\gamma) | \ell' v' J' M' \rangle \equiv & \int_{\gamma=0}^{2\pi} \int_{\Omega(\theta_i)} \Phi_{\ell v J M}^*(\gamma, \theta_i) f(\gamma) \Phi_{\ell' v' J' M'}(\gamma, \theta_i) \\ & \times d\Omega(\theta_i) |\sin 3\gamma| d\gamma \quad . \end{aligned} \quad (C.7)$$

$\Omega(\theta_i)$ and $d\Omega(\theta_i)$ are defined immediately after Equation (B.4).

We begin by considering the radial matrix element. The class of functions $h_2(\beta)$ contains $h_1(\beta)$ as a subset, so it is sufficient to evaluate

$$B^{a,p} \equiv \langle N\ell | e^{-a\beta^2} \beta^p | N'\ell' \rangle \quad . \quad (C.8)$$

Using Equation (2.26), the radial factor of each eigenfunction may be written in the form

$$f_{N\ell}(\beta) = \eta_{N\ell} \beta^\ell e^{-\frac{1}{2}\beta^2} \sum_{m=0}^n \frac{(-n, m)}{(\alpha, m)} \frac{\beta^{2m}}{m!} \quad , \quad (C.9)$$

with the normalization constant $\eta_{N\ell}$ given by Equation (B.11). When Equation (C.9) is used twice in Equation (C.6), the resulting integral may be evaluated by changing the integration variable to $x = (1+a)\beta^2$ and using (66)

$$\int_0^\infty x^t e^{-x} dx = \Gamma(t+1) \quad [t > -1] \quad . \quad (C.10)$$

We find

$$B^{a,p} = \eta_{N\ell} \eta_{N'\ell'} \frac{(1+a)^{-w} \Gamma(w)}{2} \sum_{m=0}^n \frac{(-n, m) (w, m)}{(\alpha, m) m!} \frac{1}{(1+a)^m} \\ \times \sum_{m'=0}^{n'} \frac{(-n', m') (w+m, m')}{(\alpha', m') m'!} \frac{1}{(1+a)^{m'}} \quad [p > -5] \quad , \quad (C.11)$$

with the definitions

$$\alpha = \ell + \frac{5}{2} \quad , \quad n = \frac{N-\ell}{2} \quad , \quad w = \frac{(\alpha+\alpha'+p)}{2} \quad , \\ \alpha' = \ell' + \frac{5}{2} \quad , \quad n' = \frac{N'-\ell'}{2} \quad . \quad (C.12)$$

For the special case $a = 0$, the inner sum in Equation (C.11) may be found by using Vandermonde's theorem (67):

$$\sum_{m'=0}^{n'} \frac{(-n', m') (b, m')}{(c, m') m'!} = \frac{(c-b, n')}{(c, n')} \quad . \quad (C.13)$$

In this case we have

$$B^{0,p} = \langle N\ell | \beta^p | N'\ell' \rangle = \eta_{N\ell} \eta_{N'\ell'} \frac{\Gamma(w)}{2(\alpha', n')} \sum_{m=0}^n \frac{(-n, m) (w, m) (\alpha'-w-m, n')}{(\alpha, m) m!} \quad . \quad (C.14)$$

For computational purposes the upper limit on the remaining sum is kept as small as possible. Equation (C.14) is used directly if $n \leq n'$.

Otherwise

$$\langle N\ell | \beta^p | N'\ell' \rangle = \langle N'\ell' | \beta^p | N\ell \rangle \quad , \quad (C.15)$$

which follows from the reality of the radial wavefunctions, can be used to restrict the limit on the sum to the minimum of $\{\frac{1}{2}(N-\ell), \frac{1}{2}(N'-\ell')\}$.

For small values of p , recursion relations for the associated Laguerre polynomials may be used together with Equation (B.10b) to derive more compact forms of Equation (C.14). However the general relations of Equations (C.11) and (C.14) are utilized by the MEWORK package.

We now turn our attention to the angular integral of Equation (C.7). With $\langle \theta_i | JM | K \rangle$ defined as in Equation (B.13), we may make use of Equation (2.29) to write

$$\begin{aligned}
 G &\equiv \langle \ell v JM | f(\gamma) | \ell' v' J' M' \rangle \\
 &= \sum_{\substack{J \geq 0 \\ \text{even}}}^J \sum_{\substack{J' \geq 0 \\ \text{even}}}^{J'} \int_{\gamma=0}^{2\pi} \frac{g_{\ell v JK}^{\eta*}(\gamma)}{(1 + \delta_{K,0})} f(\gamma) \frac{g_{\ell' v' J' K'}^{\eta}(\gamma)}{(1 + \delta_{K',0})} |\sin 3\gamma| d\gamma \\
 &\quad \times \int_{\Omega(\theta_i)} \langle \theta_i | JM | K \rangle^* \langle \theta_i | J' M' | K' \rangle d\Omega(\theta_i) \quad . \quad (C.16)
 \end{aligned}$$

The result of the integration over the Euler angles is given by Equation (B.19), and may be inserted to simplify the above expression:

$$\begin{aligned}
 G &= \delta_{JJ'} \delta_{MM'} \left[\frac{2}{2J+1} \sum_{\substack{K=0 \\ \text{even}}}^J \frac{(1 + (-1)^J \delta_{K,0})}{(1 + \delta_{K,0})^2} \right. \\
 &\quad \left. \times \int_0^{2\pi} g_{\ell v JK}^{\eta*}(\gamma) f(\gamma) g_{\ell' v' J' K}^{\eta}(\gamma) |\sin 3\gamma| d\gamma \right] \quad . \quad (C.17a)
 \end{aligned}$$

From Equation (A.32a), it may be seen that $g_{\ell v J 0}^{\eta}$ vanishes unless J is even. Hence $(1 + (-1)^J \delta_{K,0})$ may be replaced by $(1 + \delta_{K,0})$ in Equation (C.17a). Like its radial counterpart, the angular matrix element G is seen to be real for a real-valued potential function. Notice the G vanishes unless $(JM) = (J'M')$, and that the entire

dependence upon the projection quantum numbers is carried by the factor $\delta_{MM'}$. We may consequently write

$$G = \langle \ell v J M | f(\gamma) | \ell' v' J' M' \rangle = \delta_{JJ'} \delta_{MM'} \langle \ell v J | f(\gamma) | \ell' v' J \rangle, \quad (C.17b)$$

where $\langle \ell v J | f(\gamma) | \ell' v' J \rangle$ is the quantity in brackets in Equation (C.17a).

To proceed further we expand the g^η functions using Equation (2.30).

This results in

$$\begin{aligned} \langle \ell v J | f(\gamma) | \ell' v' J \rangle &= \frac{2}{2J+1} \sum_{\substack{K=0 \\ \text{even}}}^J \frac{1}{(1 + \delta_{K,0})} \\ &\times \sum_{\sigma} A_{\sigma}^{\eta}(\ell v J K) \sum_{\sigma'} A_{\sigma'}^{\eta}(\ell' v' J K) \mathcal{J}^{\ell+\ell'}(K+2\sigma+2\sigma') \end{aligned}, \quad (C.18)$$

with

$$\mathcal{J}^{\ell+\ell'}(K+2\sigma+2\sigma') \equiv \int_0^{2\pi} (\sin \gamma)^{K+2\sigma+2\sigma'} (\cos \gamma)^{\ell+\ell'-K-2\sigma-2\sigma'} f(\gamma) |\sin 3\gamma| d\gamma. \quad (C.19)$$

Equations (C.18) and (C.19) are the basis for the practical calculation of the angular matrix elements. Each required integral $\mathcal{J}$ is evaluated numerically by using the subroutine DQG32 (68) which performs a 32 point gauss quadrature. The exponent of $\sin \gamma$ is a non-negative, even integer. The exponent of $(\cos \gamma)$ is also a non-negative integer, its evenness or oddness being that of $(\ell + \ell')$. The assumed symmetry properties of $f(\gamma)$, Equation (C.3), may be used to narrow the region of integration. We begin by breaking $f(\gamma)$ into portions which are symmetric and antisymmetric respectively about $\gamma = \frac{1}{2}\pi$:

$$f(\gamma) = f_S(\gamma) + f_A(\gamma) \quad (C.20)$$

$$f_S(\gamma) \equiv \frac{1}{2}[f(\gamma) + f(\pi - \gamma)]$$

$$f_A(\gamma) \equiv \frac{1}{2}[f(\gamma) - f(\pi - \gamma)]$$

f_A and f_S may each be shown to satisfy Equation (C.3). In particular each is even about the midpoint of integration, $\gamma = \pi$. If $(\ell + \ell')$ is even, $f_A(\gamma)$ makes no overall contribution to $\mathcal{J}^{\ell+\ell'}(K+2\sigma+2\sigma')$, and we may make use of the symmetries of the integrand to write [symbolically]

$$\begin{aligned} \int_0^{2\pi} \sim f &= \int_0^{2\pi} \sim f_S = 4 \int_0^{\pi/2} \sim f_S \quad (\ell + \ell') \text{ even} \\ &= 4 \left[\int_0^{\pi/3} \sim f_S + \int_{\pi/3}^{\pi/2} \sim f_S \right] \quad (C.21) \end{aligned}$$

The breakup of the integral over $0 \leq \gamma \leq \pi/2$ is used to avoid numerically integrating through a cusp of $|\sin 3\gamma|$. Hence DQG32 is used twice in the calculation of each integral $\mathcal{J}$. For the remaining case we have similarly

$$\int_0^{2\pi} \sim f = \int_0^{2\pi} \sim f_A = 4 \left[\int_0^{\pi/3} \sim f_A + \int_{\pi/3}^{\pi/2} \sim f_A \right] \quad (\ell + \ell') \text{ odd} \quad (C.22)$$

The accuracy of the numerical integrations for the typical choices

$$f_1(\gamma) = (\cos 3\gamma)^p \quad p = 1, 2, 3, 4, \quad \text{and}$$

$$f_2(\gamma) = (\gamma - \gamma_0)^2 \quad 0 \leq \gamma \leq \pi/3, \quad \gamma_0 = 0, \pi/12, \pi/6,$$

was tested by further subdividing the region of integration and

recalculating $\mathcal{J}$ numerically. This was done for several values of $(\ell + \ell')$ and $(K+2\sigma+2\sigma')$. In each test case considered, the change in the calculated value of $\mathcal{J}$ was less than one part in 10^{13} .

B. Transformations Between Expansion Bases

Each state ψ_α of the generally non-orthogonal expansion basis is labeled by the five integers $\alpha = (N_\alpha, \ell_\alpha, v_\alpha, J_\alpha, M_\alpha)$. The Hamiltonian matrix of Equation (3.30) is diagonalized separately for each value of angular momentum; thus, at any one time, we require only those basis states possessing given values of J and M . [The value of M is immaterial]. Such states are distinguished by the triplets $T_\alpha = (N_\alpha, \ell_\alpha, v_\alpha)$. These may be put into one-to-one correspondence with the integers $n(\alpha) = 1, 2, 3, \dots$ through the following procedure:

- 1) The triplets T_α which occur for fixed (J, M) are ordered from left to right according to increasing values of the three labels. In particular if $T_\alpha = (N_\alpha, \ell_\alpha, v_\alpha)$ and $T_\beta = (N_\beta, \ell_\beta, v_\beta)$ are any two such triplets, then T_α appears to the left of T_β if

$$N_\alpha < N_\beta \quad , \quad \text{or}$$

$$N_\alpha = N_\beta \quad , \quad \ell_\alpha < \ell_\beta \quad , \quad \text{or}$$

$$N_\alpha = N_\beta \quad , \quad \ell_\alpha = \ell_\beta \quad , \quad v_\alpha < v_\beta \quad .$$

- 2) When all triplets have been so ordered, they are assigned the integers $n(\alpha) = 1, 2, 3, \dots$ respectively from left to right.

As an example, we have the correspondence

$$\begin{array}{rcl}
 n(\alpha) & = & 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \ 10 \ 11 \ 12 \ 13 \ 14 \ 15 \\
 N_{\alpha} & = & 4 \ 5 \ 6 \ 6 \ 7 \ 7 \ 7 \ 8 \ 8 \ 8 \ 8 \ 9 \ 9 \ 9 \ 9 \\
 \ell_{\alpha} & = & 4 \ 5 \ 4 \ 6 \ 5 \ 7 \ 7 \ 4 \ 6 \ 8 \ 8 \ 5 \ 7 \ 7 \ 9 \\
 v_{\alpha} & = & 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 1 \ 1
 \end{array}$$

for the first fifteen states [i.e., $N_{\alpha} \leq 9$] of the $J = 8$ expansion basis.

States of the associated orthonormal basis $\{\psi_i: i = (N_i, \ell_i, t_i, J, M)\}$ may have their triplets $T_i = (N_i, \ell_i, t_i)$ similarly enumerated. For convenience we may think of the label t_i as taking on the same numerical values as do the corresponding v_{α} . The orthonormal basis is completely specified when the transformation matrix $[U]$ of Equation (3.22) is given. For fixed (JM) we may write the relationship as

$$\psi_i = \sum_{\alpha} [U]_{T_i, T_{\alpha}} \psi_{\alpha}, \quad (J_i M_i) = (J_{\alpha} M_{\alpha}) = (JM) \quad (C.23)$$

$[U]$ is constructed, using the method of Section III.B, from the normalization matrix $[N]$. For fixed (JM) , the latter is

$$\begin{aligned}
 [N]_{T_{\alpha}, T_{\beta}} &= \langle N_{\alpha} \ell_{\alpha} | N_{\beta} \ell_{\beta} \rangle \langle \ell_{\alpha} v_{\alpha} J | \ell_{\beta} v_{\beta} J \rangle \\
 &= \delta_{N_{\alpha}, N_{\beta}} \delta_{\ell_{\alpha}, \ell_{\beta}} \langle \ell_{\alpha} v_{\alpha} J | \ell_{\alpha} v_{\alpha} J \rangle \quad (C.24)
 \end{aligned}$$

For $J = 8$, the low-energy portion of $[N]$ is shown in Figure C.3. The submatrices

$$\begin{bmatrix} 1 & a \\ a & 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & b \\ b & 1 \end{bmatrix}$$

occur repeatedly along the main diagonal of $[N]$. They are associated

Figure C.3. $[N]$, $[U]$ and $[U^A]$ matrices for $J = 8$, $N \leq 9$

with the v -multiplicity of $(\ell_\alpha, J) = (7, 8)$ and $(8, 8)$ respectively. In each case v_α takes on the possible values 0 and 1, and the submatrices are 2×2 . From Equations (2.34) and (2.35), it is easy to show that all such submatrices for $J = 8$ are 2×2 . That is, for fixed $(\ell_\alpha, J = 8)$, v_α can have at most two values. [v_α has exactly two values for $(\ell_\alpha, 8)$ whenever ℓ_α is greater than 6 and not a multiple of 3.] The matrix $[P]$ which diagonalizes $[N]$, and hence the transformation matrix $[U]$ [see Equations (3.24)-(3.26)] have a similar block-diagonal form. The latter is pictured in Figure C.3. In practice, the diagonal blocks of $[P]$ are found by employing the double precision subroutine EIGRS (47). The resulting matrix $[U]$ is quite sparse and is specified by the small submatrices¹

$$[u(\ell_\alpha, J)]_{t_i, v_\alpha} = [U]_{N_\alpha \ell_\alpha t_i, N_\alpha \ell_\alpha v_\alpha}, \quad N_\alpha = \ell_\alpha, \ell_\alpha + 2, \ell_\alpha + 4, \dots \quad (C.25)$$

If the matrix $[V']$,

$$\begin{aligned} [V']_{T_\alpha, T_\beta} &\equiv \langle \psi_\alpha | h(\beta) f(\gamma) | \psi_\beta \rangle && [\text{fixed (JM)}] \\ &= \langle N_\alpha \ell_\alpha | h(\beta) | N_\beta \ell_\beta \rangle \langle \ell_\alpha v_\alpha J | f(\gamma) | \ell_\beta v_\beta J \rangle, && (C.26) \end{aligned}$$

has been computed by the methods of Section A, then

$$[V]_{T_i, T_j} \equiv \langle \psi_i | h(\beta) f(\gamma) | \psi_j \rangle \quad [\text{fixed (JM)}] \quad (C.27)$$

¹For fixed (ℓ, J) within the maximal expansion basis of Table 2.3, v can take on at most four values. Thus $[u(\ell_\alpha, J)]$ in Equation (C.25) is no larger than 4×4 .

could be computed straightforwardly by performing the matrix multiplication

$$[V] = [U][V'] [U]^t .$$

In practice time is saved by realizing that the orthogonality properties of the ψ_α may be used to write Equation (C.23) more explicitly as

$$\begin{aligned} \psi_{N\ell tJM} &= \sum_v [U]_{N\ell tJM, N\ell vJM} \psi_{N\ell vJM} \\ &= \sum_v [u(\ell, J)]_{t,v} \psi_{N\ell vJM} \\ &= f_{N\ell}(\beta) \sum_v [u(\ell, J)]_{t,v} \phi_{\ell vJM}(\gamma, \theta_i) . \end{aligned} \quad (C.28)$$

Hence for matrix elements between orthonormal basis states of fixed J and M we have

$$[V]_{T_i, T_j} = \langle \psi_i | h(\beta) f(\gamma) | \psi_j \rangle = [h]_{N_i \ell_i, N_j \ell_j} [f]_{\ell_i t_i, \ell_f t_f} \quad (C.29)$$

where

$$[h]_{N_i \ell_i, N_j \ell_j} \equiv \langle N_i \ell_i | h(\beta) | N_j \ell_j \rangle , \quad (C.30)$$

$$[f]_{\ell_i t_i, \ell_f t_f} \equiv \sum_{v_i v_f} [u(\ell_i, J)]_{t_i v_i} \langle \ell_i v_i J | f(\gamma) | \ell_f v_f J \rangle [u(\ell_f, J)]_{t_f v_f} . \quad (C.31)$$

The latter matrix may be written as the product

$$[f] = [U^A][f'] [U^A]^t \quad (C.32)$$

where

$$[f']_{\ell_i v_i, \ell_f v_f} \equiv \langle \ell_i v_i J | f(\gamma) | \ell_f v_f J \rangle , \quad (C.33)$$

and where $[U^A]$ is the angular portion of the overlap matrix $[U]$:

$$\begin{aligned} [U^A]_{\ell_i t_i, \ell_f v_f} &\equiv [U]_{\ell_i \ell_i t_i J M, \ell_f \ell_f v_f J M} \\ &= \delta_{\ell_i \ell_f} [u(\ell_i, J)]_{t_i, v_f} \end{aligned} \quad (C.34)$$

For the $J = 8$ example, $[U^A]$ is shown in Figure C.3. In practice, the matrix elements of $[h]$ and $[f']$ are found using the methods of Section A. $[f]$ is then assembled from Equation (C.32), and finally Equation (C.29) is used to obtain matrix elements in the orthonormal basis. $[h]$, $[f]$, $[f']$ and $[V]$ are all symmetric matrices, and only elements on and above the main diagonal need be computed.

The elements $[V]_{n(i), n(j)}$ are written on magnetic tape in the order

$$V_{11}, V_{12}, V_{22}, V_{13}, V_{23}, V_{33}, V_{14}, \dots$$

for each potential energy function $V = h(\beta)f(\gamma)$. They are preceded on the tape by storage information specifying J , the number of potentials, and the size of the expansion basis [ie., $N_{\max}(J)$]. They are followed by the non-trivial matrices $[u(\ell, J)]^t$. Prior to use by the THEORY package, the tape file is usually transferred to a magnetic disc to speed input/output operations. THEORY then reads the necessary portion of the MEWORK output, and assembles the Hamiltonian matrix from the SR matrix elements [using, for example, Equation (3.34)]. The full expansion basis for which matrix elements have been computed need not be used by THEORY. As the elements are stored in order of increasing N , $[H]$ may be conveniently assembled for a smaller basis calculation by

reading only the leading portion of each potential matrix $[V]$. The lowest few eigenvalues of $[H]$ and their associated eigenvectors are found by using the EISPACK subroutines mentioned previously. When desired, the eigenvectors may be expressed in terms of the original basis functions ψ_α by use of the $[u(\ell, J)]^t$ matrices and Equation (3.29).

C. Preliminary Testing of Computational Techniques

Advanced testing of the MEWORK and THEORY packages, using the potential energy function of Gneuss and Greiner, is discussed at length in Chapter IV. In this section, the preliminary testing, which proceeded in several stages, is described. Initially, dummy input was used to check that each "single task" segment of code was performing as designed. The MEWORK package was then assembled and called upon to produce the matrix elements of $h(\beta)f(\gamma) = \beta^0 \cdot 1$. As would be the case in normal usage, radial matrix elements were calculated using Equation (C.14), and numerical integration of Equation (C.19) was employed in calculating the angular factors. The calculated matrix elements in the orthonormal basis were then compared with those of the unit matrix. For various values of J and $N_{\max}(J) \leq 20$, off-diagonal elements were found to be no larger in magnitude than $\sim 10^{-12}$. Diagonal elements differed from unity by amounts ranging from $\pm 10^{-16}$ to $\pm 10^{-12}$. At the conclusion of this phase of testing, MEWORK was modified so that calculated matrix elements having magnitudes $\leq 10^{-10}$ were set equal to zero. This served to prevent underflow errors in the THEORY package.

Of the tests performed on the THEORY package, the most severe

involved verifying that the output eigenvectors and eigenvalues satisfied the original-basis form of the eigenvalue problem, Equation (3.21). Such a test served to insure that the transformations between the original and orthonormal bases were being properly performed. Two potentials were employed in the test calculations:

$$V(\beta, \gamma) = \beta^2 \cos 3\gamma \quad ,$$

and

$$V(\beta, \gamma) = \text{Gneuss-Greiner potential for } {}^{124}\text{Te} \quad .$$

[see Chapter IV]

In each case the MEWORK package was used twice to produce necessary matrix elements. Initially it was run in the normal manner to produce matrix elements between orthonormal states. On the second trial, transformation via [U] was blocked, and the output file thus consisted of matrix elements between states of the original basis. The normal output file was supplied to the THEORY package which computed and stored the eigenvalues of H , E_q , and the original-basis representations of the associated eigenvectors, b_q^η . This was done for each of three angular momenta [$J = 6, 9, 12$] in which the multiplicity label v plays a non-trivial role. [E.g., for $\ell = 12$, $J = 12$, v takes on the values 0, 1, and 2]. The maximum value of the principal quantum number, $N_{\max}(J)$, was 15, 20, and 17 respectively for the three angular momenta bases. A special purpose routine EVTEST was then written. Using the secondary output from MEWORK, the output of THEORY, and the $\langle \ell v J | \ell v' J \rangle$ from the A^η tape files, EVTEST assembled

$$\underline{\Delta}_q = [H'] \underline{b}^q - E_q [N] \underline{b}^q, \quad (C.35)$$

$$[H']_{\alpha\beta} \equiv \langle \psi_{\alpha}^{\tilde{s}} | H | \psi_{\beta}^{\tilde{s}} \rangle,$$

$$[N]_{\alpha\beta} \equiv \langle \psi_{\alpha}^{\tilde{s}} | \psi_{\beta}^{\tilde{s}} \rangle = \langle \psi_{\alpha} | \psi_{\beta} \rangle = \langle \ell_{\alpha}^{\nu_{\alpha} J} | \ell_{\alpha}^{\nu_{\alpha} J} \rangle \delta_{\ell_{\alpha} \ell_{\beta}},$$

for each eigenvector $\underline{b}^q$. Ideally, as may be seen from Equation (3.18), $\underline{\Delta}_q$ should be the zero vector; its calculated components were found to range in magnitude between 10^{-12} and 10^{-16} .

For the simplest Bohr-like Hamiltonian, H_B^I , exact eigenfunctions and eigenvalues are available, and expansion techniques are not necessary. However the numerical solution of $H_B^I \phi = E \phi$ affords a simple test of the MEWORK and THEORY packages; furthermore, it provides insight into the importance of the basis parameter $\tilde{s}$. Typical investigations of reduced spectra in Chapter V employ expansion bases of 20 phonons. Thus it is a reasonable exercise to attempt the numerical solution of the standard reduced Bohr problem by expanding in a 20-phonon basis of eigenfunctions, $\psi_i^{\tilde{s}}$, of

$$H_B = -\frac{1}{2} T(\beta, \gamma, \theta_i) + \frac{1}{2} \tilde{s}^4 \beta^2. \quad (C.36)$$

For $\tilde{s} \neq 1$, truncation effects should appear in the reduced spectra. Results of such an investigation for three choices of $\tilde{s}$ are contained in Table C.1. Calculated reduced energies for states at or below 6 phonons of excitation are listed with J_i denoting the i^{th} state of spin J (arranged in order of increasing energy). Notice that the states 3_2 and 0_5 which have the same value of (N, ℓ) are calculated to be degenerate.

Table C.1. Calculated reduced energies $[(E(J_i) - E(0_1)) / (E(2_1) - E(0_1))]$ resulting from a diagonalization of H_B^1 in a ψ^S 20-phonon expansion basis

J_i^a	STATE			CALCULATED REDUCED ENERGY		
	N	ℓ	ν	$\tilde{s} = 1$	$\tilde{s} = 1.2$	$\tilde{s} = 1.4$
4_1	2	2	0	2.0	2.00000000	2.00000044
0_2	2	0	0		2.00000000	2.00000217
0_3	3	3	1	3.0	3.00000000	3.00001626
2_3	3	1	0		3.00000000	3.00005093
8_1	4	4	0	4.0	4.00000000	4.00003859
4_3	4	2	0		4.00000001	4.00013156
0_4	4	0	0		4.00000001	4.00022534
8_2	5	5	0	5.0	5.00000007	5.00039951
3_2	5	3	0		5.00000026	5.00134700
0_5	5	3	1		5.00000026	5.00134700
2_6	5	1	0		5.00000051	5.00244086
3_3	6	6	1	6.0	6.00000013	6.00072413
5_3	6	4	0		6.00000055	6.00253988
4_7	6	2	0		6.00000118	6.00488445
0_6	6	0	0		6.00000172	6.00669543

^aThe Bohr eigenstate specified by (N, ℓ , ν , J, M=J) may also be identified by $J_i \equiv i$ -th (N ℓ ν) triplet of spin J ordered by the scheme of Appendix C, Section B.

If the potential energy term of a generalized Bohr Hamiltonian H is a function of β only, ℓ remains a good quantum number [see Section E of Appendix A]. The spectrum of H then consists of ℓ -multiplets, each of which [for $\ell > 1$] contains two or more exactly degenerate states of different J . The computational procedure appears to insure that such exactly degenerate states will be calculated to be degenerate if expansion bases of the same "size" are employed. Here size refers to the value of $N_{\max}(J)$ rather than to the number of states. This result, which is independent of the choice of $\tilde{s}$, does not reflect upon the accuracy of the calculated energies. For example, the calculated energies of the 0_5 and 3_2 states, though equal, will be in considerable error if $\tilde{s} \gg 1$.

Because of the existence of the calculational degeneracies, a single representative state is listed in Table C.1 for each (N, ℓ) pair, the 0_5 - 3_2 doublet being the sole exception. The optimal choice for $\tilde{s}$ is of course unity. If $\tilde{s}$ is too large by 20%, the effect on the reduced spectrum is negligible. For a 40% error in $\tilde{s}$, the highest energies in the table are in error by $\sim 1\%$. The expansion basis is seen to become increasingly inadequate for states possessing large N and $(N - \ell)$. Figure C.4a displays the differences between the potential wells of the problem being solved [solid line] and those of the $\tilde{s} = 1.2$ and 1.4 expansion basis Hamiltonians [dashed lines]. Absolute energies of some lower states are indicated for two of the wells. It is gratifying to find that the huge difference between the $\tilde{s} = 1$ and $\tilde{s} = 1.4$ curves does not strongly manifest itself in Table C.1.

Figure C.5 displays the results of further calculations of a similar

Figure C.4. Potential energy functions, $V_{\text{Bohr}} = \frac{1}{2} \tilde{S}^4 \beta^2$, employed in test calculations

Figure C.5. The effect of mischoosing the basis parameter $\tilde{S}$

nature. In this case the expansion basis parameter was fixed at unity, and the parameter A was varied in the Bohr-like Hamiltonian being treated:

$$H = -\frac{1}{2}T(\beta, \gamma, \theta_i) + (\frac{1}{2} + A)\beta^2 \quad . \quad (C.37)$$

Only results for $-.495 \leq A \leq -.4$ and $1.75 \leq A \leq 4$ are shown, with arrows indicating the step size between successive values of A for which numerical solutions were found. For $-.4 \leq A \leq 1.75$, errors in the calculated reduced energies would not be visibly discernible on the scale of the graph. $N_{\max}(J)$ ranges from 14 to 25, and was chosen such that the number of basis states was approximately 50 for each J treated. Deviations from the true spectrum may be seen to occur earlier for those angular momenta which have smaller values of $N_{\max}(J)$ characterizing their expansion bases. The $J = 4$ and 6 states belonging to the $N = 2 = 3$, $J = 0, 3, 4, 6$ quartet were each expanded in $N_{\max}(J) = 14$ bases and were calculated to be degenerate. For the four endpoints, $A = -.495, -.4, 1.75$, and 4.0 , the optimal expansion basis parameters are $\tilde{s} = (1 + 2A)^{\frac{1}{4}} = .316, .669, 1.456$, and 1.732 respectively. The associated potential wells are shown as solid curves in Figure C.4(b). The shaded regions correspond to the calculations of Figure C.5. The $\tilde{s} = 1$ expansion basis (dashed curve) may be used with confidence to treat a Hamiltonian whose potential-well curve lies between the shaded regions. For a parabolic well at least, reduced energies of the lower states will be in error by no more than 1%.

To insure accurate calculations, optimal values of $\tilde{s}$ and basis size

should be estimated by the methods of Chapter IV. However for initial explorations an $\tilde{s} = 1$, 50-state calculation may be sufficient for treating

$$H = -\frac{1}{2}T(\beta, \gamma, \theta_i) + V(\beta, \gamma) \quad ,$$

provided that $V(\beta, \gamma)$ is "somewhat parabolic", i.e.

$$V(\beta, \gamma) \xrightarrow{\beta \rightarrow \infty} \frac{1}{2}\beta^2 \quad ,$$

and that high accuracy is not required. Such bases were used to redo calculations for two collective Hamiltonians reported in the literature.

Rabotnov and Seregin (28) treated the $J \leq 6$ eigenstates of

$$H_{RS} = -\frac{1}{2}T(\beta, \gamma, \theta_i) + \frac{1}{2}\beta^2 + C_1\beta\cos 3\gamma + C_2\beta \quad , \quad (C.38)$$

by expanding in solutions to the Bohr problem. The angular factors of the expansion eigenfunctions employed by these authors were taken from Bes (15).¹ Theoretical reduced spectra of H_{RS} for three sets of

¹The Schroedinger equation $H_B\phi = E\phi$ may be separated into radial and angular problems via the substitution $\phi = F(\beta)\Phi(\gamma, \theta_i)$. In treating the $\Phi(\gamma, \theta_i)$ problem, Bes considered each value of J in turn. For each even [or odd] spin, a basic set of $(\frac{1}{2}J + 1)$ [or $\frac{1}{2}(J - 1)$] functions $\{\psi_k(\gamma, \theta_i)\}$ was constructed. In terms of these basic functions, the general solution may be written as

$$\Phi(\gamma, \theta_i) = \sum_k W_k(\gamma)\psi_k(\gamma, \theta_i) \quad .$$

The W_k are solutions to a set of coupled differential equations, and may be obtained as polynomials in $\cos(3\gamma)$. This method of finding the $\Phi(\gamma, \theta_i)$ becomes increasingly tedious as J increases, and Bes investigated only the spins $J \leq 6$.

(C_1, C_2) were reported. [The (C_1, C_2) parameters in Equation (C.38) are related to the (α, γ_0) of Reference (28) by $C_1 = -\alpha\gamma_0$, $C_2 = \gamma_0(\alpha - 1)$]. The calculated spectra of Rabotnov and Seregin are compared with my own in Figure C.6. For each spin, I employed an $\tilde{s} = 1$ basis whose size was constrained by

- 1) $N_{\max}(J) \leq 30$, and
- 2) Number of expansion states per $J \leq 135$.

Rabotnov and Seregin confined themselves to expansion bases containing fewer than 65 states per J , and presumably used the equivalent of $\tilde{s} = 1$. Though overall agreement is good, sizeable differences may be noted between the calculated energies of the 3_1^+ and 6_1^+ states in Figure C.6. The convergence rates for these states are displayed in Table C.2. Here I have re-treated H_{RS} using the smaller $\tilde{s} = 1$ bases indicated. $N_{\max}(J) = 15$ appears to be sufficiently large. Differences in Figure C.6 may be due to the use of an inadequately small basis on the part of Rabotnov and Seregin.

In References (43) and (44), Kumar and Baranger considered the Hamiltonian

$$H_{KB} = \frac{-\hbar^2}{2B} T(\beta, \gamma, \theta_i) + \frac{C}{2} \beta^2 - f \beta^3 \cos 3\gamma + \left[G_0 + G_1 \left(\frac{\beta}{a} \right)^3 \cos 3\gamma + G_2 \left(\frac{\beta}{a} \right)^6 \cos^2 3\gamma \right] e^{-\beta^2/a^2} \quad . \quad (C.39)$$

Figure C.6. Test calculations using the potential proposed by Rabotnov and Seregin (28). Reduced energies of the states $J_i = 0_1-0_3, 2_1, 2_2, 3_1, 4_1$ and 6_1 are shown

Table C.2. Influence of expansion basis size on the calculated reduced energies of selected H_{RS} levels ($\tilde{s} = 1$)

Parameters of H_{RS}	CALCULATED REDUCED ENERGY			
	J_i	$N_{\max}(J)=8$	$N_{\max}(J)=15$	$N_{\max}(J) \geq 20^a$
$C_1 = -2.$ $C_2 = 0.$	3_1	12.586	10.491	10.484
	4_1	2.984	2.595	2.594
	6_1	5.251	4.569	4.568
$C_1 = -1.$ $C_2 = -1.$	3_1	6.657	6.437	6.437
	4_1	2.424	2.377	2.377
	6_1	4.117	4.003	4.003
$C_1 = -1.5$ $C_2 = 0.$	3_1	6.478	6.205	6.202
	4_1	2.300	2.253	2.253
	6_1	3.763	3.684	3.683

^aThe expansion basis is that indicated in Figure C.6.

Eigenfunctions of H_{KB} were expanded¹ as

$$\begin{aligned} \phi_{\alpha, JM}(\beta_0, \beta_{21}, \theta_i) = \sum_K A_{\alpha JK}(\beta_0, \beta_{21}) \left[\frac{(2J+1)}{2(8\pi^2)(1+\delta_{K,0})} \right]^{\frac{1}{2}} \\ \times \left[D_{MK}^{J*}(\theta_i) + (-1)^J D_{M, -K}^{J*}(\theta_i) \right], \end{aligned} \quad (C.40)$$

using the shape variables

$$\beta_0 \equiv \beta \cos \gamma$$

$$\beta_{21} \equiv \beta \sin \gamma.$$

The values of $A_{\alpha JK}$ at mesh points in the β - γ plane were used as variational parameters, and the Schrodinger equation was reduced to a set of linear algebraic equations in the $A_{\alpha JK}$. Results were reported for spins $J \leq 4$. For the finest mesh employed [256 points], there were 392 variational parameters in the worst case [$J = 4$], and the partial diagonalization of a matrix of this size was required. The low-energy spectrum of ^{154}Sm was shown to be reasonably reproduced by selecting the parameters in Equation (C.39) to be

$$\begin{aligned} C &= 77 \text{ MeV} & , & & G_0 &= 6.7 \text{ MeV} & , \\ f &= 9.7 \text{ MeV} & , & & G_1 &= -5.5 \text{ MeV} & , \\ \frac{B}{\hbar^2} &= 127 \text{ MeV}^{-1} & , & & G_2 &= -1.3 \text{ MeV} & , \\ a &= .3 & . & & & & \end{aligned}$$

¹Kumar and Baranger employ the volume element $d\Omega = |\sin 3\gamma| \beta^4 \sin \theta_2 d\beta d\gamma d\theta_1 d\theta_2 d\theta_3$ rather than the $d\Omega$ of Equation (2.14). The missing factor of $(8\pi^2)^{-1}$ appears as $(8\pi^2)^{-\frac{1}{2}}$ in Equation (C.40).

In treating the ^{154}Sm Hamiltonian by my methods, I began with the reduction

$$\beta' = \left[\frac{BC}{2} \right]^{\frac{1}{2}} \beta = 9.944286 \beta \quad ,$$

$$\bar{H}_{KB} = H_{KB}/\hbar\omega \quad , \quad \omega \equiv \sqrt{\frac{C}{B}} \quad .$$

The resulting Hamiltonian

$$\bar{H}_{KB} = -\frac{1}{2}T(\beta', \gamma, \theta_i) + \bar{V}_{KB}(\beta', \gamma) \quad , \quad (\text{C.41a})$$

$$\begin{aligned} \bar{V}_{KB}(\beta', \gamma) = & \frac{1}{2}(\beta')^2 - .01267(\beta')^3 \cos 3\gamma + e^{-.11236(\beta')^2} \\ & \times [8.6046 - .26602(\beta')^3 \cos 3\gamma - .002368(\beta')^6 \cos^2 3\gamma] \end{aligned} \quad (\text{C.41b})$$

was diagonalized in an $\tilde{s} = 1$ basis of approximately 75 states per spin, and the eigenvalues of H_{KB} were reconstructed. The resulting absolute energies are displayed in Figure C.7, together with a series of results reported by Kumar and Baranger. Their results may be seen to be tending toward mine as the calculational mesh becomes finer. The adequacy of my own ~ 75 state basis is indicated by $\tilde{s} = 1$ convergence calculations, the results of which are summarized in Table C.3. Incidentally, the calculated theoretical energies for H_{KB} yrast states of higher spin are [in MeV above the GS]

J_i :	5 ₁	6 ₁	7 ₁	8 ₁	10 ₁	12 ₁
$E(J_i) - E(0_1)$:	1.754	<u>.536</u>	2.088	<u>.873</u>	<u>1.271</u>	<u>1.718</u>
$N_{\max}(J)$ used :	23	17	20	16	15	15

Figure C.7. A test calculation using the potential employed by Kumar and Baranger (43, 44)

Table C.3. Convergence of absolute energies for selected states of the ^{154}Sm Hamiltonian, H_{KB}

CALCULATED ABSOLUTE ENERGY (MeV)													
Level J_i	J $N_{\text{max}}(J)$ # states:	small basis				~ 50 state basis				~ 75 state basis			
		0	2	3	4	0	2	3	4	0	2	3	4
		2	12	12	12	22	16	25	14	27	20	30	17
		9	30	12	36	52	51	52	49	75	77	75	72
3_1			6.4947				6.4867				6.4867		
2_3			6.4011				6.3852				6.3847		
2_2			6.2485				6.2222				6.2215		
0_2			6.0917				6.0733				6.0733		
4_1			5.2693				5.2656				5.2645		
2_1			5.0858				5.0805				5.0804		
0_1			4.9972				4.9954				4.9954		

where the last line specifies the size of the $\tilde{s} = 1$ expansion basis used for each spin. The 6_1 , 8_1 , 10_1 and 12_1 positive parity states of ^{154}Sm have been experimentally located at .545, .927, 1.401, and 1.934 MeV respectively (69). These may be compared with the underlined theoretical values.

D. Splitting of H_B Energies

Having concluded the preliminary testing, we are in a position to utilize the MEWORK and THEORY packages as exploratory tools. In particular we can gain insight into the effects of simple perturbations upon the H_B' spectrum. The calculations of the previous section indicate that the Bohr-like problem

$$H\phi = E\phi \quad (C.42a)$$

$$H = -\frac{1}{2}T(\beta, \gamma, \theta_1) + \frac{1}{2}\beta^2 + U(\beta, \gamma) \quad (C.42b)$$

may be adequately treated with an $\tilde{s} = 1$ expansion basis of moderate size [i.e., ~ 50 states per spin] provided that $U(\beta, \gamma)$ is a "minor" perturbation. Let us take $U(\beta, \gamma)$ to be proportional to a strength parameter A which can be slowly increased from zero. For a given value of A , the perturbation U will be considered "minor" if a modest increase in the size of the basis [say to ~ 60 states per spin] does not visibly alter the calculated low-energy spectrum. Here we will be more interested in observing general trends than in obtaining highly accurate eigenvalues, and no further convergence studies need be attempted.

We begin by considering simple γ -independent perturbations

$$U(\beta) = A\beta^p, \quad p = 1, 2, 3 \dots \quad (C.43)$$

Due to the orthogonality of the angular factors of the ψ_i , the perturbation does not mix basis states of different ℓ :

$$\langle \tilde{\psi}_i | U(\beta) | \tilde{\psi}_j \rangle = 0 \quad \text{if } \ell_i \neq \ell_j \quad (C.44)$$

The state ϕ of H which collapses smoothly to ψ_i as $A \rightarrow 0$ [i.e., as $U(\beta) \rightarrow 0$] will consequently possess ℓ_i as a good quantum number.¹ As A is increased from zero, the degenerate ψ_i with a common $U(5)$ label N will generally be split into $[(N+2)/2]_{G_1}$ ℓ -multiplets. $\ell = N, N-2, N-4, \dots, 0$ or 1 will remain a good $R(5)$ label for describing the perturbed states [see, for example, Figure 5.6].

The direction of the splitting may be anticipated from Figure 2.7. For fixed N the radial probability density $P(\beta)$ shifts toward larger β as $(N - \ell)$ increases. Hence if $U(\beta)$ rises quickly enough, unperturbed states of higher $(N - \ell)$ will have a larger integral in Equation (2.50) and will be split upwards relative to the states of lower $(N - \ell)$. To determine how fast $U(\beta)$ must rise for this to be the case, we note that for $U(\beta) \propto \beta^2$ the unperturbed spectrum is not split. $p = 2$ is evidently the break-even point. For $A > 0$ in Equation (C.43), we then expect that energies of the states arising from ψ_i of a given N will be ordered in increasing or decreasing ℓ as P is <2 or >2 respectively. Diagonal

¹ If ϕ is not degenerate with another eigenfunction ϕ' of H possessing the same angular momentum character (JM), ℓ_i must be a good quantum number of ϕ . See Section E of Appendix A.

matrix elements of the perturbing function may be seen to obey a similar rule in Table C.4 [$p = 1, 2, 3$]. The lower portion of the reduced energy spectrum, as a function of A , is shown in Figure C.8 for $p = 1, 3$. The double-ended arrow $|\leftrightarrow|$ indicates the difference between successive values of A for which diagonalizations were performed. When the calculated reduced energies of states within the same ℓ -multiplet differ by .0001 or more, the energies are labeled [for the extreme values of A only]. For $U(\beta) = A\beta^3$ with $A < 0$, the potential well turns downward at large β and normalizable solutions ϕ do not exist. However, both positive and negative values of A may be investigated if a damping exponential is included. When this is done, a spectrum similar to that for $U(\beta) = A\beta$ can be seen to result.

The ℓ -degeneracy of the perturbed spectrum may be removed by choosing U to have γ -dependence:

$$U(\beta, \gamma) = h(\beta)f(\gamma) \quad . \quad (C.45)$$

$f(\gamma)$ is presumed to be cyclic in the asymmetry angle

$$f(\gamma + 2\pi) = f(\gamma) \quad ,$$

and to possess the quadrupole surface symmetries

$$f(\gamma) = f(-\gamma) = f(\gamma - 2\pi/3) \quad . \quad (C.46)$$

If $f(\gamma)$ is expanded in a Fourier series

$$f(\gamma) = \sum_{n=0}^{\infty} [a_n \sin n\gamma + b_n \cos n\gamma] \quad ,$$

one may easily show that only the coefficients $b_0, b_3, b_6, b_9, \dots$ can

Table C.4. Diagonal radial matrix elements for
selected low-energy Bohr eigenfunctions,
 ψ_α

N	ℓ	$\langle N\ell \beta N\ell\rangle$	$\langle N\ell \beta^2 N\ell\rangle$	$\langle N\ell \beta^3 N\ell\rangle$
0	0	1.504505556	2.5	4.513516668
1	1	1.805406667	3.5	7.221626669
2	0	1.955857223	4.5	11.283791671
2	2	2.063321906	4.5	10.316609528
3	1	2.192279525	5.5	14.959083815
3	3	2.292579895	5.5	13.755479370
4	0	2.326610378	6.5	19.746635424
4	2	2.407208890	6.5	18.913784134
4	4	2.500996249	6.5	17.506973744

RESULT OF DIAGONALIZING
 $H = -\frac{1}{2} T(\beta, \gamma, \theta i) + \frac{1}{2} \beta^2 + U(\beta)$
 IN A BASIS HAVING $\tilde{S}=1$

EXPANSION BASIS						
J	:	0	2	3	4	6
$N_{\text{MAX}}(J)$	:	24	18	27	16	15
# STATES	:	61	63	61	64	61

Figure C.8. The effect of adding a radial perturbation to H_B^1

be non-zero. Consequently $f(\gamma)$ can be written in either of two equivalent forms:

$$\begin{aligned} f(\gamma) &= \sum_{m=0}^{\infty} b_{3m} \cos 3m\gamma \\ &= \sum_{m=0}^{\infty} b'_m (\cos 3\gamma)^m \end{aligned}$$

For several simple choices of $h(\beta)$ and $f(\gamma)$ in Equation (C.45), the resulting spectra appear in Figure C.9. Both

$$U_1 = A h(\beta) \cos 3\gamma$$

and

$$U_2 = -A h(\beta) \cos 3\gamma$$

give rise to identical reduced spectra, as each is the reflection about $\gamma = 30^\circ$ of the other [see Section E of Appendix A]. For this reason only $A \geq 0$ is considered in the upper portion of Figure C.9. $U = A \cos 3\gamma$ may be seen to be much more successful in splitting the $N = 2$ levels than is $U = \cos^2 3\gamma$. As pointed out below Equation (2.46), no perturbation $U = f(\gamma)$ can produce first-order splitting of these three levels.

The two functions, $f(\gamma)$, considered in Figure C.9 differ in their topographical features. Although $(-\cos 3\gamma)$ and $\cos^2 3\gamma$ each possess a single minimum on $0^\circ \leq \gamma \leq 60^\circ$, the minimum occurs at $\gamma = 0^\circ$ and $\gamma = 30^\circ$ respectively. Consequently

$$\begin{aligned} -A \cos 3\gamma &\text{ resembles } \bar{V}_{QP}(\beta, \gamma) \text{ with } \beta_0 = 0, \gamma_0 = 0^\circ; \quad \text{and} \\ A \cos^2 3\gamma &\text{ resembles } \bar{V}_{QP}(\beta, \gamma) \text{ with } \beta_0 = 0, \gamma_0 = 30^\circ \end{aligned}$$

This leads to striking similarities between the spectra of corresponding pairs [see Figures 5.40 and C.9].

Figure C.9. The effect of adding simple γ -dependent terms to H_B^I

X. APPENDIX D. COMPUTATIONAL TECHNIQUES IN THE CALCULATION OF QUADRUPOLE MOMENTS AND E2 TRANSITION RATES

The calculation of $B(E2)$ values and quadrupole moments, as outlined in Section D of Chapter III, requires the reduced matrix elements appearing on the right-hand side of Equation (3.59). Computationally useful expressions for these matrix elements are developed in Section A of this appendix. The manner in which these expressions are employed in practical calculations is the topic of Section C. There, the workings of the GAMME and BE2PRO computer codes are discussed. The testing of these two codes is described in Section D. Attempts to reproduce reported H_{GG} results (29, 30) lead to second-order discrepancies when the $J_i = 3_1$ state is involved. A number of selection rules exist which may be used to speed the calculations and to test the GAMME and BE2PRO codes. Derivations of these selection rules are outlined in Section B.

A. Reduced Matrix Elements of $\Omega_{k,\mu}^{LAB}$ Operators

We begin by considering the matrix element

$$M_{\alpha\alpha'}^{k,\mu} \equiv \langle \tilde{\psi}_{\alpha} | \Omega_{k,\mu}^{LAB} | \tilde{\psi}_{\alpha'} \rangle \quad \alpha = (N\ell vJM), \quad \alpha' = (N'\ell'v'J'M') \\ = \int_{\Omega} \tilde{\psi}_{\alpha}^*(\beta, \gamma, \theta_i) \Omega_{k,\mu}^{LAB}(\beta, \gamma, \theta_i) \tilde{\psi}_{\alpha'}(\beta, \gamma, \theta_i) d\Omega(\beta, \gamma, \theta_i) \quad (D.1)$$

The first [$k = 1$] and second-order [$k = 2$] LAB operators, $\Omega_{k,\mu}^{LAB}$, are defined in Equations (3.56). Again it must be emphasized that the subscript k does not refer to the angular momentum characterization of the operators; $J = 2$ is understood. It is convenient to express these

operators in terms of the Bohr coordinates. Mirroring Equation (2.3) which connects the LAB and BF versions of the generalized coordinates $[\alpha_\mu$ and $a_\mu]$, we introduce the body-fixed operators

$$\Omega_{k,\epsilon}^{BF} \equiv \sum_{\mu} D_{\mu\epsilon}^{2*}(\theta_i) \Omega_{k,\mu}^{LAB} \quad [k = 1, 2] \quad , \quad (D.2)$$

or equivalently

$$\Omega_{k,\mu}^{LAB} = \sum_{\epsilon} D_{\mu\epsilon}^{2*}(\theta_i) \Omega_{k,\epsilon}^{BF} \quad [k = 1, 2] \quad . \quad (D.3)$$

$\Omega_{k,\epsilon}^{BF}$ so defined plays the same role in the BF frame as $\Omega_{k,\epsilon}^{LAB}$ plays in the LAB frame. [See Section F of Appendix F.] As expected, the BF operators depend only upon the shape parameters. The evaluation of the right-hand side of Equation (D.2) leads one to

$$\Omega_{1,\epsilon}^{BF}(\beta, \gamma, \theta_i) = a_\epsilon = \beta \cdot \left\{ \begin{array}{ll} 2^{-\frac{1}{2}} \sin \gamma , & \epsilon = \pm 2 \\ 0 & , \quad \epsilon = \pm 1 \\ \cos \gamma , & \epsilon = 0 \end{array} \right\} \quad , \quad (D.4a)$$

and

$$\Omega_{2,\epsilon}^{BF}(\beta, \gamma, \theta_i) = [aa]_{2\epsilon} = \beta^2 \cdot \left\{ \begin{array}{ll} (4/7)^{\frac{1}{2}} \sin \gamma \cos \gamma , & \epsilon = \pm 2 \\ 0 & , \quad \epsilon = \pm 1 \\ (2/7)^{\frac{1}{2}} [\sin^2 \gamma - \cos^2 \gamma] , & \epsilon = 0 \end{array} \right\} \quad . \quad (D.4b)$$

Hence the BF operators may be written in the factored form

$$\Omega_{k,\epsilon}^{BF} = \beta^k \hat{\Omega}_{k,\epsilon}(\gamma) \quad (D.5)$$

with $\hat{\Omega}_{k,\epsilon}$ representing the braced quantities in Equations (D.4).

Using Equations (2.25), (2.29), (3.5) and (B.13), the Bohr eigenfunctions appearing in Equation (D.1) may be written explicitly as

$$\begin{aligned}\tilde{\psi}_{\alpha}^{\tilde{s}}(\beta, \gamma, \theta_i) &= \tilde{\psi}_{N\ell\nu JM}^{\tilde{s}}(\beta, \gamma, \theta_i) \\ &= \tilde{s}^{5/2} f_{N\ell}(\tilde{s}\beta) \sum_{\substack{J \\ K \geq 0 \\ \text{even}}} g_{\ell\nu JK}^{\eta}(\gamma) \frac{\langle \theta_i | JM | K \rangle}{(1 + \delta_{K,0})}.\end{aligned}\quad (D.6)$$

We may now express Equation (D.1) in terms of integrals over the five Bohr coordinates,

$$\begin{aligned}M_{\alpha\alpha'}^{k,\mu} &= \left[\int_0^{\infty} \tilde{s}^5 f_{N\ell}^*(\tilde{s}\beta) \beta^k f_{N'\ell'}(\tilde{s}\beta) \beta^4 d\beta \right]_{\epsilon} \sum_{\substack{J \\ K \geq 0 \\ \text{even}}} \sum_{\substack{J' \\ K' \geq 0 \\ \text{even}}} \left[\int_0^{2\pi} g_{\ell\nu JK}^{\eta}(\gamma) \hat{\Omega}_{k,\epsilon}(\gamma) \right. \\ &\quad \times g_{\ell'\nu' J' K'}^{\eta}(\gamma) |\sin 3\gamma| d\gamma \left. \right] \left[\int_{\Omega(\theta_i)} \frac{\langle \theta_i | JM | K \rangle^*}{(1 + \delta_{K,0})} D_{\mu\epsilon}^{2*}(\theta_i) \right. \\ &\quad \times \left. \frac{\langle \theta_i | J' M' | K' \rangle}{(1 + \delta_{K',0})} d\Omega(\theta_i) \right],\end{aligned}\quad (D.7a)$$

which is of the form

$$M_{\alpha\alpha'}^{k,\mu} = [B] \sum_{\epsilon} \sum_K \sum_{K'} [G] \cdot [A] \quad (D.7b)$$

By virtue of Equations (D.4), ϵ effectively ranges only over 0, ± 2 in the outer sum. The radial integral may be written in terms of an SR matrix element by the change of variable $\beta' = \tilde{s}\beta$:

$$[B] = \left(\frac{1}{\tilde{s}} \right)^k \int_0^{\infty} f_{N\ell}^*(\beta') (\beta')^k f_{N'\ell'}(\beta') \beta'^4 d\beta',$$

$$[B] = \left(\frac{1}{s} \right)^k \langle N\ell | \beta^k | N'\ell' \rangle \quad . \quad (D.8)$$

The integrand in [A] is the sum of products of three rotation matrices, and may be evaluated with the aid of Equation (F.71).

$$[A] = \frac{C(J'2J; M'\mu M)}{(2J+1)(1+\delta_{K,0})(1+\delta_{K',0})} S \begin{bmatrix} J' & 2 & J \\ K' & \epsilon & K \end{bmatrix} \quad , \quad (D.9a)$$

where the last term is a sum of Clebsch-Gordon coefficients

$$S \begin{bmatrix} J' & 2 & J \\ K' & \epsilon & K \end{bmatrix} = C(J'2J; K', \epsilon, K) + C(J'2J; K', -\epsilon, K) \\ + (-1)^{J'} [C(J'2J; -K', \epsilon, K) + C(J'2J; -K', -\epsilon, K)] \quad , \quad (D.9b) \\ K, K' \geq 0 \quad .$$

The sum has the following properties:

$$S \begin{bmatrix} J' & 2 & J \\ K' & \epsilon & K \end{bmatrix} = S \begin{bmatrix} J' & 2 & J \\ K' & -\epsilon & K \end{bmatrix} \quad (D.10a)$$

$$= 0 \quad \text{when } \epsilon = 0 \text{ unless } K' = K \quad (D.10b)$$

$$= 0 \quad \text{when } \epsilon = 2 \text{ unless } K' = K \pm 2 \quad , \quad (D.10c)$$

with K' and K assumed to be non-negative, even integers. Equations (D.10b) and (D.10c) may be thought of as selection rules for the K quantum number [projection of $J/\hbar$ upon the BF z-axis]:

$$[A] = 0 \quad \text{unless } K' = K, K \pm 2 \quad . \quad (D.11)$$

The integral [G] over the asymmetry parameter may be rewritten by using Equation (2.30),

$$g_{\ell\nu JK}^{\eta}(\gamma) = \sum_{\sigma=0}^{\sigma_{\max}} A_{\sigma}^{\eta}(\ell\nu JK) (\cos \gamma)^{\ell-2\sigma-\frac{1}{2}K} (\sin \gamma)^{2\sigma+\frac{1}{2}K} \quad (D.12)$$

We are now in a position to complete the connection between Equations (3.59) and (3.60). The reduced matrix element of $\Omega_{k,\mu}^{\text{LAB}}$ may be identified by using Equation (D.9a) in conjunction with the Wigner-Eckart theorem [Equation F.79],

$$\begin{aligned} M_{\alpha\alpha'}^{k,\mu} &= \langle \tilde{\psi}_{N\ell\nu JM}^{\tilde{s}} | \Omega_{k,\mu}^{\text{LAB}} | \tilde{\psi}_{N'\ell'\nu'J'M'}^{\tilde{s}} \rangle \\ &= C(J'2J; M'1M) \langle \tilde{\psi}_{N\ell\nu J}^{\tilde{s}} || \Omega_k^{\text{LAB}} || \tilde{\psi}_{N'\ell'\nu'J'}^{\tilde{s}} \rangle \end{aligned} \quad (D.13)$$

From Equations (D.7)-(D.13) we have

$$\langle \tilde{\psi}_{N\ell\nu J}^{\tilde{s}} || \Omega_k^{\text{LAB}} || \tilde{\psi}_{N'\ell'\nu'J'}^{\tilde{s}} \rangle = \frac{\langle N\ell | \beta^k | N'\ell' \rangle}{\tilde{s}^k} \langle \ell\nu J || \frac{\Omega_k^{\text{LAB}}}{\beta^k} || \ell'\nu'J' \rangle, \quad (D.14)$$

where the angular factor may be written in two parts

$$\langle \ell\nu J || \frac{\Omega_k^{\text{LAB}}}{\beta^k} || \ell'\nu'J' \rangle = \frac{1}{(2J+1)} \left\{ \sum_{\epsilon=0,\pm 2} F[\epsilon; \ell\nu J \ell'\nu'J'; k] \right\} \quad (D.15a)$$

$$\begin{aligned} F[\epsilon; \ell\nu J \ell'\nu'J'; k] &\equiv \sum_{\substack{J \text{ even} \\ K \geq 0}} \sum_{\substack{J' \text{ even} \\ K' \geq 0}} \frac{S \begin{bmatrix} J' & 2 & J \\ K' & \epsilon & K \end{bmatrix}}{(1+\delta_{K,0})(1+\delta_{K',0})} \sum_{\sigma} \sum_{\sigma'} A_{\sigma}(\ell\nu JK) \\ &\times A_{\sigma'}(\ell'\nu'J'K') \int_0^{2\pi} (\cos \gamma)^{\ell+\ell'-2\sigma-2\sigma'-\frac{1}{2}K-\frac{1}{2}K'} \\ &\times (\sin \gamma)^{\frac{1}{2}K+\frac{1}{2}K'+2\sigma+2\sigma'} \hat{\Omega}_{k,\epsilon}(\gamma) |\sin 3\gamma| d\gamma \end{aligned} \quad (D.15b)$$

In Equation (D.15a), the two terms having $\epsilon = +2$ and $\epsilon = -2$ respectively are equal by virtue of Equations (D.4) and (D.10a). Furthermore, their sum may be shown to equal the value of the $\epsilon = 0$ term. The numerical calculation of the radial and angular factors appearing in Equation (D.14) will be discussed shortly. We first consider the selection rules which greatly simplify these tasks.

B. E2 Selection Rules

The selection rules stated by Equations (3.62) and (3.63) are of fundamental importance for the testing and employment of Equation (D.14). These rules follow from the transformation properties of the eigenfunctions $\psi_\alpha^{\tilde{S}}$ and operators $\Omega_{k,\mu}^{LAB}$ under operations of the groups in the physical chain of Equation (2.20). In general, if the sets of functions $\{\phi_\mu^A; \mu = 1, 2, \dots, d_A\}$ and $\{\phi_\nu^B; \nu = 1, 2, \dots, d_B\}$ are bases for the [A] and [B] IR respectively of a compact, semi-simple group G , and if $\{T_\epsilon^C; \epsilon = 1, 2, \dots, d_C\}$ are the components of an irreducible tensor operator belonging to the [C] IR of G , then we have the following.¹

- 1) The set of functions $\{T_\epsilon^C \phi_\mu^A; \epsilon = 1, 2, \dots, d_C; \mu = 1, 2, \dots, d_A\}$ form a basis for the direct product representation [C] $\otimes$ [A] of G . This representation is usually reducible,

¹For precise definitions of IR basis functions, irreducible tensor operators and the direct (Kronecker) product of representations, see, for example, Reference (32). The elements T of G are realized as transformations upon the basis states $|\phi\rangle$. The invariant scalar product referred to in 2) has the property $\langle\phi'|\psi'\rangle \equiv \langle\phi|\psi\rangle$; $|\phi'\rangle \equiv T|\phi\rangle$, $|\psi'\rangle \equiv T|\psi\rangle$ where T is any element of G , and $|\phi\rangle$ and $|\psi\rangle$ are any two members of the [Hilbert] state space.

and may be decomposed into a direct sum of IR of G .

- 2) If an invariant scalar product is defined on the space of functions, then two functions belonging to different IR of G are necessarily orthogonal:

$$\langle \phi_\mu^A | \phi_\nu^B \rangle = \langle \phi_\nu^B | \phi_\mu^A \rangle^* \propto \delta_{[A], [B]} \quad (D.16)$$

- 3) From 1) and 2) above, we have that

$$\langle \phi_\nu^B | T_\epsilon^C | \phi_\mu^A \rangle = 0 \quad (D.17)$$

if $[C] \otimes [A]$ does not contain $[B]$.

To apply Equation (D.17) to the problem at hand, the IR to which $\tilde{\psi}_\alpha$ and $\Omega_{k,\mu}^{LAB}$ belong must be identified. The classification of the former is, of course, known by construction, and that of the latter may be deduced from commutation relations with the group generators. As discussed in (22), the 25 generators of $U(5)$ [i.e., the $A_{\mu\nu} = b_\mu^+ b_\nu$ of Chapter II] may be taken to be

$$Q_{J\epsilon} = [b^+ b]_{J\epsilon} = \sum_{\mu\nu} C(22J; \mu\nu\epsilon) b_\mu^+ b_\nu \quad , \quad (D.18)$$

$$J = 0, 1, 2, 3, 4 \quad ; \quad \epsilon = -J, -J+1, \dots, J$$

The ten-member subset $\{Q_{J\epsilon}; J = 1, 3\}$ then generates $R(5)$, with the three $Q_{1\epsilon}$ generating the physical $R(3)$ subgroup. We begin by considering the first-order operator $\Omega_{1,\mu}^{LAB}$. In the C/D operator representation it has the form

$$\Omega_{1,\mu}^{LAB} = \alpha_\mu \propto [b_\mu^+ + b_\mu] \quad (D.19)$$

From the commutation rules of Figure 2.1, we find

$$[b_{\mu}^{+}, Q_{J\epsilon}] = C(2J; \epsilon+\mu, -\mu, \epsilon) (-1)^{\mu+1} b_{\mu+\epsilon}^{+}$$

$$[b_{\mu}, Q_{J\epsilon}] = C(2J; \epsilon+\mu, -\mu, \epsilon) (-1)^{\mu+J} b_{\mu+\epsilon},$$

and hence that

$$[\Omega_{1,\mu}^{LAB}, Q_{J\epsilon}] \propto \Omega_{1,\mu+\epsilon}^{LAB} \quad \text{if } J = 1, 3 \quad . \quad (D.20)$$

Equation (D.20) is sufficient to show that the five components of Ω_1^{LAB} form an irreducible tensorial set under the groups R(5) and R(3). The representations to which they belong may be uniquely identified by their dimensions. We find that Ω_1^{LAB} belongs to [1, 0] of R(5) and [2] of R(3). The usual angular momentum label [J] is used here to denote the (2J + 1)-dimensional IR of the physical rotational group. As discussed in References (20) and (21), two labels are required to distinguish the IR of R(5) and the notation [ℓ , k] is employed. ℓ and k are two integers or half-integers satisfying $\ell \geq k$. For the symmetric IR to which the $\tilde{\psi}_{\alpha}^{\tilde{S}}$ belong, k is zero and ℓ is integral: $\tilde{\psi}_{N\ell\nu JM}^{\tilde{S}}$ belongs to [ℓ , 0].

We are now in a position to determine the R(3) and R(5) selection rules for the first-order E2 operator. With the aid of the direct product decomposition rules (33)

$$R(3): [2] \otimes [J'] = [J'+2] \oplus [J'+1] \oplus \dots \oplus [|J'-2|] \quad (D.21)$$

$$R(5): [1, 0] \otimes [\ell', 0] = [\ell'+1, 0] \oplus [\ell', 1] \oplus [\ell'-1, 0] \quad , (D.22)$$

we deduce from Equation (D.17)

$$M_{\alpha\alpha'}^{1,\mu} \equiv \langle \tilde{\psi}_{N\ell\nu JM}^{\tilde{S}} | \Omega_{1,\mu}^{LAB} | \tilde{\psi}_{N'\ell'\nu'J'M'}^{\tilde{S}} \rangle = 0 \quad \text{unless} \quad \begin{cases} \ell = \ell' \pm 1 \\ J'+2 \geq J \geq |J'-2| \end{cases} \quad . (D.23)$$

In Equation (D.22), it is understood that terms $[\ell, k]$ for which $k > \ell$ should be deleted from the right hand side. The angular momentum selection rule, as well as the condition that $M_{\alpha\alpha'}^{1,\mu}$ vanish unless the projections obey $M = \mu + M'$, may be obtained from the usual Wigner-Eckart theorem

$$M_{\alpha\alpha'}^{1,\mu} = C(J'2J; M'\mu M) \langle \tilde{\psi}_{N\ell\nu J}^{\tilde{s}} || \Omega_1^{LAB} || \tilde{\psi}_{N'\ell'\nu'J'}^{\tilde{s}} \rangle \quad (D.24)$$

by noting that the Clebsch-Gordon coefficient is zero unless the aforementioned conditions on the spins and their projections are satisfied. Equation (D.24) is a manifestation of general group-theoretic orthogonality relations for the simply reducible group $R(3)$.

The first-order selection rule on the principal quantum number N may be deduced in a similar fashion by classifying the $\Omega_{1,\mu}^{LAB}$ under IR's of $U(5)$ and referencing the appropriate direct product reduction rules. Such a program will not be pursued here, as it is complicated by the fact that the $\Omega_{1,\mu}^{LAB}$ do not all belong to a single IR of $U(5)$. To forge an alternative proof of the selection rule, we recall Equation (2.18a). In the C/D operator representation, any Bohr eigenstate belonging to the $[N]$ symmetric IR of $R(5)$ is realized as a linear combination of terms, each of which consists of N creation operators acting on the vacuum. Hence

$$M_{\alpha\alpha'}^{1,\mu} = \text{linear combination of terms like } \underbrace{\langle 0 | b b \dots b (b^\dagger + b) b^\dagger b^\dagger \dots b^\dagger | 0 \rangle}_{N \text{ factors}} \quad .$$

Only those terms in which the creation and destruction operators are

balanced can yield a non-zero contribution, and consequently the selection rule

$$M_{\alpha\alpha'}^{l,\mu} = 0 \quad \text{unless} \quad N = N' \pm 1 \quad (\text{D.25})$$

follows trivially. In the C/D representation, the second-order operator $\Omega_{2,\mu}^{\text{LAB}}$ consists of the products $\{b^+b^+, b^+b, bb^+, bb\}$ and similar reasoning leads quickly to the U(5) selection rule of Equation (3.63).

To obtain the second-order R(5) selection rule, we can classify the $\Omega_{2,\mu}^{\text{LAB}}$, which are linear combinations of products of the $\Omega_{1,\mu}^{\text{LAB}}$. As the latter belong to $[1, 0]$ of R(5), the former must be among

$$\begin{array}{ccccccc} [1, 0] & \otimes & [1, 0] & = & [0, 0] & \oplus & [1, 1] & \oplus & [2, 0] & & \text{R(5)} \\ (5) & & (5) & & (1) & & (10) & & (14) & & \\ \downarrow & & \downarrow & & \downarrow & & \downarrow & & \downarrow & & \\ [2] & & [2] & & [0] & & [1] \oplus [3] & & [2] \oplus [4] & & \text{R(3)} \\ (5) & & (5) & & (1) & & (3) \oplus (7) & & (5) \oplus (9) & & \end{array} \quad (\text{D.26})$$

Here the angular momentum decomposition (33), under the restriction to physical R(3) operations, has been provided for each U(5) IR. Dimensions of the IR involved are enclosed by parentheses. The $\Omega_{2,\mu}^{\text{LAB}}$ are known to be $J = 2$ tensors; we consequently deduce that they must belong to the fourteen-dimensional $[2, 0]$ IR of R(5). This together with Equation (D.17) and the decomposition (33)

$$\begin{aligned} [2, 0] \otimes [\ell', 0] &= [\ell' - 2, 0] \oplus [\ell' - 1, 1] \oplus [\ell', 0] \oplus [\ell', 2] \oplus [\ell' + 1, 1] \\ &\oplus [\ell' + 2, 0] \end{aligned} \quad (\text{D.27})$$

is sufficient to determine the second-order R(5) selection rule:

$$M_{\alpha\alpha'}^{2,\mu} = 0 \quad \text{unless} \quad \ell = \ell', \ell' \pm 2, \quad (D.28)$$

The R(3) selection rules are, of course, the same for both the first and second-order operators.

In Equation (D.7a), $M_{\alpha\alpha'}^{k,\mu}$ is written as a product of radial and angular factors. The radial variable β commutes with all R(5) generators, and hence any function of β is unaffected by operations of the R(5) and R(3) subgroups. Consequently the R(5) and R(3) selection rules are carried by the angular factor in Equation (D.7a). In particular for the reduced angular matrix element [RAME] we may write¹

$$\langle \ell v J | \frac{\Omega_k^{\text{LAB}}}{\beta^k} | \ell' v' J' \rangle = 0 \quad \text{unless} \quad \begin{cases} \ell = \ell' \pm 1 & [k = 1] \\ \ell = \ell', \ell' \pm 2 & [k = 2] \\ J'+2 \geq J \geq |J'-2| \end{cases} \quad (D.29)$$

The U(5) selection rule, on the other hand, is shared between the radial and angular factors. When the selection rule is violated and the angular factor does not vanish, the radial factor must equal zero. A general expression for $\langle N\ell | \beta^p | N'\ell' \rangle$ is given by Equation (C.14). When $p = 1, 2$, recursion relations (53) for the associated Laguerre polynomials can be used to deduce alternate expressions which illustrate the U(5) selection rules. The radial factors which appear when the RAME does not vanish

¹ In Equation (D.13), $C(J'2J; M'\mu M)$ vanishes whenever J and J' differ by more than 2, and E2 transitions between ψ_{α}^S and $\psi_{\alpha'}^S$ may not occur. However the reduced matrix element in Equation (D.13) is undefined in such cases. We define it to be zero to avoid carrying qualifying factors [such as $\Delta(J_i 2 J_f)$, which equals one when $|J_i - J_f| \leq 2$ and zero otherwise] in Equation (3.48).

are found to be

$$\langle N\ell | \beta | N', \ell+1 \rangle = [\tfrac{1}{2}(N+\ell+5)]^{\frac{1}{2}} \delta_{N', N+1} - [\tfrac{1}{2}(N-\ell)]^{\frac{1}{2}} \delta_{N', N-1} \quad (D.30)$$

$$\begin{aligned} \langle N\ell | \beta^2 | N', \ell \rangle &= \tfrac{1}{2}[2N+5] \delta_{N', N} - \tfrac{1}{2}[(N+\ell+5)(N-\ell+2)]^{\frac{1}{2}} \delta_{N', N+2} \\ &\quad - \tfrac{1}{2}[(N-\ell)(N+\ell+3)]^{\frac{1}{2}} \delta_{N', N-2} \end{aligned} \quad (D.31)$$

$$\begin{aligned} \langle N\ell | \beta^2 | N', \ell+2 \rangle &= -[(N-\ell)(N+\ell+5)]^{\frac{1}{2}} \delta_{N', N} + \tfrac{1}{2}[(N+\ell+5)(N+\ell+7)]^{\frac{1}{2}} \delta_{N', N+2} \\ &\quad + \tfrac{1}{2}[(N-\ell)(N-\ell-2)]^{\frac{1}{2}} \delta_{N', N-2} \end{aligned} \quad (D.32)$$

C. Computational Methods

To execute the calculational procedure outlined below Equation (3.61), the values of $\langle N_f \ell_f | \beta^k | N_i \ell_i \rangle$ and $\langle \ell_f v_f J_f | |\Omega_k^{\text{LAB}} / \beta^k| | \ell_i v_i J_i \rangle$ must be available. In practice the former are rapidly computed as needed by the use of Equations (D.30)-(D.32), and the latter [RAME's] are found via Equations (D.15). Equation (D.15b) contains nested sums which are moderately time consuming to compute. Consequently RAME's are calculated but once and stored for selected values of J_i and $J_f \leq J_i$. This is the task of the GAMME subroutine package.

The GAMME package assumes that A^n coefficients and integrals of the form

$$\int_0^{2\pi} (\cos \gamma)^p (\sin \gamma)^q |\sin 3\gamma| d\gamma \quad [p, q \text{ non-negative integers}]$$

have been precomputed by the methods of Appendix B. [The above integral

appears in Equation (D.15b) and vanishes unless p and q are both even; hence it may be evaluated by Equation (B.21b).] For a given pair (J_i, J_f) , Equations (D.15) are employed to obtain all desired RAME's of the first-order $[k = 1]$ operator. ℓ_f is allowed to range from 0 to the $N_{\max}(J_f)$ of Table 2.3. Some of these values of ℓ_f will not give rise to J_f [see Table 2.1] and are consequently rejected. ℓ_i is similarly restricted. Upon the computation and storage of all first-order terms, RAME's of the second-order operator $\Omega_{2,\mu}^{\text{LAB}}$ are calculated and stored. For fixed J_i, J_f , and k , the storage order for the $\langle \ell_f v_f J_f | | \Omega_k^{\text{LAB}} / \beta^k | | \ell_i v_i J_i \rangle$ is given by

$$\begin{aligned}
 P_1 \quad & \ell_f = 0, 1, 2, \dots, N_{\max}(J_f) \quad [\ell_f \text{ must yield } J_f] \\
 P_2 \quad & \begin{aligned} & \ell_i = \ell_f - 1, \ell_f + 1 \quad [k = 1] \\ & \ell_i = \ell_f - 2, \ell_f, \ell_f + 2 \quad [k = 2] \end{aligned} \quad \left\{ \begin{array}{l} \ell_i \text{ must yield } J_i \\ 0 \leq \ell_i \leq N_{\max}(J_i) \end{array} \right\} \quad (D.33) \\
 P_3 \quad & v_f \text{ increases through the values allowed by } (\ell_f, J_f) \\
 P_4 \quad & v_i \text{ increases through the values allowed by } (\ell_i, J_i).
 \end{aligned}$$

The label at vertical position P_i in the above list is swept over its full range of allowed values prior to incrementing the label at position P_{i-1} . This storage order imposes the R(5) selection rule directly. Furthermore it was chosen to speed the execution of the BE2PRO subroutine package which uses the RAME's to assemble the right-hand side of Equation (3.60). [When $J_i = J_f$, the storage scheme results in the repeated calculation of equivalent matrix elements. For example when $J_i = J_f = 7$, $\langle 507 | | \Omega_2^{\text{LAB}} / \beta^2 | | 607 \rangle$ and $\langle 607 | | \Omega_2^{\text{LAB}} / \beta^2 | | 507 \rangle$ appear successively in the list (D.33).]

Production runs of the GAMME package resulted in the creation of two data sets, GAMEVN and GAMODD. Their contents are detailed in Table D.1, where the numbers of calculated first and second-order RAME's are listed for each (J_i, J_f) pair considered. For $(J_i, J_f) = (3, 3)$, ℓ_i and ℓ_f must each be multiples of 3; hence no first-order E2 transitions are allowed by the R(5) selection rule. Furthermore the ten allowed second-order RAME's for $3 \rightarrow 3$ transitions were all calculated to be zero. For $(J_i, J_f) = (5, 5)$, all calculated first-order RAME's were found to equal $-\sqrt{6/65}$. GAMEVN and GAMODD serve as input for the BE2PRO program package, which completes the calculation of B(E2) transition rates and quadrupole moments. Eigenfunctions for the states involved, expressed as expansion coefficients multiplying the $\tilde{\psi}_\alpha^S$, are supplied by the THEORY package [see Appendix C]. The overall computational procedure is illustrated by Figure D.1. The THEORY, GAMME, and BE2PRO FORTRAN codes all employ double-precision arithmetic.

D. Testing of the GAMME and BE2PRO Codes

A number of test calculations were performed using the GAMME code prior to the production of the GAMEVN and GAMODD data sets. The most severe testing centered upon the numerical verification of the R(5) selection rule. Seventeen of the (J_i, J_f) pairs listed in Table D.1 were studied in detail. For each pair, the RAME $\langle \ell_f v_f J_f || \Omega_k^{LAB} / \beta^k || \ell_i v_i J_i \rangle$ was computed for all possible (ℓ_f, v_f) and (ℓ_i, v_i) which yield J_f and J_i respectively. The only restrictions imposed were $\ell_f \leq N_{\max}(J_f)$

Table D.1. Numbers of first and second-order RAME's,
 $\langle \ell_f v_{fJ_f} || \Omega_k^{LAB} / \beta^k || \ell_i v_{iJ_i} \rangle$, calculated and
 stored [following the scheme (D.33)]

CONTENTS OF GMEEVN				CONTENTS OF GMEODD			
J_i	J_f	$k = 1$ terms	$k = 2$ terms	J_i	J_f	$k = 1$ terms	$k = 2$ terms
2	0	18	18	3	2	17	17
2	2	18	34	3	3	0	10
4	2	32	48	4	3	16	23
4	4	46	68	5	3	16	16
6	4	59	86	5	4	30	45
8	6	95	133	5	5	16	30
10	8	124	185	6	5	44	58
10	12	160	234	7	5	28	42
14	12	195	282	7	6	55	80
16	14	219	325	7	7	40	59
18	16	243	354	8	7	66	98
20	18	257	373	9	7	51	74
6	6	72	112	9	8	88	123
8	8	104	163	9	9	62	96
10	10	144	213	10	9	98	142
12	12	176	262				
14	14	204	310				
16	16	234	345				
18	18	252	369				
20	20	256	384

Figure D.1. The interrelationship of the GAMME, THEORY, and BE2PRO computer codes

and $\ell_i \leq N_{\max}(J_i)$.¹ For example with $(J_i, J_f) = (7, 6)$, there are 630 such matrix elements for each of the first and second-order operators. Of these, only 55 first-order and 80 second-order matrix elements satisfy the R(5) selection rules and are expected to be non-zero. The remaining 495 RAME's were calculated using the GAMME package, and in every case were found to be smaller in magnitude than 10^{-10} [typical non-zero RAME's are on the order of unity]. In the course of the seventeen $J_i \rightarrow J_f$ studies, a total of eight RAME's were found which violated the R(5) selection rules and had calculated values exceeding 10^{-10} in magnitude. These occurred when both ℓ_i and ℓ_f were large, and a large number of terms consequently contributed to the nested sum of Equation (D.15b). The worst case occurred for $\langle 26, 8, 2 || \Omega_2^{\text{LAB}} / \beta^2 || 30, 9, 3 \rangle$ which was calculated to be -1.915×10^{-10} . For those RAME obeying the R(5) selection rule, GAMME was used to calculate each side of

$$\langle \ell_f \nu_f J_f || \frac{\Omega_k^{\text{LAB}}}{\beta^k} || \ell_i \nu_i J_i \rangle = (-1)^{J_i - J_f} \left[\frac{2J_i + 1}{2J_f + 1} \right]^{\frac{1}{2}} \langle \ell_i \nu_i J_i || \frac{\Omega_k^{\text{LAB}}}{\beta^k} || \ell_f \nu_f J_f \rangle \quad (\text{D.34})$$

This relationship follows from Equation (D.14) and the reversal formula, Equation (3.67). Again differences were found to be generally below the 10^{-10} level.

Having concluded the initial phase of testing, GAMEVN and GAMODD were produced. The THEORY and BE2PRO packages were then used to

¹The limiting $N_{\max}(J)$ are those of Table 2.3. For larger values of ℓ , A^n coefficients appearing in Equation (2.30) have not been calculated.

calculate model $B(E2)$'s and quadrupole moments for comparison with the results reported by Habs et al. (29, 30). These test calculations employed the twenty-three instances of the Gneuss-Greiner (GG) Hamiltonian specified by Equations (4.3)-(4.5) and Table 4.1. The five-step calculational procedure of Section III.D was followed. For each of $J = 0, 2, 3, 4, 5$, and 6, the reduced Hamiltonian, $\bar{H}_{GG}$ of Equations (4.9)-(4.13), was diagonalized in the largest available $\psi_i^{\tilde{s}}$ basis [Table 2.3]. For each set of Hamiltonian parameters [Table 4.1], $\tilde{s}$ was taken from Equation (4.14) so as to mirror the calculations of Habs et al. Model energies emerging from the IHEORY package appear in Table 4.3, while $B(E2)$'s and quadrupole moments from BE2PRO¹ may be found in Tables D.2a and D.2b. The latter two tables compare calculated results for seven of the twenty-three H_{GG} parameter sets, including the "representative" five of Chapter IV. For each parameter set and transition type, three values are listed. From top to bottom, these are:

- 1) BE2PRO result using the first-order E_2 operator;
- 2) BE2PRO result using E_2 through second-order; and
- 3) result reported by Habs et al. using E_2 through second order.

Ideally, values 2) and 3) should be equal. In practice, small differences may be expected, arising from differences in the sizes of the expansion bases. Agreement is seen to be excellent throughout Table

¹The nuclear radius was taken as $R_0 = 1.2 A^{1/3}$ Fermi.

D.2a, with the exception of BA-134. [Model calculations for the BA-134 parameter set were shown in Chapter IV to be non-converged when $N_{\max}(J) \leq 30$.] Furthermore, inclusion of the second-order operator in the BE2PRO calculations is clearly necessary to achieve the agreement. In Table D.2b, however, a problem is evident for transitions involving the $J_i = 3_1$ state. The values 2) and 3) appear to agree only when the second-order correction is negligible. In fact, inclusion of the second-order term tends to enlarge the difference between the BE2PRO result and that of Habs et al. Through second order, the electric quadrupole operator is given by Equation (3.45) as

$$E_{2\mu} = D_1 \alpha_\mu + D_2 [\alpha\alpha]_{2\mu} \quad (D.35)$$

If

$$E_{2\mu}' \equiv D_1 \alpha_\mu - D_2 [\alpha\alpha]_{2\mu} \quad (D.36)$$

is used in BE2PRO, the majority of the Table D.2b discrepancies are removed for transitions involving the 3_1 state of H_{GG} . For example in TE-122, $B(E2)$'s for the transitions $3_1 \rightarrow 2_1$, $3_1 \rightarrow 2_2$, $4_1 \rightarrow 3_1$, and $4_2 \rightarrow 3_1$ become .0075, .1904, .0582, and .0137 respectively through second order. These agree with the values .008, .19, .06, and .01 reported by Habs et al. Similar agreement results for SM-142, CE-136, XE-126, and TE-126. However for BA-130, .0036, .2932, .0900, and .0627 are calculated for the four transitions in question when Equation (D.36) is used in BE2PRO; the first two disagree with the Habs values. If Equation (D.36) is used in place of Equation (D.35) throughout the

Table D.2a. Comparison of two H_{GG} calculations. For each isotope and transition type, 3 values are given. The topmost and central were computed by BE2PRO using first and (first + second)-order E2 operators respectively. The bottommost is the (first + second)-order result cited in (29, 30). Units are $(e \cdot \text{barn})$ and $(e \cdot \text{barn})^2$ for $Q(J_i)$ and $B(E2:J_i \rightarrow J_f)$ respectively

Isotope	$Q(2_1)$	$Q(2_2)$	$Q(4_1)$	$2_1 \rightarrow 0_1$	$2_2 \rightarrow 0_1$	$2_2 \rightarrow 2_1$	$4_1 \rightarrow 2_1$	$4_1 \rightarrow 2_2$
BA-130	.403	- .400	.309	.157	.0048	.180	.234	.0023
	.351	- .353	.214	.150	.0089	.189	.225	.0027
	.35	- .35	.21	.15	.009	.19	.23	.003
BA-134	.0391	- .0889	-.232	.1387	.00135	.227	.221	.0071
	-.0120	- .0360	-.332	.1396	.00376	.234	.227	.0078
	-.18	.10	-.33	.135	.0003	.22	.23	.002
CE-136	-.098	.084	-.114	.178	.000016	.2691	.268	9.6×10^{-6}
	-.157	.145	-.225	.181	.000603	.2687	.272	2.2×10^{-5}
	-.15	.14	-.22	.18	.0006	.27	.27	.000
SM-142	.507	-1.077	-.727	.179	.0049	.175	.252	.280
	.450	-1.139	-.898	.171	.0089	.194	.260	.325
	.45	-1.14	-.91	.17	.009	.19	.26	.33
TE-122	-.279	.130	-.530	.127	.001257	.2102	.235	.0072
	-.339	.141	-.640	.132	.000087	.2099	.250	.0113
	-.34	.14	-.64	.13	.00009	.21	.25	.01

Table D.2a. Continued

Isotope	$Q(2_1)$	$Q(2_2)$	$Q(4_1)$	$2_1 \rightarrow 0_1$	$2_2 \rightarrow 0_1$	$2_2 \rightarrow 2_1$	$4_1 \rightarrow 2_1$	$4_1 \rightarrow 2_2$
TE-126	-.171	-.1113	-.516	.100	.00049	.180	.193	.023
	-.221	-.1147	-.620	.103	.000003	.183	.203	.031
	-.22	-.11	-.62	.10	.0000	.18	.20	.03
XE-126	-.078	.032	-.182	.149	3.4×10^{-5}	.219	.221	.0011
	-.132	.076	-.278	.151	.00106	.221	.227	.0017
	-.13	.08	-.28	.15	.001	.22	.23	.002

Table D.2b. Comparison of two H_{GG} calculations. [See caption for Table D.2a]

Isotope	$4_2 \rightarrow 2_1$	$4_2 \rightarrow 2_2$	$4_2 \rightarrow 4_1$	$3_1 \rightarrow 2_1$	$3_1 \rightarrow 2_2$	$4_1 \rightarrow 3_1$	$4_2 \rightarrow 3_1$
BA-130	.0003	.100	.078	.0087	.2809	.0921	.0487
	.00002	.094	.084	.0161	.2688	.0942	.0365
	.000	.09	.08	.01	.09	.09	.06
BA-134	.00049	.0922	.0619	.0023	.305	.116	.047
	.00002	.1048	.0593	.0070	.307	.115	.062
	.001	.10	.06	.003	.29	.12	.03
CE-136	.00078	.112	.0617	.00007	.356	.1454	.0276
	.00259	.122	.0605	.00097	.361	.1453	.0406
	.003	.12	.06	.002	.35	.15	.02
SM-142	.0538	.245	.231	.0089	.193	.127	.0201
	.0419	.285	.241	.0174	.162	.122	.0323
	.04	.28	.24	.003	.23	.13	.01
TE-122	.00164	.169	.135	.00275	.1945	.0554	.0207
	.00013	.175	.133	.00033	.1987	.0527	.0291
	.0001	.18	.13	.008	.19	.06	.01
TE-126	.0033	.123	.077	.00111	.1671	.0519	.0072
	.0018	.144	.087	.00002	.1659	.0495	.0095
	.002	.14	.09	.004	.168	.05	.005
XE-126	5×10^{-8}	.105	.083	3×10^{-7}	.258	.0883	.0218
	.00053	.113	.081	.0011	.261	.0878	.0316
	.0005	.11	.08	.001	.25	.09	.01

BE2PRO calculations, agreement is generally lost if the 3_1 state is not involved. To force overall agreement in the majority of cases, a mechanism is evidently required which reverses the phase of the second-order term when an odd-spin state is involved.

In an attempt to discover an error in the GAMME/BE2PRO code, by-hand calculations of the matrix elements

$$\langle \psi_{\bar{f}}^{\bar{s}} | | \alpha | | \psi_i^{\bar{s}} \rangle \quad (i = N_i, \ell_i, v_i = t_i, J_i)$$

and

(D.37)

$$\langle \psi_{\bar{f}}^{\bar{s}} | | [\alpha\alpha]_2 | | \psi_i^{\bar{s}} \rangle$$

were performed in the C/D operator representation. Wavefunctions for Bohr eigenstates, expressed as creation operators on the vacuum, are given for $N \leq 3$ in Reference (3). These were used in the by-hand calculations, and all allowed first and second-order transitions between the $N \leq 3$ states were considered. Resulting first and second-order matrix elements are listed in Tables D.3 and D.4 respectively. The Bohr eigenstates are labeled simply by J_i as in Figure 3.3. When similar numerical calculations¹ were performed using THEORY and BE2PRO, it was found in every case that

¹The $\psi^{\bar{s}}$ in expressions (D.37) are eigenstates of $H_B = -(\hbar^2/2B)T + \frac{1}{2}CB^2$ [i.e., $\bar{s} = (BC/\hbar^2)^{1/2}$]. In the numerical calculations, H_B was diagonalized in an $N_{\max}(J) = 10$, $\bar{s} = 1$ basis. Magnitudes of matrix elements calculated numerically and by hand differed by less than 10^{-12} .

$$\left[\begin{array}{c} \text{numerically calculated} \\ \text{matrix element} \end{array} \right] = e^{i\phi} \left[\begin{array}{c} \text{by-hand calculated} \\ \text{matrix element} \end{array} \right] , \quad e^{i\phi} = \pm 1 .$$

The phase factors $e^{i\phi}$ appear in Tables D.3 and D.4. These factors are not all expected to be +1, since the wavefunctions used in the two calculations are taken from different sources. However, it should be possible to find phase factors $e^{i\eta(k)}$ connecting the two sets of states

$$\begin{array}{ccc} [\tilde{\psi}_k^{\tilde{s}}] & = e^{i\eta(k)} & [\tilde{\psi}_k^{\tilde{s}}] \\ \text{num.} & & \text{B-H} \end{array}$$

such that the $e^{i\phi}$ appearing in Table D.3 or D.4 and in

$$\begin{array}{cccc} \langle \tilde{\psi}_f^{\tilde{s}} | | \alpha \text{ or } [\alpha\alpha]_2 | | \tilde{\psi}_i^{\tilde{s}} \rangle & = e^{i\phi} \langle \tilde{\psi}_f^{\tilde{s}} | | \alpha \text{ or } [\alpha\alpha]_2 | | \tilde{\psi}_i^{\tilde{s}} \rangle \\ \text{num.} & \text{num.} & \text{B-H} & \text{B-H} \end{array}$$

is given by

$$e^{i\phi} = e^{-i\eta(f)} e^{i\eta(i)} \quad (\text{D.38})$$

in all instances. Such is indeed the case. If we assume the phase relationship

$$e^{i\eta(0_1)} = +1 ,$$

phase factors for the remaining states are found to be -1, -1, +1, -1, -1, +1, +1, -1, and +1 for 0_2 , 0_3 , 2_1 , 2_2 , 2_3 , 3_1 , 4_1 , 4_2 , and 6_1 respectively. Equation (D.38) is then seen to be satisfied throughout Tables D.3 and D.4. In summary, I have been unable to discover any errors or inconsistencies in my work which would account for the second-

Table D.3. Exact first-order reduced matrix elements for Hg eigenstates [$N \leq 3$]. See Figure (3.3) for (N&v) quantum numbers

J_i	J_f	By hand calculation $\frac{1}{s} \langle \bar{\psi}_f \alpha \bar{\psi}_i \rangle$	Numerical calculation phase factor, $e^{i\phi}$
0_2	2_1	$\sqrt{1/5}$	-1
0_3	2_2	$\sqrt{3/10}$	+1
2_1	0_1	$\sqrt{5/2}$	+1
2_2	2_1	1	-1
2_3	0_2	$\sqrt{7/2}$	+1
2_3	2_2	$\sqrt{2/7}$	+1
2_3	4_1	$\sqrt{2/7}$	-1
3_1	2_2	$\sqrt{3/2}$	-1
3_1	4_1	$-\sqrt{1/3}$	+1
4_1	2_1	$\sqrt{9/5}$	+1
4_2	2_2	$\sqrt{99/70}$	+1
4_2	4_1	$\sqrt{5/7}$	-1
6_1	4_1	$\sqrt{13/6}$	+1

Table D.4. Exact second-order reduced matrix elements for H_B eigenstates [$N \leq 3$]. See Figure (3.3) for (N, ν) quantum numbers

J_i	J_f	By hand calculation $\frac{1}{-2} \langle \psi_f^{\bar{5}} [\alpha\alpha]_2 \psi_i^{\bar{5}} \rangle$	Numerical calculation phase factor, $e^{i\phi}$
0_3	2_1	$\sqrt{3/10}$	-1
2_1	2_1	1	+1
2_2	0_1	$\sqrt{5/2}$	-1
2_2	0_2	2	+1
2_2	2_2	$-3/7$	+1
2_3	0_3	$\sqrt{12/7}$	+1
2_3	2_1	$\sqrt{2/7}$	-1
2_3	2_3	$11/7$	+1
3_1	2_1	$-\sqrt{3/2}$	+1
3_1	2_3	$-\sqrt{12/7}$	-1
3_1	3_1	0	--
4_1	2_2	$\sqrt{144/245}$	-1
4_1	4_1	$\sqrt{110/49}$	+1
4_2	2_1	$\sqrt{99/70}$	-1
4_2	2_3	$\sqrt{396/245}$	+1
4_2	3_1	$-\sqrt{66/49}$	-1
4_2	4_2	$\sqrt{160/539}$	+1
6_1	4_2	$\sqrt{208/231}$	-1
6_1	6_1	$\sqrt{45/11}$	+1

order discrepancies in Table D.2b.

On a final note, a few comments should be made concerning the convergence properties of transition rate calculations. As in Section C of Appendix C, the unperturbed Bohr Hamiltonian may serve as a vehicle for test calculations. Transition rates between eigenstates of

$$H_B = A_1 [-\frac{1}{2}T(\beta, \gamma, \theta_i)] + A_2 [\frac{1}{2}\beta^2]$$

are given in the final section of Chapter III for $N \leq 5$. In their computation, a transformation to the SR problem [$A_1 = A_2 = 1$] was made. The natural expansion basis [$\tilde{s} = 1$] was then used in treating the reduced Hamiltonian. The use of any other finite basis would result in truncation errors, as indicated in Table D.5. Here both the size and $\tilde{s}$ parameter of the expansion basis have been varied, and the effect upon the calculated B(E2) rate may be observed for four representative transitions. Only the first-order E2 operator contributes, and the units are those of Figure 3.3 [$(D_1/\tilde{s})^2$ with $\tilde{s} = [A_2/A_1]^{\frac{1}{4}}$]. Notice that if B(E2: $J_i \rightarrow J_f$) were graphed as a function of $\tilde{s}$, the resulting curve would not have the concave-upward shape characteristic of energy-vrs- $\tilde{s}$ plots. At the 20-phonon level, underestimating the optimal $\tilde{s}$ by 40% results in B(E2) errors of ~1%. As may be seen from the table, it is very much safer to overestimate $\tilde{s}$ than to underestimate it.

Table D.5. Calculated $B(E2)$ rates for Hg transitions, using different choices of the expansion basis. Units are those of $[D_1/s]^2$. See Figure 3.3

Expansion		$B(E2:J_i \rightarrow J_f)$			
		band _i		band _f	
Basis		$8_1 \rightarrow 6_1$	$2_1 \rightarrow 0_1$	$2_3 \rightarrow 0_2$	$2_2 \rightarrow 0_3$
$N_{\max}$	$\tilde{s}$	GS GS	GS GS	β β	GS γ
-	1.0	2.0	.5	.7	.3
10	.6	2.652961	.507576	.763154	.318747
	.8	2.016247	.500004	.700241	.300051
	1.2	1.995335	.499998	.699635	.299938
	1.4	1.883236	.499416	.673819	.294723
15	.6	2.055010	.502145	.762027	.310948
	.8	2.000016	.500000	.700020	.300003
	1.2	1.999996	.500000	.699998	.300000
	1.4	1.996574	.499985	.698267	.299752
20	.6	2.023309	.500055	.703136	.300535
	1.4	1.999863	.500000	.699987	.299998

XI. APPENDIX E: MISCELLANEOUS TABLES

Table E.1. Best estimates of E , $\tilde{s}$, and K_1 resulting from an analysis of the GG-model, representative-isotope calculations. Method 1 [Equation 4.23] has been used, and absolute energies are listed

			$E_B(J_i)$ in MeV			$\tilde{s}_B$			K_1		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:	1		2	3		1	2	3	1	2	3
ISOTOPE SPIN NMAX											
TE-122	0	15	1.0946	2.3921	3.1085	0.93	0.93	0.97	0.44E-03	0.16E-01	0.13E-01
	0	20	1.0946	2.3920	3.1084	1.02	1.02	1.01	0.31E-05	0.32E-03	0.74E-04
	0	25	1.0946	2.3920	3.1084	1.07	1.05	1.05	0.12E-06	0.15E-04	0.11E-04
	0	30	1.0946	2.3920	3.1084	1.04	1.11	1.10	0.29E-07	0.23E-06	0.35E-06
	3	15	3.0788	4.8538	5.8066	1.02	0.98	1.03	0.12E-01	0.17E 00	0.21E 00
	3	20	3.0788	4.8527	5.8061	1.06	1.02	1.09	0.26E-03	0.70E-02	0.55E-02
	3	25	3.0788	4.8527	5.8061	1.15	1.08	1.08	0.99E-05	0.10E-03	0.32E-04
	3	30	3.0788	4.8527	5.8061	1.21	1.07	1.15	0.35E-06	0.59E-05	0.22E-05
	9	15	5.4724	6.4639	7.5398	1.02	0.98	1.00	0.18E 00	0.31E 00	0.35E 00
	9	20	5.4711	6.4602	7.5330	1.04	1.03	1.06	0.33E-02	0.93E-02	0.50E-02
	9	25	5.4710	6.4601	7.5328	1.10	1.07	1.09	0.14E-03	0.24E-03	0.31E-03
	10	15	4.3712	5.3174	6.3340	0.97	0.93	0.96	0.83E-01	0.25E 00	0.37E 00
	10	20	4.3702	5.3150	6.3283	0.99	1.00	1.01	0.44E-02	0.46E-02	0.20E-01
	10	25	4.3702	5.3149	6.3281	1.04	1.07	1.05	0.39E-04	0.72E-04	0.36E-03
	20	15	8.7710	10.1931	11.5372	0.98	0.99	0.98	0.42E 01	0.28E 01	0.15E 02
	20	20	8.7108	10.0434	11.3246	1.00	1.01	1.03	0.28E 00	0.44E 00	0.76E 00
	20	25	8.7087	10.0381	11.3125	1.05	1.06	1.06	0.24E-02	0.68E-02	0.39E-01

Table E.1. Continued

			$E_B(J_i)$ in MeV			$\tilde{S}_B$			K_1		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE	SPIN	NMAX									
XE-126	0	15	-5.0535	-2.9488	-0.5969	0.92	0.92	1.01	0.44E 00	0.81E 00	0.28E 00
	0	20	-5.0614	-2.9663	-0.6241	1.01	1.01	1.06	0.25E-01	0.85E-01	0.30E-01
	0	25	-5.0622	-2.9679	-0.6270	1.06	1.05	1.07	0.33E-02	0.57E-02	0.78E-02
	0	30	-5.0623	-2.9681	-0.6272	1.12	1.11	1.14	0.20E-03	0.45E-03	0.35E-03
	3	15	-3.6856	-0.5972	2.2576	0.95	0.87	0.95	0.73E 00	0.28E 01	0.25E 01
	3	20	-3.7085	-0.6425	2.1745	1.00	1.02	1.04	0.82E-01	0.37E 00	0.31E 00
	3	25	-3.7105	-0.6489	2.1663	1.05	1.01	1.08	0.32E-02	0.74E-02	0.14E-01
	3	30	-3.7106	-0.6493	2.1655	1.14	1.10	1.14	0.42E-03	0.55E-03	0.18E-02
	9	15	-0.8152	0.7856	2.1796	0.92	0.93	0.93	0.21E 01	0.31E 01	0.46E 01
	9	20	-0.8695	0.6866	2.0546	1.01	1.02	1.01	0.14E 00	0.54E 00	0.26E 00
	9	25	-0.8758	0.6785	2.0415	1.05	1.08	1.06	0.13E-01	0.28E-01	0.43E-01
	10	15	-1.6326	0.3527	1.4017	0.93	0.92	0.91	0.76E 00	0.14E 01	0.27E 01
	10	20	-1.6843	0.2797	1.3137	1.01	1.00	1.02	0.18E 00	0.15E 00	0.52E 00
	10	25	-1.6884	0.2734	1.3046	1.06	1.06	1.04	0.69E-02	0.42E-02	0.23E-01
	20	15	4.8697	8.6235	10.3043	0.93	0.96	0.95	0.60E 01	0.26E 02	0.49E 02
	20	20	4.5830	7.9922	9.5005	0.99	0.99	0.99	0.81E 00	0.21E 01	0.24E 01
	20	25	4.5521	7.9318	9.3973	1.05	1.08	1.07	0.76E-01	0.22E 00	0.13E 00

Table E.1. Continued

			$E_B(J_i)$ in MeV			S_B			K_1		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:	1	2	3	1	2	3	1	2	3		
ISOTOPE SPIN NMAX											
BA-130	0	15	-3.7782	-0.7726	-0.2987	0.95	0.94	0.94	0.29E-00	0.50E-00	0.89E-00
	0	20	-3.7829	-0.7852	-0.3116	1.04	1.00	1.00	0.56E-02	0.23E-01	0.24E-01
	0	25	-3.7833	-0.7864	-0.3125	1.06	1.07	1.09	0.97E-03	0.16E-02	0.22E-02
	0	30	-3.7833	-0.7865	-0.3125	1.13	1.13	1.15	0.31E-04	0.10E-03	0.99E-04
	3	15	-2.4736	1.5762	2.4277	0.95	0.97	0.96	0.41E-00	0.25E-01	0.13E-01
	3	20	-2.4824	1.5374	2.3912	1.04	1.02	1.02	0.82E-02	0.84E-01	0.23E-00
	3	25	-2.4832	1.5331	2.3872	1.06	1.06	1.10	0.29E-02	0.15E-01	0.59E-02
	3	30	-2.4833	1.5329	2.3870	1.10	1.11	1.16	0.47E-04	0.56E-03	0.69E-03
	9	15	0.4414	2.0488	3.3433	0.97	0.94	0.93	0.16E-01	0.18E-01	0.51E-01
	9	20	0.4039	2.0011	3.2544	1.00	1.01	1.00	0.56E-01	0.14E-00	0.23E-00
	9	25	0.4014	1.9967	3.2475	1.09	1.06	1.09	0.50E-02	0.14E-01	0.74E-02
	10	15	-0.3963	1.7574	3.0325	0.96	0.92	0.94	0.71E-00	0.26E-01	0.10E-01
	10	20	-0.4190	1.7138	2.9587	1.00	1.03	1.03	0.56E-01	0.75E-01	0.17E-00
	10	25	-0.4207	1.7106	2.9541	1.07	1.10	1.09	0.22E-02	0.52E-02	0.77E-02
	20	15	6.2852	10.0998	12.3566	0.96	1.00	1.00	0.60E-01	0.64E-01	0.12E-02
	20	20	6.0454	9.6540	11.6976	1.01	1.02	1.03	0.46E-00	0.13E-01	0.24E-01
	20	25	6.0309	9.6184	11.6318	1.07	1.09	1.07	0.12E-01	0.42E-01	0.11E-00

Table E.1. Continued

			$E_B(J_i)$ in MeV			σ_B			K_1		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE SPIN NMAX											
SM-142	0	15	-0.3212	1.4576	4.5907	0.87	0.83	0.80	0.44E 00	0.75E 01	0.36E 01
	0	20	-0.3365	1.2022	4.4956	0.95	0.89	0.89	0.81E-01	0.78E 00	0.73E 00
	0	25	-0.3414	1.0797	4.4262	0.93	0.92	0.92	0.23E-01	0.50E 00	0.24E 00
	0	30	-0.3420	1.0679	4.4193	1.00	1.00	0.99	0.30E-02	0.68E-01	0.38E-01
	3	15	2.4554	4.4955	9.0204	0.81	0.81	0.83	0.84E 01	0.75E 01	0.98E 01
	3	20	2.1600	4.2434	8.3857	0.91	0.86	0.86	0.12E 01	0.10E 01	0.27E 01
	3	25	2.0910	4.1976	8.2215	0.94	0.93	0.92	0.36E 00	0.31E 00	0.73E 00
	3	30	2.0716	4.1840	8.1769	0.99	0.99	0.98	0.72E-01	0.40E-01	0.93E-01
	9	15	5.7335	8.1164	9.9728	0.83	0.81	0.80	0.62E 01	0.40E 01	0.12E 02
	9	20	4.8255	7.1907	9.4716	0.87	0.89	0.89	0.17E 01	0.21E 01	0.25E 01
	9	25	4.6698	6.8723	9.2718	0.95	0.92	0.93	0.40E 00	0.12E 01	0.74E 00
	10	15	4.5739	6.8092	8.0684	0.80	0.81	0.87	0.62E 01	0.11E 02	0.15E 01
	10	20	4.0183	5.9461	7.5982	0.89	0.90	0.90	0.13E 01	0.39E 01	0.25E 01
	10	25	3.8655	5.7490	7.4229	0.94	0.93	0.95	0.35E 00	0.47E 00	0.54E 00
	20	15	12.7919	18.6349	20.1353	0.80	0.84	0.83	0.28E 02	0.30E 02	0.47E 02
	20	20	10.7904	15.2896	17.9348	0.86	0.89	0.89	0.54E 01	0.87E 01	0.12E 02
	20	25	10.3222	14.5223	16.9857	0.94	0.94	0.95	0.11E 01	0.26E 01	0.40E 01

Table E.1. Continued

			$E_B(J_i)$ in MeV			ξ_B			K_1		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:	1		2	3		1	2	3	1	2	3
ISOTOPE SPIN NMAX											
BA-134	0	15	-2.0063	0.2612	5.1069	0.94	0.93	0.91	0.37E 01	0.16F 02	0.11E 02
	0	20	-2.0713	0.0869	4.7219	1.04	1.02	1.00	0.18E 00	0.79E 00	0.32E 01
	0	25	-2.3514	-0.6383	3.8322	1.03	1.02	1.00	0.94E 00	0.18E 01	0.45E 01
	0	30	-2.4657	-0.8178	3.5493	1.11	1.10	1.08	0.62E 00	0.93E 00	0.18E 01
	3	15	0.8120	5.1723	11.6521	1.00	0.89	0.92	0.64E 01	0.01E 01	0.26E 02
	3	20	-0.2884	3.7896	9.3888	1.01	1.03	0.94	0.23E 01	0.54E 01	0.04E 01
	3	25	-0.7487	3.3203	8.4931	1.06	1.03	0.99	0.28E 01	0.24E 01	0.51E 01
	3	30	-0.9800	3.0627	7.9307	1.15	1.07	1.06	0.14E 01	0.66E 00	0.22E 01
	9	15	5.5814	8.3335	10.7844	0.95	0.94	0.97	0.79E 01	0.21E 02	0.19E 02
	9	20	3.8195	6.1146	8.1039	0.99	1.02	0.99	0.94E 01	0.80E 01	0.55E 01
	9	25	2.9025	5.0046	6.6183	1.06	1.05	1.05	0.23E 01	0.51E 01	0.88E 01
	10	15	4.8242	8.3546	10.1577	0.94	0.95	0.92	0.77E 01	0.13E 02	0.15E 02
	10	20	2.8487	6.3975	8.0746	1.01	1.03	0.98	0.30E 01	0.79E 01	0.11E 02
	10	25	2.0616	4.8978	6.8854	1.05	1.02	1.05	0.24E 01	0.19E 01	0.31E 01
	20	15	16.7519	26.7476	28.1702	0.96	0.94	0.97	0.23E 02	0.65E 02	0.40E 02
	20	20	12.7605	18.6563	22.2363	0.99	1.00	0.96	0.12E 02	0.22E 02	0.16E 02
	20	25	10.4932	16.1719	19.3544	1.05	1.04	1.02	0.43E 01	0.84E 01	0.65E 01

Table E.2. Best estimates of E , $\tilde{s}$, and K_2 resulting from an analysis of the GG-model, representative-isotope calculations. Method II [Equations (4.24)-(4.26)] has been used, and absolute energies are listed

			$E_B(J_i)$ in MeV			$\tilde{s}_B$			K_2		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE	SPIN	NMAX									
TE-122	0	15	1.0946	2.3921	3.1085	0.98	0.91	0.98	0.78E-10	0.55E-07	0.41E-07
	0	20	1.0946	2.3920	3.1084	1.04	1.04	1.04	0.58E-14	0.46E-10	0.44E-11
	0	25	1.0946	2.3920	3.1084	1.07	1.04	1.04	0.57E-17	0.70E-13	0.31E-13
	0	30	1.0946	2.3920	3.1084	1.11	1.11	1.11	0.56E-17	0.13E-16	0.30E-16
	3	15	3.0788	4.8543	5.8071	0.98	0.98	0.98	0.70E-08	0.84E-05	0.30E-05
	3	20	3.0788	4.8527	5.8061	1.04	1.04	1.04	0.70E-11	0.52E-09	0.82E-09
	3	25	3.0788	4.8527	5.8061	1.11	1.11	1.11	0.12E-14	0.26E-11	0.76E-12
	3	30	3.0788	4.8527	5.8061	1.07	1.11	1.11	0.17E-16	0.90E-15	0.47E-15
	9	15	5.4727	6.4649	7.5412	0.98	0.98	0.98	0.14E-05	0.23E-04	0.77E-04
	9	20	5.4711	6.4602	7.5330	1.04	1.04	1.04	0.26E-09	0.28E-07	0.14E-07
	9	25	5.4710	6.4601	7.5328	1.11	1.11	1.11	0.62E-11	0.36E-10	0.52E-10
	10	15	4.3714	5.3180	6.3353	0.98	0.98	0.98	0.18E-05	0.55E-05	0.59E-04
	10	20	4.3702	5.3150	6.3284	1.04	0.98	0.98	0.35E-08	0.13E-07	0.20E-06
	10	25	4.3702	5.3149	6.3281	1.04	1.04	1.04	0.37E-12	0.40E-11	0.44E-10
	20	15	8.7850	10.1927	11.5873	0.98	0.98	0.98	0.45E-02	0.24E-02	0.58E-01
	20	20	8.7117	10.0449	11.3272	1.04	0.98	1.04	0.22E-04	0.77E-04	0.20E-03
	20	25	8.7087	10.0381	11.3126	1.04	1.04	1.04	0.17E-08	0.24E-07	0.58E-06

Table E.2. Continued

		$E_B(J_i)$ in MeV			$\bar{s}_B$			K_2			
		ENERGIES			S-TILDA			CURVATURE			
LEVEL #:		1	2	3	1	2	3	1	2	3	
ISOTOPE SPIN NMAX											
XE-126	0	15	-5.0505	-2.9429	-0.5943	0.98	0.91	0.98	0.50E-04	0.21E-03	0.70E-04
	0	20	-5.0613	-2.9658	-0.6238	1.04	0.98	1.04	0.34E-06	0.10E-05	0.46E-06
	0	25	-5.0622	-2.9679	-0.6270	1.11	1.04	1.11	0.25E-08	0.84E-08	0.19E-08
	0	30	-5.0623	-2.9691	-0.6272	1.11	1.11	1.17	0.16E-10	0.50E-10	0.29E-10
	3	15	-3.6763	-0.5866	2.2777	0.85	0.91	0.98	0.22E-03	0.24E-03	0.35E-02
	3	20	-3.7081	-0.6412	2.1766	0.98	0.98	1.04	0.12E-05	0.29E-05	0.24E-04
	3	25	-3.7104	-0.6488	2.1664	1.04	1.04	1.11	0.15E-08	0.43E-07	0.12E-06
	3	30	-3.7106	-0.6493	2.1656	1.11	1.11	1.17	0.18E-11	0.85E-10	0.16E-09
	9	15	-0.8012	0.8095	2.2068	0.98	0.91	0.98	0.10E-02	0.43E-02	0.42E-02
	9	20	-0.8686	0.6896	2.0571	0.98	0.98	0.98	0.69E-05	0.44E-04	0.66E-04
	9	25	-0.8757	0.6786	2.0418	1.04	1.04	1.04	0.46E-07	0.94E-07	0.67E-06
	10	15	-1.6265	0.3625	1.4204	0.91	0.91	0.91	0.31E-03	0.53E-03	0.18E-02
	10	20	-1.6834	0.2809	1.3160	0.98	0.98	0.98	0.39E-05	0.12E-04	0.19E-04
	10	25	-1.6883	0.2734	1.3048	1.04	1.04	1.04	0.25E-07	0.64E-08	0.13E-06
	20	15	4.9068	8.7455	10.5613	0.91	0.91	0.91	0.64E-02	0.60E-01	0.34E 00
	20	20	4.5889	8.0075	9.5175	0.98	0.98	0.98	0.23E-03	0.14E-02	0.17E-02
	20	25	4.5526	7.9327	9.3984	1.04	1.04	1.04	0.16E-05	0.17E-05	0.12E-04

Table E.2. Continued

			$E_B(J_i)$ in MeV			$\bar{s}_B$			K_2		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE	SPIN	NMAX									
EA-130	0	15	-3.7764	-0.7688	-0.2932	0.91	0.91	0.91	0.23E-04	0.14E-03	0.19E-03
	0	20	-3.7829	-0.7851	-0.3114	1.04	1.04	1.04	0.77E-08	0.16E-07	0.25E-06
	0	25	-3.7833	-0.7864	-0.3124	1.11	1.11	1.11	0.29E-09	0.25E-08	0.23E-08
	0	30	-3.7833	-0.7865	-0.3125	1.11	1.11	1.11	0.87E-13	0.75E-12	0.65E-12
	3	15	-2.4704	1.5887	2.4367	0.98	0.91	0.98	0.90E-04	0.75E-03	0.53E-03
	3	20	-2.4823	1.5378	2.3922	1.04	0.98	1.04	0.17E-07	0.79E-06	0.62E-05
	3	25	-2.4832	1.5332	2.3872	1.11	1.04	1.11	0.24E-08	0.80E-07	0.29E-08
	3	30	-2.4833	1.5329	2.3870	1.11	1.11	1.11	0.55E-12	0.75E-10	0.50E-10
	9	15	0.4496	2.0640	3.3669	0.91	0.98	0.98	0.31E-03	0.24E-02	0.24E-02
	9	20	0.4042	2.0019	3.2553	1.04	1.04	1.04	0.88E-06	0.54E-05	0.27E-05
	9	25	0.4015	1.9968	3.2476	1.04	1.11	1.11	0.13E-07	0.35E-07	0.30E-07
	10	15	-0.3914	1.7723	3.0418	0.91	0.98	0.98	0.17E-03	0.12E-02	0.96E-03
	10	20	-0.4187	1.7143	2.9599	1.04	1.04	1.04	0.44E-06	0.18E-05	0.93E-05
	10	25	-0.4207	1.7106	2.9542	1.04	1.11	1.11	0.42E-08	0.11E-07	0.36E-07
	20	15	6.3155	10.1487	12.4535	0.98	0.98	0.98	0.41E-02	0.20E-01	0.90E-01
	20	20	6.0481	9.6634	11.7145	1.04	1.04	1.04	0.52E-04	0.72E-03	0.19E-02
	20	25	6.0310	9.6187	11.6325	1.11	1.11	1.11	0.51E-07	0.82E-06	0.26E-05

Table E.2. Continued

			$E_B(J_i)$ in MeV			$\bar{s}_B$			K_2		
			ENERGIES			S-TILDA			CURVATURE		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE SPIN NMAX											
SM-142	0	15	-0.3167	1.5052	4.6296	0.91	0.78	0.85	0.64E-04	0.33E-02	0.49E-02
	0	20	-0.3360	1.2103	4.4911	0.91	0.85	0.85	0.52E-06	0.21E-03	0.61E-04
	0	25	-0.3412	1.0850	4.4288	0.98	0.91	0.91	0.72E-07	0.69E-04	0.19E-04
	0	30	-0.3419	1.0687	4.4197	1.04	1.04	0.98	0.20E-08	0.20E-05	0.51E-06
	3	15	2.5116	4.5319	9.1000	0.85	0.85	0.85	0.50E-02	0.57E-03	0.13E-01
	3	20	2.1730	4.2530	8.4078	0.91	0.85	0.85	0.39E-03	0.21E-03	0.74E-03
	3	25	2.0941	4.2005	8.2292	0.98	0.98	0.91	0.28E-04	0.22E-04	0.14E-03
	3	30	2.0721	4.1843	8.1778	0.98	0.98	0.98	0.45E-06	0.12E-07	0.23E-05
	9	15	5.8010	8.1727	10.1086	0.85	0.78	0.85	0.13E-01	0.15E-01	0.69E-01
	9	20	4.8481	7.2049	9.4996	0.85	0.91	0.91	0.23E-02	0.21E-02	0.25E-02
	9	25	4.6742	6.8850	9.2801	0.98	0.91	0.91	0.13E-03	0.46E-03	0.23E-03
	10	15	4.6275	6.9160	8.0881	0.85	0.85	0.85	0.75E-02	0.38E-01	0.17E-02
	10	20	4.0340	5.9780	7.6252	0.91	0.85	0.85	0.10E-02	0.21E-02	0.21E-02
	10	25	3.8701	5.7548	7.4280	0.91	0.91	0.91	0.96E-04	0.13E-03	0.76E-04
	20	15	13.0693	18.9462	20.6548	0.85	0.85	0.85	0.23E 00	0.23E 00	0.82E 00
	20	20	10.8501	15.3807	18.0435	0.91	0.85	0.91	0.12E-01	0.27E-01	0.23E-01
	20	25	10.3353	14.5548	17.0180	0.91	0.91	0.91	0.70E-03	0.44E-02	0.15E-02

Table E.2. Continued

		$E_B(J)$ in MeV			$\tilde{S}_B$			K_2			
		ENERGIES			S-TILDA			CURVATURE			
LEVEL #:		1	2	3	1	2	3	1	2	3	
ISOTOPE SPIN NMAX											
BA-134	0	15	-1.9667	9.4528	5.2314	0.98	0.91	0.91	0.45E-02	0.10E 00	0.30E-01
	0	20	-2.0692	0.0974	4.7400	1.04	1.04	0.98	0.80E-05	0.38E-03	0.14E-02
	0	25	-2.3402	-0.6165	3.8788	1.04	1.04	1.04	0.32E-03	0.14E-02	0.58E-02
	0	30	-2.4588	-0.8071	3.5736	1.11	1.11	1.11	0.93E-04	0.25E-03	0.21E-02
	3	15	1.0624	5.3013	12.4363	0.85	0.85	0.78	0.34E-02	0.14E-01	0.17E 00
	3	20	-0.2639	3.8604	9.5849	1.04	0.91	0.91	0.13E-02	0.10E-02	0.58E-01
	3	25	-0.7114	3.3470	8.5548	1.04	1.04	0.98	0.47E-02	0.15E-02	0.10E-01
	3	30	-0.9616	3.0710	7.9519	1.04	1.04	1.04	0.18E-03	0.14E-03	0.85E-03
	9	15	5.6880	8.6133	10.9996	0.98	0.98	0.98	0.39E-01	0.28E 00	0.11E 00
	9	20	3.9278	6.2101	8.1667	0.98	0.98	0.98	0.26E-01	0.26E-01	0.86E-02
	9	25	2.9316	5.0615	6.7172	1.04	1.04	1.04	0.26E-02	0.64E-02	0.20E-01
	10	15	4.9297	8.5322	10.3285	0.98	0.98	0.91	0.41E-01	0.11E 00	0.62E-01
	10	20	2.9066	6.4761	8.1969	0.98	0.98	0.98	0.13E-01	0.13E-01	0.29E-01
	10	25	2.0898	4.9214	6.9203	1.04	1.04	1.04	0.18E-02	0.16E-02	0.26E-02
	20	15	17.0273	27.2135	28.6345	0.98	0.98	0.98	0.19E 00	0.28E 00	0.51E 00
	20	20	12.8986	18.9435	22.4274	0.98	0.98	0.98	0.43E-01	0.28E 00	0.10E 00
	20	25	10.5419	16.2664	19.4440	1.04	1.04	1.04	0.49E-02	0.17E-01	0.29E-01

Table E.3. Best estimates of E , $\tilde{s}$, and K_1 [Equation (4.23)] for 23 instances of H_{GG} . Energies reported in (29, 30) appear below those of the present work. The absolute energy is given for $J_i=0_1$. Estimated errors are for points 1σ above the LSSL [Figure 4.13]

			$E_B(J_i)-E_B(0_1)$ in MeV			$\tilde{s}_B$			$\Delta E(J_i)$ in MeV		
			ENERGIES			S-TILDA			EST ERROR		
LEVEL #:			1	2	3	1	2	3	1	2	3
ISOTOPE	SPIN	NMAX									
BA-128	0	30	-8.2087	3.0853	4.3031	1.12	1.10	1.13	0.00000	0.00001	0.00002
			-8.209	3.085	4.303						
	2	27	0.2813	0.8802	3.5640	1.07	1.09	1.08	0.00003	0.00011	0.00002
			0.281	0.879	3.563						
	3	30	1.2069	5.3908	6.3951	1.13	1.12	1.13	0.00001	0.00003	0.00021
			1.207	5.390							
	4	25	0.7704	1.6392	2.3478	1.05	1.04	1.10	0.00018	0.00022	0.00042
			0.770	1.638	2.347						
	5	27	1.9585	2.9773	6.4128	1.11	1.09	1.08	0.00025	0.00005	0.00022
			1.956								
	6	25	1.4052	2.6231	3.5164	1.07	1.06	1.02	0.00024	0.00041	0.00073
			1.405	2.621							
BA-130	0	30	-3.7833	2.9968	3.4708	1.10	1.14	1.10	0.00000	0.00000	0.00001
			-3.783	2.997	3.469						
	2	27	0.3560	0.9074	3.5921	1.09	1.11	1.09	0.00001	0.00001	0.00003
			0.356	0.906	3.591						
	3	30	1.3000	5.3162	6.1703	1.14	1.14	1.15	0.00000	0.00002	0.00002
			1.300	5.316							
	4	25	0.9033	1.8156	2.4153	1.05	1.05	1.06	0.00008	0.00005	0.00007
			0.903	1.813	2.414						
	5	27	2.1263	3.1345	6.4268	1.10	1.09	1.10	0.00003	0.00007	0.00029
			2.126								
	6	25	1.5915	2.9248	3.7162	1.08	1.08	1.07	0.00004	0.00012	0.00027
			1.591	2.923							
BA-132	0	30	-3.6340	2.9386	4.7496	1.16	1.15	1.20	0.00001	0.00005	0.00002
			-3.634	2.939	4.748						
	2	27	0.4655	1.0336	3.6214	1.11	1.15	1.07	0.00003	0.00004	0.00012
			0.465	1.032	3.621						
	3	30	1.5070	5.6690	8.1447	1.17	1.15	1.17	0.00003	0.00012	0.00008
			1.507	5.669							
	4	25	1.1257	2.2067	2.7642	1.12	1.10	1.11	0.00006	0.00019	0.00035
			1.125	2.205	2.762						
	5	27	2.4970	3.6303	6.9622	1.17	1.11	1.10	0.00017	0.00023	0.00017
			2.496								
	6	25	1.9405	3.5726	4.3716	1.11	1.10	1.10	0.00021	0.00026	0.00108
			1.940	3.570							

Table E.3. Continued

		$E_B(J_i)-E_B(0_i)$ in MeV			$\tilde{s}_B$			$\Delta E(J_i)$ in MeV			
		ENERGIES			S-TILDA			EST ERROR			
	LEVEL #:	1	2	3	1	2	3	1	2	3	
BA-134	0	30	-2.4657	1.6479	6.0149	1.11	1.10	1.08	0.05647	0.08630	0.16878
			-2.339	1.725	6.200						
	2	27	0.6606	1.1894	2.6676	1.10	1.05	1.08	0.05486	0.09389	0.06092
			0.600	1.178	2.672						
	3	30	1.4858	5.5277	10.3969	1.15	1.08	1.10	0.13261	0.07319	0.31975
			1.701	5.708							
	4	25	1.4659	2.4963	3.2418	1.05	1.05	1.07	0.08265	0.23989	0.04629
			1.361	2.433	3.123						
	5	27	2.5925	3.8876	7.4773	1.06	1.10	1.02	0.14236	0.05741	0.18352
			2.714								
	6	25	2.3183	4.0193	4.9503	1.06	1.03	1.04	0.15604	0.23791	0.17369
			2.192	3.935							
BA-134P	0	30	-2.5286	1.6832	6.0027	1.11	1.10	1.09	0.03940	0.07567	0.16353
			-2.431	1.771							
	2	27	0.6608	1.2125	2.6496	1.10	1.05	1.08	0.05387	0.08159	0.09071
			0.607	1.164							
	3	30	1.5217	5.4555	10.3374	1.15	1.13	1.10	0.10906	0.05359	0.25954
			1.622								
	4	25	1.4837	2.5566	3.2084	1.06	1.05	1.08	0.06782	0.17026	0.06698
			1.369	2.413							
	5	27	2.6293	3.8866	7.3671	1.06	1.10	1.02	0.09864	0.08290	0.14816
			2.3561	4.0683	4.9757	1.06	1.04	1.05	0.12713	0.12618	0.16641
	6	25	2.190								
BA-136	0	30	1.7235	1.5825	2.1765	1.09	1.02	1.01	0.00000	0.00013	0.00016
			1.723	1.589	2.181						
	2	27	0.8193	1.6164	1.9824	1.02	1.01	0.98	0.00000	0.00062	0.00128
			0.819	1.616	1.985						
	3	30	2.5168	3.0296	4.5956	1.03	1.03	1.02	0.00026	0.00180	0.00417
			2.521	3.047							
	4	25	1.6769	2.0298	2.8286	0.98	0.98	0.97	0.00054	0.00314	0.00117
			1.679	2.033	2.826						
	5	27	3.0166	3.7409	4.4018	1.01	1.01	0.99	0.00183	0.00101	0.00289
			3.034								
	6	25	2.1954	2.7951	3.2593	0.97	0.97	0.94	0.00402	0.00209	0.00913
			2.201	2.795							

Table E.3. Continued

		LEVFL #:	$E_B(J_i) - E_B(0_i)$ in MeV			$\frac{S}{S_B}$			$\Delta E(J_i)$ in MeV		
			ENERGIES			S-TILDA			EST ERROR		
			1	2	3	1	2	3	1	2	3
CE-136	0	30	-2.6315	2.9117	6.8016	1.12	1.17	1.13	0.00178	0.00535	0.01354
			-2.620	2.927	6.852						
	2	27	0.5471	1.1121	3.9238	1.13	1.20	1.09	0.00683	0.00618	0.00969
			0.545	1.102	3.931						
	3	30	1.5682	6.2365	11.4916	1.18	1.16	1.14	0.00659	0.02434	0.06803
			1.578	6.276							
	4	25	1.3061	2.5384	3.1163	1.13	1.12	1.13	0.00670	0.00508	0.01618
			1.295	2.518	3.108						
	5	27	2.7225	3.9687	7.8920	1.16	1.13	1.13	0.00717	0.02419	0.03396
			2.716								
	6	25	2.2431	4.1624	5.0344	1.12	1.13	1.11	0.01385	0.00786	0.05621
			2.223	4.148							
CE-138	0	30	0.1047	1.3849	4.3894	1.01	1.00	0.96	0.00010	0.00375	0.00141
			0.105	1.392	4.393						
	2	27	0.7805	1.4791	2.4630	0.99	0.91	0.98	0.00021	0.00137	0.00631
			0.780	1.481	2.469						
	3	30	2.5126	4.3595	8.1080	0.98	0.97	0.99	0.00303	0.00181	0.01099
			2.529	4.370							
	4	25	1.7305	2.3171	3.0262	0.93	0.93	0.95	0.01075	0.00981	0.01154
			1.725	2.314	3.024						
	5	27	3.1862	5.1163	6.0294	0.97	0.99	0.93	0.00621	0.00663	0.02300
			3.197								
	6	25	2.4300	3.5747	4.1276	0.94	0.94	0.96	0.01668	0.01351	0.01249
			2.414	3.557							
ND-138	0	30	-2.5154	2.7837	6.5023	1.11	1.16	1.15	0.00273	0.00386	0.01502
			-2.504	2.798	6.553						
	2	27	0.5231	1.0634	3.7505	1.13	1.20	1.11	0.00715	0.00161	0.02169
			0.521	1.050	3.758						
	3	30	1.4995	5.9622	10.9858	1.20	1.16	1.14	0.00600	0.02312	0.06934
			1.500	6.001							
	4	25	1.2488	2.4267	2.9793	1.13	1.07	1.13	0.00604	0.01206	0.01592
			1.236	2.411	2.965						
	5	27	2.5031	3.7942	7.5458	1.16	1.13	1.14	0.00307	0.02501	0.00529
			2.593								
	6	25	2.1446	3.9795	4.8132	1.12	1.13	1.11	0.01324	0.00751	0.05373
			2.131	3.963							

Table E.3. Continued

	LEVEL	#	$E_B(J_i) - E_B(0_i)$ in MeV			S_B			$\Delta E(J_i)$ in MeV		
			ENERGIES			S-TILDA			EST EPROP		
			1	2	3	1	2	3	1	2	3
ND-140	0	30	0.1038	1.3741	4.3555	1.01	1.00	0.96	0.00010	0.00373	0.00140
			0.104	1.382	4.359						
	2	27	0.7745	1.4676	2.4439	0.99	0.91	0.98	0.00021	0.00136	0.00627
			0.774	1.469	2.450						
	3	30	2.4932	4.3248	8.0454	0.98	0.97	0.94	0.00301	0.00180	0.01090
			2.510	4.336							
	4	25	1.7170	2.2991	3.0025	0.93	0.93	0.95	0.00982	0.01090	0.01466
			1.712	2.296	3.001						
	5	27	3.1615	5.0768	5.9829	0.97	1.02	0.92	0.00579	0.00586	0.02410
			3.172								
	6	25	2.4109	3.5471	4.0959	0.94	0.95	0.94	0.02027	0.00974	0.00912
			2.405	3.542							
SM-142	0	30	-0.3420	1.4099	4.7612	1.00	1.00	1.00	0.00017	0.00541	0.00332
			-0.342	1.426	4.770						
	2	27	0.7680	1.4950	2.3833	1.00	0.93	0.97	0.00019	0.00287	0.01042
			0.768	1.498	2.398						
	3	30	2.4136	4.5261	8.5188	0.99	0.98	0.95	0.00776	0.00281	0.01000
			2.442	4.545							
	4	25	1.7432	2.3691	2.9831	0.93	0.92	0.95	0.01384	0.01872	0.02177
			1.741	2.367	2.986						
	5	27	3.1231	5.0115	6.2041	0.97	1.02	0.92	0.00786	0.00802	0.02947
			3.144								
	6	25	2.4844	3.6119	4.2319	0.95	0.96	0.94	0.01880	0.02016	0.00647
			2.481	3.609							
SM-142F	0	30	1.7096	1.4287	2.3429	1.03	1.02	1.02	0.00000	0.00452	0.00141
			1.709	1.420							
	2	27	0.7679	1.5123	2.0198	1.02	0.93	0.99	0.00002	0.00001	0.00238
			0.768	1.496							
	3	30	2.1603	2.9303	4.8894	1.00	1.02	1.01	0.00321	0.00298	0.01628
			2.162								
	4	25	1.6331	1.8958	2.3915	0.94	0.94	0.96	0.00509	0.01130	0.01975
			1.623	1.882							
	5	27	2.5075	3.6674	3.9762	0.97	0.95	0.94	0.00972	0.01263	0.01343
			2.0722	2.7225	2.9570	0.96	0.95	0.95	0.00997	0.01030	0.00774
	6	25	2.048								

Table E.3. Continued

		$E_B(J_i)-E_B(0_1)$ in MeV			s_B			$\Delta E(J_i)$ in MeV			
		ENERGIES			S-TILDA			EST ERROR			
LEVEL #:		1	2	3	1	2	3	1	2	3	
TE-120	0	30	1.8171	1.2168	1.8693	1.13	1.12	1.11	0.00000	0.00000	0.00000
			1.817	1.216	1.868						
	2	27	0.5599	1.2005	2.0382	1.14	1.11	1.10	0.00000	0.00000	0.00000
			0.560	1.200	2.038						
	3	30	1.8305	3.8041	4.1250	1.10	1.12	1.11	0.00000	0.00000	0.00000
			1.830	3.803							
	4	25	1.1515	1.8536	2.5472	1.05	1.07	1.03	0.00000	0.00000	0.00000
			1.151	1.853	2.545						
	5	27	2.5317	3.3045	4.7376	1.11	1.07	1.13	0.00000	0.00000	0.00001
			2.531								
	6	25	1.8003	2.5549	3.3107	1.13	1.03	1.08	0.00000	0.00000	0.00000
			1.800	2.553							
TE-122	0	30	1.0946	1.2974	2.0138	1.10	1.10	1.11	0.00000	0.00000	0.00000
			1.094	1.291	2.008						
	2	27	0.5650	1.2263	2.0276	1.12	1.10	1.06	0.00000	0.00000	0.00000
			0.564	1.215	2.018						
	3	30	1.9842	3.7581	4.7115	1.16	1.12	1.14	0.00000	0.00000	0.00000
			1.982	3.755							
	4	25	1.1776	1.9004	2.7493	1.06	1.05	1.07	0.00000	0.00000	0.00000
			1.175	1.881	2.736						
	5	27	2.7422	3.6237	4.6564	1.16	1.10	1.08	0.00000	0.00000	0.00000
			2.742								
	6	25	1.8342	2.6250	3.5324	1.07	1.04	1.06	0.00000	0.00000	0.00000
			1.831	2.602							
TE-124	0	30	0.9535	1.1473	1.9448	1.16	1.14	1.14	0.00000	0.00000	0.00001
			0.953	1.144	1.942						
	2	27	0.6025	1.2396	1.6685	1.17	1.13	1.14	0.00000	0.00000	0.00002
			0.602	1.234	1.663						
	3	30	2.0667	3.0543	4.1162	1.19	1.12	1.11	0.00000	0.00004	0.00011
			2.066	3.053							
	4	25	1.1513	1.7782	2.3136	1.09	1.09	1.09	0.00001	0.00008	0.00014
			1.190	1.773	2.302						
	5	27	2.7344	3.4602	3.9329	1.11	1.07	1.05	0.00001	0.00029	0.00013
			2.734								
	6	25	1.7032	2.3599	3.0070	1.10	1.05	1.06	0.00002	0.00009	0.00032
			1.830	2.601							

Table E.3. Continued

		$E_B(J_i) - E_B(0_i)$ in MeV			S_B			$\Delta E(J_i)$ in MeV				
		ENERGIES			S-TILDA			EST ERROR				
LEVEL #:		1	2	3	1	2	3	1	2	3		
TF-126	0	30	1.3923 1.392	1.3412 1.338	1.8106 1.811	1.19	1.10	1.09	0.00000	0.00001	0.00023	
	2	27	0.6692 0.668	1.3608 1.354	1.7439 1.740	1.16	1.11	1.07	0.00000	0.00000	0.00015	
	3	30	2.1391 2.138	2.9389 2.954	3.5397	1.16	1.12	1.07	0.00000	0.00031	0.00052	
	4	25	1.3450 1.343	1.8463 1.840	2.1793 2.170	1.05	1.03	0.99	0.00000	0.00025	0.00011	
	5	27	2.8316 2.833	3.1468	3.7290	1.06	1.05	0.99	0.00015	0.00152	0.00012	
	6	25	1.9072 1.852	2.2043 2.136	2.8020	1.03	1.03	1.03	0.00018	0.00057	0.00079	
	TF-128	0	30	1.1712 1.171	1.3202 1.318	1.9323 1.935	1.03	0.99	0.99	0.00000	0.00009	0.00037
		2	27	0.7432 0.743	1.4582 1.452	1.7934 1.789	0.97	0.93	0.93	0.00000	0.00017	0.00022
		3	30	2.6634 2.663	4.2219 4.229	5.2519	1.07	1.05	1.03	0.00000	0.00009	0.00020
		4	25	1.4321 1.429	1.8714 1.867	2.5695 2.562	0.94	0.94	0.94	0.00060	0.00353	0.00317
		5	27	3.6039 3.603	4.6231	5.0869	1.00	0.99	0.98	0.00004	0.00155	0.00236
		6	25	1.8733 1.828	2.5104 2.502	3.3814	0.97	0.97	0.96	0.00246	0.00364	0.00230
TF-130	0	30	1.3307 1.331	1.3284 1.329	2.0875 2.089	1.05	1.01	1.01	0.00000	0.00005	0.00011	
	2	27	0.8385 0.838	1.4674 1.468	1.9171 1.917	0.98	0.98	0.97	0.00000	0.00024	0.00014	
	3	30	2.9193 2.919	4.2327 4.235	5.3867	1.06	1.05	1.01	0.00000	0.00041	0.00087	
	4	25	1.5197 1.520	1.9621 1.963	2.9275 2.824	0.95	0.95	0.94	0.00064	0.00102	0.00106	
	5	27	3.9010 3.901	4.6692	5.4124	1.00	0.97	0.96	0.00004	0.00253	0.00159	
	6	25	1.8929 1.894	2.7902 2.791	3.7400	0.96	0.95	0.96	0.00115	0.00083	0.00204	

Table E.3. Continued

		$E_B(J_i) - E_B(0_i)$ in MeV			ξ_B			$\Delta E(J_i)$ in MeV			
		ENERGIES			S-TILDA			EST ERROR			
LEVEL #:		1	2	3	1	2	3	1	2	3	
XF-126	0	30	-5.0623	2.0942	4.4351	1.12	1.07	1.13	0.00001	0.00002	0.00002
			-5.060	2.094	4.432						
	2	27	0.3882	0.8913	2.6415	1.11	1.08	1.04	0.00003	0.00006	0.00007
			0.388	0.890	2.641						
	3	30	1.3517	4.4130	7.2278	1.14	1.08	1.09	0.00001	0.00005	0.00017
			1.351	4.412							
	4	25	0.9444	1.8045	2.3851	1.06	1.07	1.07	0.00009	0.00026	0.00044
			0.944	1.803	2.383						
	5	27	2.1740	3.2218	5.5319	1.08	1.11	1.06	0.00010	0.00006	0.00005
			2.174								
	6	25	1.6319	2.8689	3.6049	1.07	1.03	1.03	0.00016	0.00081	0.00068
			1.632	2.867							
XF-129	0	30	1.2084	1.9206	4.0995	1.11	1.11	1.11	0.00003	0.00007	0.00013
			1.210	1.920	4.099						
	2	27	0.4435	0.9665	2.8794	1.10	1.06	1.10	0.00004	0.00031	0.00020
			0.444	0.965	2.879						
	3	30	1.3505	4.9003	7.2961	1.15	1.09	1.15	0.00014	0.00024	0.00017
			1.351	4.902							
	4	25	1.0377	1.9872	2.4254	1.04	1.07	1.06	0.00052	0.00050	0.00135
			1.038	1.985	2.425						
	5	27	2.2004	3.1245	6.0947	1.05	1.10	1.04	0.00024	0.00022	0.00357
			2.200								
	6	25	1.7458	3.1780	3.8626	1.06	1.04	1.05	0.00031	0.00285	0.00189
			1.746	3.177							
XF-130	0	30	1.4749	1.8769	3.5725	1.11	1.07	1.13	0.00000	0.00001	0.00000
			1.475	1.877	3.571						
	2	27	0.5289	1.1231	2.8938	1.08	1.07	1.05	0.00000	0.00002	0.00000
			0.529	1.121	2.893						
	3	30	1.6035	5.0409	6.6585	1.08	1.09	1.14	0.00001	0.00004	0.00001
			1.603	5.040							
	4	25	1.1880	2.1983	2.6683	1.04	1.07	1.07	0.00007	0.00011	0.00025
			1.188	2.196	2.666						
	5	27	2.5041	3.4838	6.2845	1.04	1.05	1.04	0.00011	0.00008	0.00061
			2.504								
	6	25	1.9553	3.4177	4.1080	1.06	1.04	1.04	0.00004	0.00026	0.00014
			1.955	3.415							

Table E.3. Continued

			$E_B(J_i) - E_B(0_1)$ in MeV			ξ_B			$\Delta E(J_i)$ in MeV		
			ENERGIES			S-TILDA			EST ERROR		
	LEVEL	#:	1	2	3	1	2	3	1	2	3
XE-132	0	30	1.0311	1.6136	3.1662	1.58	1.54	1.51	0.00001	0.00045	0.00466
			1.032	1.638	3.340						
	2	27	0.6673	1.3346	2.2853	1.55	1.52	1.51	0.00001	0.00033	0.00050
			0.668	1.342	2.328						
	3	30	1.8015	3.5729	5.4962	1.55	1.50	1.49	0.00013	0.00237	0.01230
			1.817	3.750							
	4	25	1.3902	2.3327	2.6845	1.49	1.49	1.49	0.00044	0.00113	0.00143
			1.397	2.350	2.729						
	5	27	2.5682	3.3027	4.3966	1.50	1.50	1.45	0.00118	0.00021	0.01270
			2.631								
	6	25	2.1234	3.3550	3.7177	1.50	1.46	1.44	0.00075	0.00677	0.00309
			2.138	3.421							
XE-134	0	30	1.7837	1.5015	2.0881	1.06	1.04	0.99	0.00000	0.00398	0.00089
			1.789	1.513	2.089						
	2	27	0.8479	1.5714	1.8918	0.99	0.98	0.95	0.00001	0.00638	0.00203
			0.843	1.577	1.888						
	3	30	2.3910	2.7784	4.3254	1.02	1.01	1.00	0.00605	0.00185	0.01302
			2.407	2.783							
	4	25	1.6935	1.8755	2.5243	0.96	0.96	1.00	0.00928	0.00925	0.04319
			1.694	1.876	2.521						
	5	27	2.6237	3.7094	3.9117	0.99	0.99	0.97	0.00959	0.00278	0.02530
			2.627								
	6	25	1.9939	2.7415	2.8449	0.96	0.93	0.93	0.01857	0.02651	0.01346
			2.000	2.735							

Table E.4. Values of $\tilde{s}$ used in GRID diagonalizations of $\bar{H}_{QP}(\beta_0, \gamma_0, c_\gamma)$ [Figure 5.3]. For fixed (β_0, c_γ) , $\tilde{s}$ varied linearly as γ_0 ranged over $0^\circ, 2.5^\circ, 5^\circ, \dots, 30^\circ$; the value of $\tilde{s}$ is consequently given only for $\gamma_0 = 0^\circ$ and 30°

β_0	c_γ	$\tilde{s}(\gamma_0=0^\circ)$	$\tilde{s}(\gamma_0=30^\circ)$	β_0	c_γ	$\tilde{s}(\gamma_0=0^\circ)$	$\tilde{s}(\gamma_0=30^\circ)$
0	0	1.001	1.001	1	0	1.00	1.00
	10	1.22	1.22		10	1.13	1.13
	20	1.20	1.20		20	1.15	1.15
	30	1.20	1.20		30	1.10	1.16
	40	1.20	1.25		40	1.10	1.15
	50	1.18	1.26		50	1.10	1.16
	60	1.18	1.26		60	1.10	1.14
	70	1.18	1.26		70	1.08	1.12
2	0	1.00	1.00	3	0	.90	.90
	10	1.00	1.00		10	.90	.95
	20	1.00	1.05		20	.90	.95
	30	1.00	1.05		30	.90	.95
	40	1.00	1.05		40	.90	.95
	50	1.00	1.08		50	.90	.95
	60	1.00	1.08		60	.90	.95
	70	1.00	1.08		70	.90	.95
4	0	.78	.78	5	0	.74	.74
	10	.78	.82		10	.72	.75
	20	.78	.82		20	.72	.75
	30	.78	.82		30	.72	.75
	40	.80	.84		40	.72	.75
	50	.80	.84		50	.72	.75
	60	.80	.84		60	.72	.75
	70	.80	.84		70	.72	.75
6	0	.67	.67	6	40	.67	.67
	10	.67	.67		50	.67	.67
	20	.67	.67		60	.67	.67
	30	.67	.67		70	.67	.67

Table E.5. Particulars of energy and $B(E2)$ curves for $\bar{H}_{qp}$ drawn using the I.S.U. Simplotter program [mode = 2, see Reference (49)]. x and y refer respectively to the horizontal and vertical coordinates of the figure. In column (C), $[xL0, xH1, \Delta x]$ indicates that x ranged from $xL0$ to $xH1$ in steps of Δx . Within each such interval, $\tilde{s}$ used in the diagonalization ranged linearly from $\tilde{s}(xL0)$ to $\tilde{s}(xH1)$. In column (B), "*" indicates secondary figures constructed from data at one value of x only [e.g., Figure 5.9 is essentially a "detail" of Figure 5.6]. When "GRID" appears in column (B), the figure is based upon the results of the GRID calculations, and graphing particulars may be deduced from Figure 5.3 and Table E.4

(A)	(B)	(C)	(D)	(E)	(F)
Figure(s)	x	Values of x for which y was calculated by diagonalization	$\tilde{s}(xL0)$	$\tilde{s}(xH1)$	$N_{\max}(J)$
5.5	GRID				
5.6-5.8	β_O	$[0, 3, .3]$ $[3.3, 5.1, .3]$	1.0 .92	.93 .76	$\left\{ \begin{array}{l} 20 \text{ for each of} \\ J = 0, 2, 3, 4, 5, 7, 9 \end{array} \right\}$
5.9	β_O^*	$[3, 3, 0]$	.93	.93	as above
5.10-5.11	c_γ	$[0, 80, 1]$	1.1025	1.1025 ^a	$\left\{ \begin{array}{l} 25 \text{ for each of} \\ J = 0, 2 \end{array} \right\}$
5.12	c_β	$[1, 10, .1]$	.95	1.55	25 for $J = 0$
5.13	GRID				
5.14, 5.15, 5.20	c_γ	$[0, 24, 2]$	.92	.92	$\left\{ \begin{array}{l} 22 \text{ for } J = 0; \\ 20 \text{ for each of} \\ J = 2, 3, 4, 5, 6, 7 \end{array} \right\}$
5.23, 5.25 5.27 ($\gamma_O=15^\circ$), 5.28, 5.30	c_γ^*	$[18, 18, 0]$	.92	.92	as above

5.16, 5.17 5.21, 5.22 ^b	C_Y	[0, 24, 2]	.95	.95	$\left\{ \begin{array}{l} 22 \text{ for } J = 0; \\ 20 \text{ for each of} \\ J = 2, 3, 4, 5, 6, 7 \end{array} \right\}$
5.24, 5.26, 5.27 ($\gamma_0=30^\circ$), 5.29, 5.31	C_Y^*	[24, 24, 0]	.95	.95	as above
5.32-5.39	GRID				
5.40 ($\gamma_0=0^\circ, 15^\circ$)	C_Y	[0, 24, 2]	1.0	1.2	$\left\{ 15 \text{ for each of} \right. \\ \left. J=0, 2, 3, 4, 5, 6, 7, 8 \right\}$
5.40 ($\gamma_0=30^\circ$)	C_Y	[0, 24, 2]	1.0	1.25	as above
5.41-5.46 ^c 5.48-5.49	GRID				

^aOriginally each of the $\gamma_0=0^\circ, 15^\circ, 30^\circ$ calculations was made with $\tilde{s}$ fixed at 1.1025. It was later found that the optimal $\tilde{s}$ was somewhat smaller ($\approx .95$). It was found necessary to repeat only the $\gamma_0=0^\circ$ calculations. These were redone with $\tilde{s}(xL0)=.90, \tilde{s}(xH1)=.95$.

^bFor the most part, curves appearing in the figures of this table represent the relative or reduced energy of the state J_i as a function of x . This method is usually appropriate since H_{qp} energies of the states J_i and J_{i+1} are generally forbidden to cross. However in those instances [$C_Y=0; C_Y \neq 0, \gamma_0=30^\circ$] where crossing can occur, $E(J_i)$ -vrs- x curves constructed from a limited number of points will not illustrate the crossing. [See, for example, Figure 5.15. There the $J=0, \beta$ and γ band heads should intersect.] Such intersecting levels have been drawn as exactly intersecting [i.e., followed smoothly through intersections] only in Figures 5.6-5.8, 5.21 and 5.22.

^cThe curves representing 0_Y in Figures 5.41-5.46 do not reflect interference effects from the 2β band head.

Table E.6. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of
 ^{166}Er . [See Figure 6.7]

Band	J	Exp. Energy ^a	DC Model	QP#1 Model (High C_γ)	QP#2 Model (Low C_γ)
GS (K=0)	2	.0806	.081	.082	.082
	4	.265	.263	.265	.265
	6	.545	.535	.534	.530
	8	.911	.883	.871	.861
	10	1.350	1.291	1.261	1.245
GS (K=2)	2	.786	.787	.777	.764
	3	.859	.859	.853	.848
	4	.956	.958	.958	.959
	5	1.075	1.074	1.076	1.086
	6	1.216	1.225	1.237	1.250
	7	1.376	1.374	1.383	1.406
	8	1.556	1.584	1.610	1.623
β (K=0)	0	1.460	1.450	1.446	1.431
	2	1.528	1.541	1.539	1.527
	4		1.746	1.746	1.735
γ (K=0)	0			3.426	2.112
	2			3.497	2.196
	4			3.657	2.382

^aFrom Reference (59). The 1.460 and 1.528 MeV experimental levels may not be β -vibrational in character. However, during model fitting these two levels were assumed to belong to the first β -band.

Table E.7. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of
 ^{182}W . [See Figure 6.8]

Band	J	Exp. Energy ^a	DC Model	QP#1 Model (High C_γ)	QP#2 Model (Low C_γ)
GS (K=0)	2	.100	.101	.104	.107
	4	.329	.325	.329	.336
	6	.681	.649	.648	.657
	8	(1.145)	1.053	1.038	1.046
	10	(1.712)	1.516	1.481	1.487
GS (K=2)	2	1.221	1.250	1.249	1.219
	3	1.331	1.326	1.338	1.327
	4	1.443	1.428	1.451	1.443
	5	1.624	1.551	1.587	1.604
	6		1.702	1.748	1.756
	7		1.862	1.920	1.960
β (K=0)	0	1.138	1.154	1.131	1.095
	2	1.257	1.274	1.258	1.237
	4	1.510	1.536	1.519	1.514
γ (K=0)	0			3.057	2.406
	2			3.136	2.513
	4			3.313	2.759

^aFrom Reference (60).

Table E.8. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of
 ^{122}Te . [See Figure 6.9]

Band	J	Exp. Energy ^a	QP Model	GG Model ^b
GS (K=0)	2	.564	.559	.565
	4	1.181	1.182	1.178
	6	1.751	1.847	1.834
	8	2.669	2.541	2.534
	10	3.290	3.257	3.276
GS (K=2)	2	1.257	1.235	1.226
	3		1.862	1.984
	4		1.918	1.900
	5		2.553	2.742
	6		2.618	2.625
	7		3.267	
GS (K=4)	4		2.582	2.749
	5		3.284	
	6		3.317	
β (K=0)	0	1.357	1.366	1.297
	2		2.012	2.027
	4		2.691	
β (K=2)	2		2.735	
γ (K=0)	0	1.940	1.971	2.014
	2		2.622	
	4		3.315	
γ (K=2)	2		3.347	

^aFrom References (29) and (30), and the works cited therein.

^bFrom References (29) and (30), and Chapter IV of the present work.

Table E.9. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of ^{186}Os .
 [See Figure 6.12].

Band	J	Exp. Energy ^a	DC Model	HQP($\beta\gamma$) Model	HQP($\gamma\beta$) Model	HQP($\gamma 0$) Model
GS (K=0)	2	.137	.138	.138	.143	.144
	4	.434	.424	.394	.400	.400
	6	.869	.807	.724	.741	.733
	8	1.421	1.249	1.104	1.147	1.122
	10	2.070	1.732	1.522	1.606	1.554
GS (K=2)	2	.768	.782	.729	.634	.710
	3	.910	.889	.876	.857	.904
	4	1.071	1.036	1.025	.977	1.028
	5	1.276	1.193	1.207	1.237	1.258
	6	1.491	1.421	1.388	1.360	1.391
	7	1.752	1.596	1.594	1.678	1.665
	8		1.919	1.803	1.801	1.800
	9		2.073	2.024	2.169	2.113
	10			2.255	2.290	2.246
GS (K=4)	4	1.352	2.457	1.549	1.373	1.462
	5	1.560		1.788	1.757	1.790
	6	1.776		1.993	1.866	1.918
	7			2.225	2.259	2.247
	8			2.445	2.379	2.364
0 ₂ (K=0)	0 ₂	1.061	1.072	.985	1.077	1.015
	2	1.208	1.242	1.179	1.383	1.241
	4		1.584	1.485	1.772	1.564
0 ₃ (K=0)	0 ₃	1.456	2.152	1.549	1.451	1.307
	2		2.351	1.710	1.632	1.532
	4			1.988	1.937	1.862
	0 ₄	1.953		1.993	2.372	2.080
	0 ₅			2.599	2.625	2.388

^aFrom Reference (62) and the works cited therein.

Table E.10. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of ^{188}Os .
 [See Figure 6.13]

Band	J	Exp. Energy ^a	DC Model	HQP($\beta\gamma$) Model	HQP($\gamma\beta$) Model	HQP($\gamma 0$) Model
GS (K=0)	2	.155	.157	.163	.162	.159
	4	.478	.470	.440	.431	.424
	6	.940	.870	.782	.776	.770
	8	1.515	1.322	1.172	1.183	1.178
	10	2.170	1.817	1.599	1.642	1.640
GS (K=2)	2	.633	.650	.594	.562	.578
	3	.790	.776	.769	.801	.837
	4	.965	.960	.953	.928	.928
	5	1.182	1.130	1.138	1.194	1.230
	6	1.425	1.429	1.380	1.343	1.327
	7		1.587	1.560	1.646	1.679
	8		2.022	1.855	1.808	1.777
	9		2.115	2.021	2.146	2.178
	10			2.359	2.315	2.272
GS (K=4)	4	1.280	2.055	1.363	1.295	1.308
	5	1.516	2.216	1.654	1.691	1.725
	6		2.405	1.874	1.809	1.795
	7			2.145	2.209	2.232
	8			2.381	2.347	2.312
0 ₂ (K=0)	0 ₂	1.085	1.111	1.069	1.071	.989
	2	1.305	1.305	1.291	1.386	1.330
	4		1.680	1.619	1.780	1.746
0 ₃ (K=0)	0 ₃	1.478	2.234	1.486	1.416	1.422
	2		2.461	1.675	1.616	1.620
	4			1.986	1.931	1.932
	0 ₄	1.704		2.162	2.407	2.307
	0 ₅	1.765		2.644	2.610	2.527

^aFrom Reference (62) and the works cited therein.

Table E.11. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of ^{190}Os .
 [See Figure 6.14]

Band	J	Exp. Energy ^a	DC Model	HQP($\beta\gamma$) Model	HQP($\gamma\beta$) Model	HQP($\gamma 0$) Model
GS (K=0)	2	.187	.191	.200	.184	.179
	4	.548	.532	.490	.457	.450
	6	1.050	.934	.827	.802	.795
	8	1.667	1.375	1.197	1.210	1.204
	10		1.851	1.597	1.672	1.667
GS (K=2)	2	.558	.589	.546	.483	.497
	3	.756	.733	.734	.783	.808
	4	.955	.958	.945	.851	.849
	5	1.204	1.124	1.107	1.191	1.213
	6		1.490	1.394	1.275	1.258
	7		1.600	1.515	1.654	1.673
	8		2.116	1.869	1.747	1.719
	9		2.124	1.950	2.166	2.181
	10			2.354	2.263	2.226
GS (K=4)	4	1.163	1.758	1.260	1.215	1.234
	5	1.446	1.938	1.556	1.661	1.684
	6	1.836	2.149	1.771	1.707	1.708
	7		2.383	2.034	2.183	2.197
	8			2.308	2.241	2.226
0_2 (K=0)	0_2	.912	.950	.884	.911	.870
	2	1.115	1.191	1.149	1.279	1.254
	4		1.601	1.489	1.716	1.701
0_3 (K=0)	0_3	1.546	1.938	1.513	1.474	1.463
	2		2.214	1.740	1.694	1.681
	4			2.074	2.014	1.997
	0_4	1.734		1.810	2.289	2.235
	0_5			2.517	2.513	2.459

^aFrom Reference (62) and the works cited therein.

Table E.12. Experimental and model relative energies
 $[E(J_i) - E(0_1)]$ in MeV for selected states of ^{192}Os .
 [See Figure 6.15]

Band	J	Exp. Energy ^a	DC Model	HQP($\beta\gamma$) Model	HQP($\gamma\beta$) Model	HQP($\gamma 0$) Model
GS (K=0)	2	.206	.207	.215	.196	.180
	4	.580	.549	.497	.470	.457
	6	1.089	.947	.824	.804	.800
	8	1.708	1.392	1.189	1.190	1.189
	10		1.875	1.586	1.619	1.616
GS (K=2)	2	.489	.507	.480	.468	.617
	3	.690	.669	.709	.752	.874
	4	.909	.960	.910	.845	.965
	5	1.143	1.106	1.089	1.143	1.248
	6	1.362	1.573	1.365	1.266	1.345
	7	1.713	1.614	1.502	1.578	1.663
	8	1.967	2.229	1.829	1.719	1.759
	9		2.155	1.939	2.050	2.110
	10			2.296	2.201	2.203
GS (K=4)	4	1.069	1.510	1.141	1.166	1.334
	5		1.733	1.498	1.578	1.715
	6	1.465	1.996	1.652	1.641	1.789
	7		2.272	1.979	2.068	2.172
	8			2.184	2.151	2.255
0_2 (K=0)	0_2	.956	.982	.914	.944	.916
	2	1.125	1.243	1.187	1.280	1.198
	4		1.653	1.522	1.676	1.544
0_3 (K=0)	0_3	1.206	2.002	1.236	1.161	1.123
	2		2.300	1.451	1.404	1.401
	4			1.801	1.728	1.767
	0_4	1.924		1.867	2.239	1.927
	0_5			2.301	2.253	2.183

^aFrom Reference (62) and the works cited therein.

Table E.13. $B(E2:J_i \rightarrow J_f)$ in units of $B(E2:2_1 \rightarrow 0_1)$, and $\bar{Q}(J_i) \equiv Q(J_i)/[B(E2:2_1 \rightarrow 0_1)]^{1/2}$ for ^{186}Os . Experimental and GG-model values are taken from Reference (63)

	Exp. ^a	DC Model	GG Model	$\bar{H}_{QP}(\beta\gamma)$ Model	$\bar{H}_{QP}(\gamma\beta)$ Model
$2_2 \rightarrow 0_1$	.078		.033	.0829	.0742
$2_2 \rightarrow 2_1$	.172	.177	.330	.362	.506
$4_1 \rightarrow 2_1$	1.51	1.539	1.58	1.571	1.527
$4_1 \rightarrow 2_2$		.0561	.006	.0123	.0097
$6_1 \rightarrow 4_1$	1.8			1.963	1.851
$2_1 \rightarrow 0_2$				.0795	.0225
$2_2 \rightarrow 0_2$		.0126		.0001	.2050
$\bar{Q}(2_1)$	-1.86		-1.91	-1.902	-1.757
$\bar{Q}(2_2)$			1.75	1.940	1.752
$\bar{Q}(4_1)$			-2.37	-2.246	-1.996
$\bar{Q}(4_2)$			-.79	-1.162	-.317

^aRatios calculated from values cited in References (61) and (63).

Table E.14. $B(E2:J_i \rightarrow J_f)$ in units of $B(E2:2_1 \rightarrow 0_1)$, and $\bar{Q}(J_i) \equiv Q(J_i)/[B(E2:2_1 \rightarrow 0_1)]^{1/2}$ for ^{188}Os . Experimental and GG-model values are taken from Reference (63)

	Exp. ^a	DC Model	GG Model	$\bar{H}_{QP}(\beta\gamma)$ Model	$\bar{H}_{QP}(\gamma\beta)$ Model
$2_2 \rightarrow 0_1$	.091		.029	.0791	.0634
$2_2 \rightarrow 2_1$	.27	.295	.55	.625	.739
$4_1 \rightarrow 2_1$	1.42	1.560	1.60	1.577	1.529
$4_1 \rightarrow 2_2$		.0282	.002	.0219	.0117
$6_1 \rightarrow 4_1$	2.5			2.010	1.879
$2_1 \rightarrow 0_2$				.0794	.0186
$2_2 \rightarrow 0_2$		.0126		.0011	.2002
$\bar{Q}(2_1)$	-1.78		-1.75	-1.689	-1.546
$\bar{Q}(2_2)$			1.64	1.720	1.544
$\bar{Q}(4_1)$			-2.07	-1.744	-1.631
$\bar{Q}(4_2)$			-.92	-1.319	.353

^aRatios calculated from values cited in References (61) and (63).

Table E.15. $B(E2:J_i \rightarrow J_f)$ in units of $B(E2:2_1 \rightarrow 0_1)$, and $\bar{Q}(J_i) \equiv Q(J_i)/[B(E2:2_1 \rightarrow 0_1)]^{1/2}$ for ^{190}Os . Experimental and GG-model values are taken from Reference (63)

	Exp. ^a	DC Model	GG Model	$\bar{H}_{QP}(\beta\gamma)$ Model	$\bar{H}_{QP}(\gamma\beta)$ Model
$2_2 \rightarrow 0_1$	.087		.00004	.0548	.0188
$2_2 \rightarrow 2_1$	.48	.483	1.37	.979	1.261
$4_1 \rightarrow 2_1$	1.17	1.618	1.47	1.632	1.495
$4_1 \rightarrow 2_2$		.0481	.005	.0222	.0035
$6_1 \rightarrow 4_1$	2.8			2.185	1.832
$2_1 \rightarrow 0_2$				.1236	.0051
$2_2 \rightarrow 0_2$		.0172		.0052	.2851
$\bar{Q}(2_1)$	-1.33		- .54	-1.391	- .840
$\bar{Q}(2_2)$			.57	1.433	.839
$\bar{Q}(4_1)$			- .40	-1.262	- .830
$\bar{Q}(4_2)$			.34	-1.566	+ .137

^aRatios calculated from values cited in References (61) and (63).

Table E.16. $B(E2:J_i \rightarrow J_f)$ in units of $B(E2:2_1 \rightarrow 0_1)$, and $\bar{Q}(J_i) \equiv Q(J_i)/[B(E2:2_1 \rightarrow 0_1)]^{1/2}$ for ^{192}Os . Experimental and GG-model values are taken from Reference (63)

	Exp. ^a	DC Model	GG Model	$\bar{H}_{QP}(\beta\gamma)$ Model	$\bar{H}_{QP}(\gamma\beta)$ Model
$2_2 \rightarrow 0_1$	.097		.0058	0.0	.0009
$2_2 \rightarrow 2_1$	.82	.797	1.50	1.568	1.498
$4_1 \rightarrow 2_1$	1.23	1.591	1.50	1.576	1.513
$4_1 \rightarrow 2_2$		.05608	.0006	0.0	.002
$6_1 \rightarrow 4_1$				2.083	1.901
$2_1 \rightarrow 0_2$				.1138	.0005
$2_2 \rightarrow 0_2$		.0118		0.0	.2618
$\bar{Q}(2_1)$	- .75		- .138	0.0	- .188
$\bar{Q}(2_2)$			.121	0.0	.188
$\bar{Q}(4_1)$			- .199	0.0	- .178
$\bar{Q}(4_2)$			.188	0.0	- .0026

^aRatios calculated from values cited in Reference (63).

XII. APPENDIX F: ANGULAR MOMENTUM CONVENTIONS

This final appendix sets forth the angular momentum conventions assumed throughout Reference (22) and the present work. In the initial section, the "active" rotations of points, functions and physical systems are defined with reference to an arbitrary "fixed" LAB coordinate frame. Two methods of enumerating the distinct rotations are described. These employ the usual Euler angles, θ_i , and the Mielnik-Plebanski vector (70), b , respectively. The latter parameterization is used to illustrate some of the general concepts. Observers in two reference frames, LAB and $\overline{\text{LAB}}$, generally assign different sets of parameters to a given active rotation. The relationship between the two sets of parameters, and its application to the rigid body problem are the final topics of Section A. The following two sections then outline the procedure for constructing rotation matrix elements $D_{m,m}^j(\theta_i)$. Group representations are introduced in Section B, and commutation relationships are derived for the generators (J_i) of infinitesimal rotations. These commutation relations, together with a phase convention, lead to the expression for $D_{m,m}^j(\theta_i)$ presented in Section C. Sections D and E discuss the spherical harmonic functions and Clebsch-Gordon coefficients respectively. In each case the adoption of a phase convention leads to a specific closed expression. The final section serves to define irreducible tensor operators and to present the adopted form of the Wigner-Eckart theorem.

Sections C-F essentially summarize relevant portions of the text by M. E. Rose (31), and the reader is referred there for further details of

the derivations. For a more complete discussion of properties of continuous groups near the identity [in particular, the relationships between group generators, structure constants, and the form of the product mapping] the interested reader may consult References (32) and (71). Equations (F.11)-(F.13) and (F.15), which involve the Mielnik-Plebanski vector, are due to D. L. Pursey (72).

A. The Active Viewpoint

An n -parameter continuous group G consists of a collection of elements $\{a, b, c, \dots\}$ together with a mapping m of $G \times G$ onto G . Each element b requires n real numbers $(b_1, b_2, \dots, b_n)$ for its specification, and the mapping may consequently be represented by a set of n functions:

$$m_i(a_1, a_2, \dots, a_n; b_1, b_2, \dots, b_n) = c_i, (i = 1, 2, \dots, n) \quad (F.1a)$$

We assume that each of the m_i is a smooth function of its arguments and possesses continuous first and second derivatives. By definition, four conditions must be satisfied by the elements and mapping for G to be a group. If the group product of Equation (F.1a) is written in the abbreviated form

$$a \cdot b = c, \quad (F.1b)$$

these conditions may be expressed as follows:

- 1) Closure. If a and b are arbitrary elements of G , then their product $a \cdot b$ is a unique element of G .
- 2) Identity. There exists a unique element e of G with the property

$$e \cdot b = b \cdot e = b \quad (F.2a)$$

for arbitrary b .

- 3) Inverse. For every element b of G there exists a unique element of G , denoted by b^{-1} , with the property

$$b \cdot b^{-1} = b^{-1} \cdot b = e \quad . \quad (F.2b)$$

- 4) Associativity. For arbitrary elements a , b , and c of G , the product mapping satisfies

$$a \cdot (b \cdot c) = (a \cdot b) \cdot c \quad . \quad (F.2c)$$

In a physical setting, the explicit form of the product [Equation (F.1a)] may be found once we have specified:

- 1) the meaning of each element [or "operation"] of G as it is realized in the physical setting;
- 2) the meaning of the group product of two operations; and
- 3) a scheme for enumerating the elements of G .

We now consider each of these points in turn for the group of physical rotations, $G = R(3)$.

We begin by selecting a set of right-handed, mutually perpendicular [LAB] axes. With respect to these axes, points in the surrounding three-dimensional Euclidean space $[E_3]$ may be assigned cartesian coordinates $\underline{x} = (x_1, x_2, x_3)$. Each rotation b of $R(3)$ is a mapping of E_3 onto E_3 , and associates with each point $\underline{x}$ a "rotated image" $\underline{x}'$. We write

$$\boxed{b: \underline{x} \rightarrow \underline{x}' \quad \text{or} \quad \underline{x}' = \underline{f}(b, \underline{x})} \quad . \quad (F.3)$$

By definition, the mapping has the properties:

- 1) lengths are preserved $\left[\sum_{i=1}^3 x_i' x_i' = \sum_{i=1}^3 x_i x_i \right]$; and
- 2) for every b there is some straight line passing through the LAB origin [axis of rotation] such that

$$x_i' = x_i \quad (i = 1, 2, 3)$$

for points on the line.

If the relationship between $\underline{x}$ and $\underline{x}'$ is expressed as

$$x_i' = \sum_j [F(b)]_{ij} x_j \quad ,$$

the above properties assure that $[F]$ is an orthogonal matrix (i.e., $[F]^t = [F]^{-1}$) having a determinant of +1. The relationship between $\underline{x}$ and $\underline{x}'$ is depicted in Figure F.1a. In this case the [directed] axis of rotation is along the unit vector $\hat{n}$, and the rotation is through the positive angle θ . [A right-handed screw, lying along $\hat{n}$ with its head facing the origin, is advanced away from the origin by a rotation about $\hat{n}$ through a positive angle θ .] A rotation of $-\theta$ or $(2\pi - \theta)$ about the vector $-\hat{n}$ would have an equivalent effect upon $\underline{x}$. The group identity e is the null rotation $[\underline{x}' = \underline{x}$ for arbitrary $\underline{x}]$, and a rotation about $\hat{n}$ through $-\theta$ is the inverse of the rotation depicted in Figure F.1a.

We view every rotation b as acting actively upon objects situated in E_3 . For example, a point mass at $\underline{x}$ is transported to $\underline{x}'$ by the action of b . Both the original and rotated mass are viewed from the LAB axes which provide a reference frame for gauging the effects of b . Thus the orientations of the LAB axes are not altered by b . However, point

P' is the image of P under a rotation through the positive angle θ about the $\hat{n}$ axis. The arc $\widehat{PP'}$ shown lies in a plane perpendicular to $\hat{n}$.

$\phi'(\underline{x})$ is the image of $\phi(\underline{x})$ under a rotation through the positive angle θ about the $\hat{z}$ axis. In this example the values of $\phi(\underline{x})$ and $\phi'(\underline{x})$ at selected points in the xy plane are indicated by the contour lines. Notice that if P' is the image of P , then

$$\phi'(P') = \phi(P) \quad .$$

Figure F.1. Actively rotated points (a) and functions (b) as viewed from the LAB reference frame.

masses situated at LAB coordinates $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ would all be actively rotated, with their final positions dictated by Equation (F.3). There will be some reference frame in which the final positions of the three masses are $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ respectively. We designate this frame LAB' , write

$$\boxed{b: \text{LAB} \rightarrow \text{LAB}'}, \quad (\text{F.4})$$

and refer to coordinate system LAB' as the "image of LAB under b ". Let S denote an arbitrarily complex physical system, and let S' denote the rotated version of S , obtained by applying b [of Equation (F.4)] actively. The characteristics of S' as they appear to a LAB' observer, are identical to the characteristics of S as they appear to a LAB observer. This last statement may be viewed as defining the rotated version of S in the general case.

Suppose now that $\underline{q} = (q_1, q_2, \dots, q_m)$ and $\underline{q}'$ are the generalized coordinate sets used by a LAB observer to specify the configurations of S and S' respectively. Then $\underline{q}'$ is said to be the image of $\underline{q}$ under b and we write

$$\boxed{b: \underline{q} \rightarrow \underline{q}' \quad \text{or} \quad \underline{q}' = \underline{h}(b, \underline{q})}, \quad (\text{F.5})$$

Hence the active rotation b changes the generalized coordinates of S from $\underline{q}$ to $\underline{q}'$. If S consists of a single point particle whose only characteristic is its location, we may take $q_i = x_i$ ($i = 1, 2, 3$), in which case Equations (F.3) and (F.5) become identical. [The fact that the elements b satisfy the defining conditions for a group [Equations (F.2)] imposes certain conditions upon the functions $\underline{h} = (h_1, h_2, \dots, h_m)$.

We will return to this point shortly when the "product" of rotations is defined.] Let $\phi(q)$ and $\phi'(q)$ be the LAB versions of the S and S' wave-functions in the q -coordinate representation. We may insist that the phase of the latter be chosen such that

$$\phi'(q') = \phi(q) \quad , \quad (F.6a)$$

from which

$$\phi'(q) = \phi(h(b^{-1}, q)) \quad (F.6b)$$

follows. The function $\phi'(q)$ defined by Equation (F.6b) is said to be the actively rotated counterpart of $\phi(q)$, and we write

$$\boxed{b: \phi(q) \rightarrow \phi'(q) \text{ or } R(b)\phi(q) = \phi'(q) = \phi(h(b^{-1}, q))} \quad . \quad (F.6c)$$

$R(b)$ satisfying Equation (F.6c) would be realized as a differential operator on the space of functions of q . The relationship between ϕ and ϕ' is pictured in Figure F.1b for the case $q = x$.

We now assign a meaning to the product mapping for $R(3)$ operations. By $a \cdot b$ we shall mean the successive application of the active rotations, b followed by a . Thus in the equation

$$a \cdot b = c \quad ,$$

c identifies that single rotation whose effect [as gauged from Figure (F.1a) or Equation (F.3)] is equivalent to that of b followed by a . If x'' denotes the rotated image of x under c , then

$$c = a \cdot b: x \rightarrow x'' \text{ implies } x'' = f(a, x') = f(a, f(b, x)) \quad (F.7)$$

where x' is the vector in Equation (F.3). By virtue of Equations (F.2),

(F.3) and (F.7) we have the conditions

$$\underline{f}(a \cdot b, \underline{x}) = \underline{f}(a, \underline{f}(b, \underline{x})) \quad , \quad (\text{F.8a})$$

$$\underline{f}(e, \underline{x}) = \underline{x} \quad , \quad (\text{F.8b})$$

and

$$\underline{x}' = \underline{f}(b, \underline{x}) \text{ implies } \underline{x} = \underline{f}(b^{-1}, \underline{x}') \quad . \quad (\text{F.8c})$$

Similar conditions [obtained by replacing $\underline{f}$ by $\underline{h}$ and $\underline{x}$ by $\underline{q}$ in Equations (F.8a)-(F.8c)] are assumed to be satisfied by the $\underline{h}(b, \underline{q})$ of Equation (F.5). We are then assured that the operator $R(b)$ in Equation (F.6c) has the properties

$$R(a)R(b)\phi(\underline{q}) = R(c)\phi(\underline{q}) \text{ if } a \cdot b = c \quad , \quad (\text{F.8d})$$

$$R(e)\phi(\underline{q}) = \phi(\underline{q}) \quad , \quad (\text{F.8e})$$

and

$$R(b)\phi(\underline{q}) = \phi'(\underline{q}) \text{ implies } R(b^{-1})\phi'(\underline{q}) = \phi(\underline{q}) \quad . \quad (\text{F.8f})$$

When operating on an arbitrary function of $(\underline{q})$, $R(b)$ effectively replaces every occurrence of $\underline{q}_i$ with $\underline{h}_i(b^{-1}, \underline{g})$. The conditions expressed by Equations (F.8a)-(F.8c) appear, in the notation of Equation (F.4), as

$$\left. \begin{array}{l} b: \text{ LAB} \rightarrow \text{LAB}' \\ a: \text{ LAB}' \rightarrow \text{LAB}'' \end{array} \right\} \text{ imply } a \cdot b: \text{ LAB} \rightarrow \text{LAB}'' \quad , \quad (\text{F.8g})$$

$$e: \text{ LAB} \rightarrow \text{LAB} \quad , \quad (\text{F.8h})$$

$$b: \text{ LAB} \rightarrow \text{LAB}' \text{ implies } b^{-1}: \text{ LAB}' \rightarrow \text{LAB} \quad . \quad (\text{F.8i})$$

Again we emphasize that the orientations of all sets of coordinate axes [LAB, LAB', LAB'' in Equations (F.8g)-(F.8i)] are regarded as fixed

against rotations. The notation

$$b: LAB \rightarrow LAB' ,$$

which is used to describe the relative orientation of two sets of coordinates axes, should be interpreted in terms of the hypothetical point masses described above Equation (F.4).

Thus far little has been said about methods of assigning group coordinates $(b_1, b_2, \dots b_n)$ to the general element b of $R(3)$. In effect such coordinates would specify the relative orientations of two frames, LAB and LAB' , connected by

$$b: LAB \rightarrow LAB' .$$

In as much as every b leaves some "rotation axis" unchanged, a LAB observer may parameterize b , as in Figure F.1a, by specifying

- 1) the unit vector $\hat{n}$ along the directed rotation axis, and
- 2) the angle of rotation θ about $\hat{n}$.

All rotations may be enumerated by extending $\hat{n}$ over all unit vectors from the origin, and restricting θ to $0 \leq \theta \leq \pi$. [Rotations through π about $\hat{n}$ and $-\hat{n}$ are equivalent]. From $\hat{n}$ and θ we may construct the Mielnik-Plebanski [MP] vector (70)

$$\underline{b} \equiv \hat{n} \tan(\tfrac{1}{2}\theta) . \quad (F.9a)$$

The direction and magnitude of $\underline{b}$ then specify the axis and angle of

rotation respectively.¹ The projections of $\underline{b}$ along the LAB axes $\{b_i; i = 1, 2, 3\}$ may be taken as group parameters. From the restriction of θ to $[0, \pi]$, the ranges of the MP parameters are then

$$-\infty < b_i < \infty \quad i = 1, 2, 3 \quad . \quad (F.9b)$$

Two rotations having MP vectors $\underline{b}^1$ and $\underline{b}^2$ are equivalent if

$$\underline{b}^1 = -\underline{b}^2 \quad \text{and} \quad |\underline{b}^1| = |\underline{b}^2| = \infty \quad . \quad (F.9c)$$

The null rotation has the MP parameterization

$$\underline{e} = \underline{e} - \underline{0} = (0, 0, 0) \quad , \quad (F.9d)$$

and the rotation inverse to $\underline{b}$ is clearly $-\underline{b}$:

$$(\underline{b}^{-1}) = -\underline{b} \quad . \quad (F.9e)$$

The MP parameters are useful tools for the exploration of $R(3)$ properties. The rotation associated with $\underline{b}$ may be immediately visualized, and the parameterization is well-defined in the neighborhood of $\underline{e}$.

A more common method of specifying $R(3)$ elements employs Euler angles $(\theta_i) = (\theta_1, \theta_2, \theta_3)$. In particular we consider here the version of the Euler angles employed by Rose (31). Three successive "simple" rotations are performed whose cumulative effect is equivalent to

$$\underline{b}: \text{LAB} \rightarrow \text{LAB}' \quad .$$

¹We will continue to use $\underline{b}$ to denote a general element of $R(3)$. $\underline{b}$ and (θ_i) will be used to denote the MP parameters and Euler angles of $\underline{b}$ respectively.

In order of application,¹ these are

- 1) A rotation through θ_3 about the LAB $\hat{x}_3 = \hat{z}$ axis,
 - 2) A rotation through θ_2 about the LAB $\hat{x}_2 = \hat{y}$ axis, and
 - 3) A rotation through θ_1 about the LAB $\hat{x}_3 = \hat{z}$ axis.
- (F.10)

All possible rotations may be accounted for by restricting the angles to $\Omega(\theta_i)$ defined below Equation (B.4). Alternatively, ranges symmetric about zero may be chosen so that the element inverse to $(\theta_1, \theta_2, \theta_3)$ may be written as $(-\theta_3, -\theta_2, -\theta_1)$. In the latter event, b^{-1} lies near the origin of Euler-angle-space if b does; however, $(\theta_1, 0, -\theta_1)$ then represents the null rotation for any value of θ_1 . This last property renders the Euler angle parameterization inappropriate for exploring differential properties of Equation (F.1a) near the identity. For such an exploration we desire that the parameters of all infinitesimal rotations lie near the parameters of e , and that all such rotations be uniquely parameterized. The MP parameters, on the other hand, satisfy these requirements.

If the rotation b is parameterized by a LAB observer to have MP components $\underline{b} = (b_1, b_2, b_3)$ and Euler angles $(\theta_i) = (\theta_1, \theta_2, \theta_3)$, then the two sets of parameters are connected by

$$\begin{aligned} b_1 &= [\tan \tfrac{1}{2}\theta_2 / \cos \tfrac{1}{2}(\theta_1 + \theta_3)] [-\sin \tfrac{1}{2}(\theta_1 - \theta_3)] \\ b_2 &= [\tan \tfrac{1}{2}\theta_2 / \cos \tfrac{1}{2}(\theta_1 + \theta_3)] [\cos \tfrac{1}{2}(\theta_1 - \theta_3)] \end{aligned} \quad (F.11)$$

¹Rose (31) begins with an equivalent definition in which the order of application is reversed, and rotations are performed about rotated images of the LAB axes.

$$b_3 = \tan \frac{1}{2}(\theta_1 + \theta_3)$$

These may be inverted to give

$$\begin{aligned}\tan \theta_1 &= [b_2 b_3 - b_1] / [b_2 + b_1 b_3] \\ \cos \theta_2 &= [1 + (b_3)^2 - (b_1)^2 - (b_2)^2] / [1 + (b_1)^2 + (b_2)^2 + (b_3)^2] \\ \tan \theta_3 &= [b_2 b_3 + b_1] / [b_2 - b_1 b_3]\end{aligned}\quad (F.12)$$

In the MP parameterization, the relationship between the original and rotated image positions [$\underline{x}$ and $\underline{x}'$ in Figure F.1a] of an arbitrary point may be written explicitly as

$$\underline{x}' = \underline{f}(\underline{b}, \underline{x}) = [1 + \underline{b} \odot \underline{b}]^{-1} \{ (1 - \underline{b} \odot \underline{b}) \underline{x} + 2(\underline{x} \odot \underline{b}) \underline{b} + 2 \underline{b} \boxtimes \underline{x} \} \quad (F.13)$$

In Equation (F.13), $\odot$ and $\boxtimes$ denote the usual scalar and cross products:

$$\begin{aligned}\underline{b} \odot \underline{c} &\equiv \sum_{i=1}^3 b_i c_i \\ \underline{b} \boxtimes \underline{c} &\equiv \sum_{ijk} \epsilon_{ijk} b_i c_j \hat{x}_k \quad ; \quad \epsilon_{ijk} = \begin{cases} +1 & (ijk) = (123), (312), (231) \\ -1 & (ijk) = (213), (132), (321) \\ 0 & \text{otherwise} \end{cases}\end{aligned}$$

One may readily verify that $\underline{f}(\underline{b}, \underline{x})$ given by Equation (F.13) satisfies Equations (F.8b) and (F.8c). Furthermore,

$$\underline{c} = \underline{a} \cdot \underline{b} \text{ implies } \underline{f}(\underline{c}, \underline{x}) = \underline{f}(\underline{a}, \underline{f}(\underline{b}, \underline{x})) \quad (F.14)$$

may be used to deduce the form of the group product [Equation (F.1a)] under the MP parameterization:

$$\underline{c} = \underline{m}(\underline{a}; \underline{b}) = \frac{\underline{a} + \underline{b} + \underline{a} \boxtimes \underline{b}}{[1 - \underline{a} \odot \underline{b}]} \quad (F.15)$$

The group postulates [Equations (F.2)] are found to be satisfied by the set of elements and product mapping defined in Equations (F.9) and (F.15) respectively. When Equation (F.15) is used, care must be taken to refer all components a_i , b_i , c_i to a single set of reference axes [LAB for example] whose orientations are fixed against the rotations in question.

Occasionally in physical problems, one becomes interested in translating expressions between two or more reference frames. We now briefly consider the problem of translating rotation parameters. Let LAB and $\overline{\text{LAB}}$ denote two distinct reference frames possessing a common origin, and suppose that observers in each frame agree to parameterize active rotations according to a common scheme. Each observer, for example, could adopt the Euler angle scheme, and refer $(\theta_1, \theta_2, \theta_3)$ to his own coordinate axes. It is clear that the observers will generally not assign identical parameters to a given rotation. For example in the MP scheme, the projections of $\underline{b}$ upon corresponding LAB and $\overline{\text{LAB}}$ axes will generally differ. Let us suppose that:

- 1) The two reference frames are connected by the rotation a in the sense of Equation (F.4)

$$a: \text{LAB} \rightarrow \overline{\text{LAB}} \quad .$$

- 2) a is assigned the parameters $(a_i^{\text{LAB}}; i = 1, 2, 3)$ by a LAB observer.
- 3) Some other rotation b is assigned parameters $(b_i^{\text{LAB}}; i = 1, 2, 3)$ by a LAB observer.

We ask, "what parameters $(b_i^{\overline{\text{LAB}}}; i = 1, 2, 3)$ are assigned to b by the

$\overline{LAB}$ observer?" This question may be immediately answered if two auxiliary reference frames, $\overline{LAB}^*$ and LAB^* , are introduced. By definition the first is the image of $\overline{LAB}$ under b

$$b: \overline{LAB} \rightarrow \overline{LAB}^*,$$

and second is defined from the first by

$$a: LAB^* \rightarrow \overline{LAB}^*.$$

The relationships between the four reference frames [in the sense of Equation (F.4)] may thus be summarized by

$$\begin{array}{ccc} LAB & \xrightarrow{a} & \overline{LAB} \\ & \downarrow b & \\ LAB^* & \xrightarrow{a} & \overline{LAB}^* \end{array} \quad (F.16)$$

We may think of the rotation "a" as simultaneously taking LAB and LAB^* into their respective images $\overline{LAB}$ and $\overline{LAB}^*$. The relative orientation between LAB and LAB^* is not altered during this process, and consequently

$$\left[\begin{array}{l} \text{The appearance of } LAB^* \\ \text{as seen from } LAB \end{array} \right] \text{ is identical to } \left[\begin{array}{l} \text{the appearance of } \overline{LAB}^* \\ \text{as seen from } \overline{LAB} \end{array} \right].$$

Thus the parameters assigned by $\overline{LAB}$ to b must equal the parameters assigned by LAB to

$$b^*: LAB \rightarrow LAB^*.$$

However from Equations (F.8g), (F.8i) and (F.16), b^* is clearly equivalent to the group product $a^{-1} \cdot b \cdot a$. Hence if $a: LAB \rightarrow \overline{LAB}$, then for arbitrary b

$$\overline{b_i^{LAB}} = [a^{-1} \cdot b \cdot a]_i^{LAB}, \quad i = 1, 2, 3, \quad (F.17a)$$

where the right-hand side denotes the i^{th} parameter assigned by LAB to the single rotation equivalent to $a^{-1} \cdot b \cdot a$. $[a^{-1} \cdot b \cdot a]_i^{LAB}$ may be computed by using the a_i^{LAB} and b_i^{LAB} together with the appropriate multiplication law [Equation (F.15) in the MP parameterization]. An immediate consequence of Equation (F.17a) is obtained by taking $b = a$:

$$\overline{a_i^{LAB}} = a_i^{LAB}. \quad (F.17b)$$

The two frames, LAB and $\overline{LAB}$, assign identical parameter sets to the rotation which connects them. In the MP scheme, this result is obvious. When the LAB axes are "spun about" the rotation vector $\underline{a}$, the projections of $\underline{a}$ along the moving axes do not change. Consequently all instantaneous images of LAB encountered during this spinning process must assign identical parameter sets to $\underline{a}$.

Because both LAB and $\overline{LAB}$ observers agree on the parameters of $\underline{a}$, the result of Equation (F.17a) may be expressed in an alternative form:

$$\begin{aligned} &\text{If } \underline{a}: \text{ LAB} \rightarrow \overline{LAB}, \\ &\text{then for any rotation } b \end{aligned} \quad (F.17c)$$

$$[a \cdot b]_i^{\overline{LAB}} = [b \cdot a]_i^{LAB}, \quad i = 1, 2, 3.$$

This form finds an immediate application in the rigid body problem. To specify the configuration of a rigid body, it suffices to describe the orientation of a set of axes (BF) fixed in the body. For this purpose, a LAB observer may choose as generalized coordinates (q_1, q_2, q_3) the

LAB parameters describing the rotation

$$q_i = a_i^{\text{LAB}}, \quad a: \text{LAB} \rightarrow \text{BF} \quad . \quad (\text{F.18a})$$

Let us suppose now that the LAB observer wishes to find the generalized coordinates q'_i describing the orientation of a different set of axes $[\overline{\text{BF}}]$ fixed in the same body. Again he writes

$$q'_i = [a']_i^{\text{LAB}}, \quad a': \text{LAB} \rightarrow \overline{\text{BF}} \quad . \quad (\text{F.18b})$$

If the second body-fixed frame is specified by

$$b: \text{BF} \rightarrow \overline{\text{BF}}, \quad (\text{F.18c})$$

the parameters b_i^{BF} will be independent of the orientation of BF relative to LAB and hence independent of the values of the q_i . This is not true of the b_i^{LAB} . From Equations (F.18) and (F.17c) we have $a' = b \cdot a$ and

$$q'_i = [a']_i^{\text{LAB}} = [b \cdot a]_i^{\text{LAB}} = [a \cdot b]_i^{\text{BF}} \quad . \quad (\text{F.19a})$$

Since LAB and BF agree upon the parameters of a ,

$$q_i = a_i^{\text{LAB}} = a_i^{\text{BF}}, \quad ,$$

we may rewrite Equation (F.19a) in the more explicit form

$$q'_i = m_i(q_1, q_2, q_3; b_1^{\text{BF}}, b_2^{\text{BF}}, b_3^{\text{BF}}) \quad (\text{F.19b})$$

and conclude that right multiplication of the generalized coordinates by a constant rotation corresponds to a change of BF axes. This result was used in Appendix A [see Equation (A.18)] under the Euler angle parameterization scheme.

B. Angular Momentum Operators

When a complete set of expansion states is introduced, the effect of an active rotation upon a system in the quantum state $|\psi\rangle$ [or $\psi(q)$] may be represented by a linear transformation connecting the expansion coefficients of the original and rotated states. This procedure is summarized in Figure F.2. The rotation b is replaced by a matrix $[D(b)]$ which acts upon the vector of expansion coefficients, and matrix multiplication plays the role of the group product. The set of matrices

$$M \equiv \{[D(b)]; b \text{ an element of } R(3)\} \quad (F.20a)$$

with the property

$$a \cdot b = c \quad \text{implying} \quad [D(a)][D(b)] = [D(c)] \quad (F.20b)$$

is said to be a representation of $R(3)$. The possible effects of $R(3)$ operations upon quantum states may be ascertained by cataloging all possible sets M which satisfy Equation (F.20b). This latter task reduces to a search for irreducible representations [IR] of $R(3)$, i.e., sets M for which there exists no matrix $[U]$ with the property¹

$$[U][D(b)][U]^{-1} \quad \text{has the partitioned form} \quad \left[\begin{array}{c|c} [D'(b)] & [0] \\ \hline [G(b)] & [D''(b)] \end{array} \right] \quad \text{for all } [D(b)] \text{ in } M. \quad (F.21)$$

Here $[0]$ denotes a matrix with only zeros as its elements. If M is an

¹ If such a $[U]$ does exist, then both $\{[D'(b)]\}$ and $\{[D''(b)]\}$ are easily shown to be representations of $R(3)$.

Figure F.2. Mapping the group elements onto a set of matrices, $b \rightarrow [D(b)]$, by introducing a complete set of expansion states

IR consisting of square matrices of side d , then the set of functions $\{\phi_m(q); m = 1, 2, \dots, d\}$ is said to be a basis for M [in the q -coordinate representation] if

$$R(b)\phi_n(q) = \phi_n(h(b^{-1}, q)) = \sum_{m=1}^d D_{mn}(b)\phi_m(q), [n = 1, 2, \dots, d]. \quad (F.22a)$$

From Figure F.2, the appropriate matrix elements in Equation (F.22a) are

$$D_{mn}(b) = \langle \phi_m(q) | R(b) | \phi_n(q) \rangle. \quad (F.22b)$$

The $\phi_m(q)$ may be thought of as spanning the space $\mathfrak{S}$ consisting of all possible linear combinations $\sum_{m=1}^d \alpha_m \phi_m(q)$. The restriction that M be an IR assures that there is no set $\{\bar{\phi}_n(q) \text{ in } \mathfrak{S}; n = 1, 2, \dots, \bar{d} < d\}$ such that

$$R(b)\bar{\phi}_n(q) = \sum_{m=1}^{\bar{d}} \bar{D}_{mn}(b)\bar{\phi}_m(q)$$

with $\{\bar{D}(b)\}$ a representation of $R(\mathfrak{S})$.

In Figure F.2, the effect of $R(b)$ upon a general function $\psi(q)$ is easily gauged if

- 1) the complete set of expansion functions is chosen to consist of orthogonal sets of irreducible basis functions, and
- 2) the matrix elements $D_{mn}(b)$ of Equation (F.22b) are determined for each such basis set.

In the present section, the angular momentum operators J_i are introduced and their commutation relations are derived. In the following section, simultaneous eigenfunctions of J^2 and J_z are adopted as the appropriate

expansion functions for step 1) above, and the explicit construction of the $D_{mn}(b)$ in step 2) is outlined.

It is clear that the general rotation b may be built up by the successive application of infinitesimal rotations about the LAB x_1 , x_2 and x_3 axes. We introduce the angular momentum operators as the generators of these infinitesimal rotations. In particular, let δb denote a rotation about the unit axis $\hat{n}$ through the infinitesimal angle $\delta\theta$. We define the [dimensionless] vector angular momentum $\underline{J}$ by insisting that $R(\delta b)$ have the form

$$R(\delta b) = e^{-i\delta\theta \hat{n} \otimes \underline{J}}, \quad \delta b = \text{rotation through } \delta\theta \text{ about the } \hat{n} \text{ axis} \quad i \equiv \sqrt{-1}, \quad (\text{F.23a})$$

and we denote the components of $\underline{J}$ along the LAB x_i axis by

$$J_i \equiv \underline{J} \otimes \hat{x}_i.$$

A rotation b about $\hat{n}$ through the finite angle θ may be expressed as a sequential product of the infinitesimal rotations appearing in Equation (F.23a)

$$R(b) = \dots e^{-i\delta\theta_2 \hat{n} \otimes \underline{J}} e^{-i\delta\theta_1 \hat{n} \otimes \underline{J}},$$

$$\theta = \delta\theta_1 + \delta\theta_2 + \dots$$

Using (39)

$$e^A e^B = e^{A+B} \quad \text{if} \quad [A, B] = 0,$$

we consequently obtain the finite form of Equation (F.23a)

$$R(b) = e^{-i\theta \hat{n} \cdot \underline{J}} \quad , \quad b = \begin{array}{l} \text{rotation through } \theta \\ \text{about the } \hat{n} \text{ axis} \end{array} \quad . \quad (F.23b)$$

The physical angular momentum operator referred to elsewhere in this thesis is the $\underline{J}$ of Equations (F.23) multiplied by $\hbar$. In this appendix, however, only the dimensionless form is used so as to avoid carrying factors of $\hbar$. $\underline{J}$ is assumed to be an Hermitian operator with respect to the q -space inner product of normalizable functions, i.e.,

$$\langle J_i \phi_1(\underline{q}) | \phi_2(\underline{q}) \rangle = \langle \phi_1(\underline{q}) | J_i \phi_2(\underline{q}) \rangle \quad i = 1, 2, 3 \quad . \quad (F.24)$$

This assures that $R(b)$ preserves the norm of the function on which it operates.

In the q -coordinate representation [$\underline{q} = (q_1, q_2, \dots, q_m)$], the form of J_i is fixed by its definition and by Equation (F.6c) which we may write as

$$R(b)\psi(\underline{q}) = \psi'(\underline{q}) = \psi(\underline{h}(\underline{c}, \underline{q})) \quad , \quad \underline{c} = \underline{b}^{-1} \quad . \quad (F.25)$$

To facilitate the discussion we use the MP parameterization and consider an infinitesimal rotation through $\delta\theta$ about the $\hat{x}_\ell$ axis. Then

$$\underline{b} = \hat{x}_\ell \tan \frac{\delta\theta}{2} = \hat{x}_\ell \frac{\delta\theta}{2} \quad \text{or} \quad b_j = \frac{\delta\theta}{2} \delta_{\ell j}$$

and

$$\underline{c} = -\underline{b} \quad \text{or} \quad c_j = -\frac{\delta\theta}{2} \delta_{\ell j} \quad .$$

We now expand the right-hand side of Equation (F.25) about $\underline{c} = 0$, keeping only terms of order $\delta\theta$ and larger.

$$\begin{aligned}
\psi'(\underline{q}) &= \psi(h(\underline{0}, \underline{q})) + \sum_{j=1}^3 \left[\frac{\partial \psi(h(\underline{c}, \underline{q}))}{\partial c_j} \right]_{\underline{c}=\underline{0}} c_j \\
&= \psi(\underline{q}) + \sum_{j=1}^3 \sum_{\alpha=1}^m \left[\frac{\partial \psi(h(\underline{c}, \underline{q}))}{\partial h_\alpha} \frac{\partial h_\alpha}{\partial c_j} \right]_{\underline{c}=\underline{0}} c_j \\
&= \psi(\underline{q}) + \sum_{j=1}^3 \sum_{\alpha=1}^m \frac{\partial \psi(\underline{q})}{\partial q_\alpha} \left[\frac{\partial h_\alpha(\underline{c}, \underline{q})}{\partial c_j} \right]_{\underline{c}=\underline{0}} c_j \\
&= \psi(\underline{q}) - \sum_{j=1}^3 c_j [X_j] \psi(\underline{q}) \\
&= \psi(\underline{q}) + \frac{\delta \theta}{2} [X_\ell] \psi(\underline{q}) \quad , \tag{F.26}
\end{aligned}$$

where the definition

$$X_j \equiv - \sum_{\alpha=1}^m \left[\frac{\partial h_\alpha(\underline{c}, \underline{q})}{\partial c_j} \right]_{\underline{c}=\underline{0}} \frac{\partial}{\partial q_\alpha} \tag{F.27}$$

has been introduced. We may similarly expand

$$\begin{aligned}
\psi'(\underline{q}) &= R(b) \psi(\underline{q}) = e^{-i \delta \theta J_\ell} \psi(\underline{q}) \\
&= \psi(\underline{q}) - i \delta \theta J_\ell \psi(\underline{q}) \tag{F.28}
\end{aligned}$$

and compare with Equation (F.26) to deduce that

$$J_\ell = \frac{i}{2} X_\ell \quad . \tag{F.29}$$

The explicit form of X_ℓ , and hence J_ℓ , depends on the manner in which

the generalized coordinates are chosen. However, the constants $C_{\ell jk}$ appearing in the commutation relation

$$[X_\ell, X_j] = X_\ell X_j - X_j X_\ell = \sum_k C_{\ell jk} X_k \quad (F.30)$$

may be shown to be determined solely by the form of the group product in the vicinity of the identity. [The function $h(c, q)$ must be smooth and satisfy Equations (F.8a)-(F.8c)]. In particular if we expand Equation (F.1a) in a Taylor's series about $a = b = e = (0, 0, \dots, 0)$

$$m_k(a; b) = a_k + b_k + \sum_{\ell j} p_{\ell jk} a_\ell b_j + \dots,$$

then the structure constant $C_{\ell jk}$ in Equation (F.30) is given quite generally by

$$C_{\ell jk} = p_{\ell jk} - p_{j\ell k}.$$

For the MP parameterization, expanding Equation (F.15) results in

$$p_{\ell jk} = \epsilon_{\ell jk}, \quad C_{\ell jk} = 2\epsilon_{\ell jk} \quad (F.31)$$

Consequently from Equations (F.29)-(F.31) we have

$$\boxed{[J_\ell, J_j] = i \sum_k \epsilon_{\ell jk} J_k} \quad (F.32)$$

As an example of these general results, consider a point mass located by LAB cartesian coordinates $q = x$. In this case

$$h(b, q) = f(b, x) \text{ of Equation (F.13),}$$

and we may easily evaluate Equation (F.27):

$$X_\ell = -2 \sum_{jk} \epsilon_{jkl} x_j \frac{\partial}{\partial x_k}$$

Then Equation (F.29) leads to the well-known form

$$J_\ell = \sum_{jk} \epsilon_{jkl} x_j \left[-i \frac{\partial}{\partial x_k} \right] \text{ or } \left\{ \begin{array}{l} \tilde{J} = \tilde{x} \otimes \frac{\tilde{p}}{\hbar} \\ \tilde{p} = \text{linear momentum} \end{array} \right\}, \quad (\text{F.33})$$

and the commutation relations of Equation (F.32) are seen to be satisfied.

Rewriting Equation (F.33) in terms of spherical polar coordinates

(R, θ, ϕ) [See Figure F.3] results in

$$J_1 = J_x = i \left[\cot \theta \cos \phi \frac{\partial}{\partial \phi} + \sin \phi \frac{\partial}{\partial \theta} \right] \quad (\text{F.34a})$$

$$J_2 = J_y = i \left[\cot \theta \sin \phi \frac{\partial}{\partial \phi} - \cos \phi \frac{\partial}{\partial \theta} \right] \quad (\text{F.34b})$$

$$J_3 = J_z = -i \frac{\partial}{\partial \phi} \quad (\text{F.34c})$$

C. Rotation Matrices

Equation (F.23b) allows us to assemble the rotation matrix element $D_{nn'}(b) = \langle \phi_n | R(b) | \phi_{n'} \rangle$ from a knowledge of the $\langle \phi_n | J_i | \phi_{n'} \rangle$. The latter may be found from the commutation relations of the J_i if the orthonormal expansion states $\phi_n(q)$ appearing in Figure F.2 are properly chosen.

For this purpose it is convenient to introduce the pseudo-spherical components of the angular momentum operator $\{J_\mu; \mu = 0, \pm 1\}$ defined by¹

¹To avoid confusion between the first member of $(J_1, J_2, J_3) = (J_x, J_y, J_z)$ and the pseudo-spherical component J_μ with $\mu = 1$, the latter will be written as J_{+1} . Greek $[\mu, \nu, \dots]$ and Roman $[i, j, \dots]$ subscripts will be used to refer to the pseudo-spherical and cartesian components of J respectively.

$$J_0 \equiv J_z \quad (F.35)$$

$$J_{\pm 1} \equiv \mp \frac{1}{\sqrt{2}} (J_x \pm iJ_y)$$

From Equation (F.32), the J_μ are found to obey

$$[J_{+1}, J_{-1}] = -J_0 \quad (F.36)$$

$$[J_0, J_{\pm 1}] = \pm J_{\pm 1}$$

The [Casimer] operator

$$J^2 \equiv (J_x)^2 + (J_y)^2 + (J_z)^2 = (J_0)^2 - J_1 J_{-1} - J_{-1} J_1 \quad (F.37)$$

has the property of commuting with each of the J_i or J_μ :

$$[J^2, J_\mu] = [J^2, J_i] = 0 \quad \begin{matrix} i = 1, 2, 3 \\ \mu = 0, \pm 1 \end{matrix} \quad (F.38)$$

In a given representation (q), simultaneous eigenfunctions of J^2 and J_0 can consequently be found. We choose the $\phi_n(q)$ to be such eigenfunctions and write $\phi_n(q) = \phi_{jm}(q)$. Here m is the eigenvalue of J_0 , and j labels the eigenvalue $w(j)$ of J^2 :

$$J^2 \phi_{jm} = w(j) \phi_{jm} \quad (F.39a)$$

$$J_0 \phi_{jm} = m \phi_{jm} \quad (F.39b)$$

As J^2 and J_0 are Hermitian operators, two ϕ_{jm} with different eigenvalues of either J^2 or J_0 are necessarily orthogonal. Assuming the ϕ_{jm} to be normalized we have then

$$\langle \phi_{jm} | \phi_{j'm'} \rangle = \delta_{jj'} \delta_{mm'} \quad (F.39c)$$

With no other assumptions about the character of $\phi_{jm}(q)$, we may use Equations (F.36)-(F.39) to show:

- 1) For fixed j , m is bounded: $[w(j) - m^2 \geq 0]$. Consequently for fixed j , there are largest and smallest values of m [$m_>$ and $m_<$ respectively].
- 2) $J_{\pm 1} \phi_{jm} \propto \phi_{j, m \pm 1}$.
 m may be raised or lowered in steps of unity.
- 3) $m_> = -m_<$.
 For fixed $j \equiv m_>$, m can range from $-j$ to $+j$.
- 4) j may be either integral or half-integral, and the associated eigenvalue $w(j)$ is $j(j+1)$.

In summary

$$J^2 \phi_{jm} = j(j+1) \phi_{jm} \quad j = 0, 1/2, 1, 3/2, \dots \quad (\text{F.40a})$$

$$J_0 \phi_{jm} = m \phi_{jm} \quad m = j, j-1, \dots, (-j) \quad (\text{F.40b})$$

for fixed j .

Furthermore, Equations (F.36)-(F.40) may be used to deduce matrix elements of the J_μ between the basis states:

$$\langle \phi_{jm} | J_0 | \phi_{j, m'} \rangle = m \delta_{jj'} \delta_{mm'} \quad (\text{F.41a})$$

$$\langle \phi_{jm} | J_{\pm 1} | \phi_{j, m'} \rangle = \mp \frac{1}{\sqrt{2}} [(j \mp m')(j \pm m' + 1)]^{\frac{1}{2}} \delta_{jj'} \delta_{m, m' \pm 1} \quad (\text{F.41b})$$

[The commutation relations determine only the absolute value of the matrix elements in Equation (F.41b). A phase choice has been made.]

By virtue of Equations (F.23) and (F.41), eigenstates of J^2 with different eigenvalues are not connected by rotations:

$$\langle \phi_{jm} | R(b) | \phi_{j'm'} \rangle = 0 \quad \text{if } j \neq j'.$$

Consequently, when the actively rotated eigenfunction $R(b)\phi_{jm}$ is expanded in the complete set of $\phi_{j'm'}$, we find

$$R(b)\phi_{jm} = \sum_{m'} D_{m',m}^j(b) \phi_{jm'} \quad (\text{F.42a})$$

$$D_{m',m}^j(b) \equiv \langle \phi_{jm'} | R(b) | \phi_{jm} \rangle \quad (\text{F.42b})$$

The matrices defined by Equation (F.42a) comprise a $(2j + 1)$ -dimensional irreducible representation of the rotation group. The group product has been replaced by matrix multiplication,

$$a \cdot b = c \quad \text{implies} \quad D_{mm'}^j(c) = \sum_{m''} D_{mm''}^j(a) D_{m''m'}^j(b), \quad (\text{F.43a})$$

and the $(2j + 1) \times (2j + 1)$ unit matrix represents the group identity [i.e., the null rotation]

$$D_{m,m'}^j(e) = \delta_{m,m'} \quad (\text{F.43b})$$

Furthermore, from Equation (F.23b) and the hermicity of J , we may deduce that the rotation matrices defined by Equation (F.42b) are unitary:

$$D_{mm'}^j(b^{-1}) = D_{m',m}^{j*}(b) \quad (\text{F.43c})$$

The orthonormality properties

$$\sum_{m''} D_{mm''}^{j*}(b) D_{m',m''}^j(b) = \delta_{m,m'} \quad (\text{F.44a})$$

$$\sum_{m'} D_{m'm}^{j*}(b) D_{m'm'}^j(b) = \delta_{m,m'} \quad (\text{F.44b})$$

then follow from Equations (F.43).

Having specified the form of the general rotation operator [Equation (F.23b)] and the matrix elements of the rotation generators [Equations (F.41)], $D_{m'm}^j(b)$ may be unambiguously constructed if a parameterization for b is chosen. The Euler angles are particularly appropriate for this task. Because of the manner of their definition we have

$$R(b) = R(\theta_i) = e^{-i\theta_1 J_z} e^{-i\theta_2 J_y} e^{-i\theta_3 J_z},$$

and we may immediately write

$$D_{m'm}^j(\theta_i) = e^{-im'\theta_1} d_{m'm}^j(\theta_2) e^{-im\theta_3} \quad (\text{F.45a})$$

$$\begin{aligned} d_{m'm}^j(\theta_2) &\equiv \langle \phi_{jm'} | e^{-i\theta_2 J_y} | \phi_{jm} \rangle \\ &= \langle \phi_{jm'} | e^{\theta_2 (J_{+1} + J_{-1}) / \sqrt{2}} | \phi_{jm} \rangle \end{aligned} \quad (\text{F.45b})$$

The latter matrix element may be evaluated as

$$\begin{aligned} d_{m'm}^j(\theta_2) &= [(j+m)!(j-m)!(j+m')!(j-m')!]^{\frac{1}{2}} \\ &\times \sum_k (-1)^k [(j-m'-k)!(j+m-k)!(k+m'-m)!k!]^{-1} \\ &\times \left[\cos \frac{\theta_2}{2} \right]^{2j+m-m'-2k} \left[-\sin \frac{\theta_2}{2} \right]^{m'-m+2k}, \end{aligned} \quad (\text{F.45c})$$

where the integer k ranges over those values for which all factorial arguments are non-negative. A number of useful relationships may be

Table F.1. The twenty-five $d_{m,m}^j(\theta)$ for $j = 2$. The superscript 2 and argument (θ) have been omitted from the right-hand portion of the table

$d_{2,2}^2(\theta) = \frac{1}{4}[1 + \cos\theta]^2$	$= d_{-2,-2}$
$d_{2,1}^2(\theta) = -\frac{1}{2} \sin\theta[\cos\theta + 1]$	$= d_{-1,-2} = -d_{1,2} = -d_{-2,-1}$
$d_{2,0}^2(\theta) = \frac{\sqrt{6}}{4} \sin^2\theta$	$= d_{0,-2} = d_{0,2} = d_{-2,0}$
$d_{2,-1}^2(\theta) = \frac{1}{2} \sin\theta[\cos\theta - 1]$	$= d_{1,-2} = -d_{-1,2} = -d_{-2,1}$
$d_{2,-2}^2(\theta) = \frac{1}{4}[\cos\theta - 1]^2$	$= d_{2,2}$
$d_{1,1}^2(\theta) = [1 + \cos\theta][\cos\theta - \frac{1}{2}]$	$= d_{-1,-1}$
$d_{1,0}^2(\theta) = -\frac{\sqrt{6}}{4} \sin\theta \cos\theta$	$= d_{0,-1} = -d_{0,1} = -d_{-1,0}$
$d_{1,-1}^2(\theta) = [1 - \cos\theta][\cos\theta + \frac{1}{2}]$	$= d_{-1,1}$
$d_{0,0}^2(\theta) = \frac{1}{2}[3 \cos^2\theta - 1]$	

deduced from Equation (F.45c) and the unitarity property

$$d_{mm'}^j(-\theta_2) = d_{m'm}^j(\theta_2) \quad . \quad (F.46a)$$

In particular,

$$d_{m'm}^j(\theta_2) = (-1)^{m'-m} d_{mm'}^j(\theta_2) = d_{-m,-m'}^j(\theta_2) = (-1)^{m'-m} d_{-m',-m}^j(\theta_2) \quad . \quad (F.46b)$$

Recalling that the rotation with Euler angles $(-\theta_3, -\theta_2, -\theta_1)$ is inverse to the rotation specified by $(\theta_1, \theta_2, \theta_3)$, Equations (F.43c), (F.45a), and (F.46) may be used to deduce

$$D_{m'm}^{j*}(\theta_i) = (-1)^{m'-m} D_{-m',-m}^j(\theta_i) \quad . \quad (F.46c)$$

The $D_{m'm}^j(\theta_i)$ of Equations (F.45) are orthogonal¹ on the surface of the unit sphere:

$$\int_0^{2\pi} \int_0^\pi \int_0^{2\pi} D_{\mu_1 m_1}^{j_1*}(\theta_i) D_{\mu_2 m_2}^{j_2}(\theta_i) \sin\theta_2 d\theta_1 d\theta_2 d\theta_3 = \frac{8\pi^2}{2j_1+1} \delta_{\mu_1 \mu_2} \delta_{m_1 m_2} \delta_{j_1 j_2} \quad . \quad (F.47)$$

$\theta_1 \quad \theta_2 \quad \theta_3$

The $d_{m'm}^j(\theta_2)$ are used extensively throughout this thesis, and may be found in Table F.1. Their explicit forms are required in Section C of Appendix A.

From Figure F.1a, it is clear that the two rotations

b: about the $\hat{n}$ axis through the angle θ ,

¹ A proof may be found in Section 16 of Reference (31).

and

$b_{2\pi}$: about the $\hat{n}$ axis through the angle $(\theta + 2\pi)$,

are equivalent in their effects. Hence operators representing physical rotations must generally satisfy

$$R(b)\phi(q) = R(b_{2\pi})\phi(q) \quad . \quad (F.48a)$$

Equation (F.48a) imposes the condition

$$D_{m'm}^j(b) = D_{m'm}^j(b_{2\pi}) \quad (F.48b)$$

on IR matrix elements of $R(3)$. For example if $\theta = 0$ and $\hat{n} = \hat{z}$ in Equation (F.48b), we have

$$D_{m'm}^j(0, 0, 0) = D_{m'm}^j(0, 0, 2\pi) \quad (F.49)$$

in the Euler angle parameterization. $D_{m'm}^j(\theta_i)$ given by Equation (F.45a) clearly fails to satisfy Equation (F.49) if j [and hence m] is half integral. The half-integral representations which we have constructed are then not to be associated with the group $R(3)$. Recall that the entire construction procedure for the $D_{m'm}^j$ proceeded from a knowledge of $\underline{m}(a; b)$ in the vicinity of $a = b = e$. There is another three-parameter continuous group, namely $SU(2)$, which is isomorphic with $R(3)$ in the vicinity of the group identity. The $j = 1/2, 3/2, 5/2, \dots$ representations of Equation (F.45a) are in fact IR of $SU(2)$ ¹ [under a

¹See, for example, Appendix II of Reference (31).

parameterization similar to the Euler angle parameterization of $R(3)$, but with extended ranges for the θ_i . Representations of $SU(2)$ play no role in the mathematical developments required in this thesis. However, they are often encountered in the treatment of other physical phenomena [e.g., electron spin]. Henceforth in this appendix, we shall continue to use the letter j [as in $D_{m,m}^j$, ϕ_{jm}] in all relationships which hold true for both the integral and half-integral representations of Equation (F.45a). L will be used exclusively to denote integral representations.

D. Spherical Harmonics

In the q -coordinate representation, orthonormal basis functions $\phi_{jm}(q)$ may be obtained by solving the differential equations implied by Equations (F.40). If the phases of the solutions are chosen such that Equations (F.41) are satisfied, we are then guaranteed that Equation (F.42a) will hold with $D_{m,m}^j(\theta_i)$ given by Equations (F.45). This procedure requires that the q -coordinate representatives of the angular momentum operators be known. When the generalized coordinates (q) are the spherical polar coordinates of a point mass, the appropriate J_i are given by Equations (F.34). Since the J_i are independent of the radial coordinate, we may write

$$\phi_{LM}(q) = R(r)Y_{LM}(\theta, \phi) \quad L = 0, 1, 2, \dots, \quad (F.50)$$

where the radial function is arbitrary. The $Y_{LM}(\theta, \phi)$ satisfying Equations (F.40) and (F.41) may then be deduced¹ to be

¹See Appendix III of Reference (31).

$$Y_{LM}(\theta, \phi) = \left[\frac{(2L+1)(L-M)!}{4\pi(L+M)!} \right]^{\frac{1}{2}} \frac{1}{2^L L!} e^{iM\phi} (-\sin\theta)^M \left[\frac{d}{d(\cos\theta)} \right]^{L+M} (\cos^2\theta - 1)^L. \quad (\text{F.51})$$

The above expression is unique to within a phase factor depending upon

L. The Y_{LM} obey the orthonormality condition

$$\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} Y_{LM}^*(\theta, \phi) Y_{L'M'}(\theta, \phi) \sin\theta d\theta d\phi = \delta_{LL'} \delta_{MM'}, \quad (\text{F.52})$$

and satisfy the identity

$$Y_{LM}^*(\theta, \phi) = (-1)^M Y_{L,-M}(\theta, \phi). \quad (\text{F.53})$$

The Y_{LM} may also be related to the Euler angle form of the rotation matrices:

$$Y_{LM}(\theta, \phi) = \left[\frac{2L+1}{4\pi} \right]^{\frac{1}{2}} D_{M0}^{L*}(\phi, \theta, 0). \quad (\text{F.54})$$

The explicit forms for the Y_{2M} , obtained by evaluating Equation (F.51), may be found in Figure F.3.

Consider two reference frames, LAB and BF, which are related by the active rotation b ,

$$b: \text{LAB} \rightarrow \text{BF}.$$

Recall that both frames will assign identical parameters [such as Euler angles] to b . Let $Y_{LM}(\theta, \phi)$ be a spherical harmonic with (θ, ϕ) measured with respect to LAB axes. We now endeavor to express this same function in terms of the coordinates (θ', ϕ') measured with

cartesian (x, y, z) and spherical (R, θ, ϕ) coordinates of a point P:

$$x = R \sin \theta \cos \phi$$

$$y = R \sin \theta \sin \phi$$

$$z = R \cos \theta$$

$$Y_{0,0}(\theta, \phi) = \left[\frac{1}{4\pi} \right]^{\frac{1}{2}}$$

$$Y_{2,2}(\theta, \phi) = \frac{1}{4} \left[\frac{15}{2\pi} \right]^{\frac{1}{2}} \sin^2 \theta e^{2i\phi}$$

$$Y_{1,1}(\theta, \phi) = -\frac{1}{2} \left[\frac{3}{2\pi} \right]^{\frac{1}{2}} \sin \theta e^{i\phi}$$

$$Y_{2,1}(\theta, \phi) = -\frac{1}{2} \left[\frac{15}{2\pi} \right]^{\frac{1}{2}} \sin \theta \cos \theta e^{i\phi}$$

$$Y_{2,0}(\theta, \phi) = \frac{1}{4} \left[\frac{5}{\pi} \right]^{\frac{1}{2}} [3 \cos^2 \theta - 1]$$

$$Y_{1,0}(\theta, \phi) = \frac{1}{2} \left[\frac{3}{\pi} \right]^{\frac{1}{2}} \cos \theta$$

$$Y_{2,-1}(\theta, \phi) = \frac{1}{2} \left[\frac{15}{2\pi} \right]^{\frac{1}{2}} \sin \theta \cos \theta e^{-i\phi}$$

$$Y_{1,-1}(\theta, \phi) = \frac{1}{2} \left[\frac{3}{2\pi} \right]^{\frac{1}{2}} \sin \theta e^{-i\phi}$$

$$Y_{2,-2}(\theta, \phi) = \frac{1}{4} \left[\frac{15}{2\pi} \right]^{\frac{1}{2}} \sin^2 \theta e^{-2i\phi}$$

Figure F.3. Some spherical harmonics

respect to BF axes. That is, we seek an expression for

$$Y_{LM}^{BF}(\theta', \phi') \equiv Y_{LM}(\theta, \phi) \quad \text{rewritten in terms of the BF coordinates } (\theta', \phi') \quad . \quad (F.55a)$$

We may define a new scalar function by actively rotating Y_{LM} [and hence Y_{LM}^{BF}] through the rotation b . By construction, the appearance of the new function to BF is identical with the appearance of the old function to LAB. Consequently a BF observer may write

$$R(b)Y_{LM}^{BF}(\theta', \phi') = Y_{LM}(\theta', \phi') \quad ,$$

or equivalently,

$$Y_{LM}^{BF}(\theta', \phi') = R(b^{-1})Y_{LM}(\theta', \phi') \quad .$$

Using Equation (F.42a) [which holds for an arbitrary cartesian reference frame], we obtain the desired result

$$Y_{LM}^{BF}(\theta', \phi') = \sum_{M'} D_{M'M}^L(b^{-1})Y_{LM'}(\theta', \phi') \quad . \quad (F.55b)$$

Suppose that observers in the LAB and BF frames view a common quadrupole surface. In the manner of Equations (2.1) and (2.2), the two observers may express the surface as

$$R = R_O [1 + \sum_{\mu} \alpha_{\mu} Y_{2\mu}^*(\theta, \phi)]$$

and

$$R = R_O [1 + \sum_{\mu} a_{\mu} Y_{2\mu}^*(\theta', \phi')]$$

respectively. Since the observers agree upon the radius R to a given point on the surface, we may write

$$\begin{aligned}\sum_{\mu} a_{\mu} Y_{2\mu}^*(\theta', \phi') &= \sum_{\mu} \alpha_{\mu} Y_{2\mu}^*(\theta, \phi) \\ &= \sum_{\mu} \alpha_{\mu} \sum_{\mu'} D_{\mu'\mu}^{2*}(b^{-1}) Y_{2\mu'}^*(\theta', \phi')\end{aligned}$$

Equations (F.55) have been used in deducing the last equality. Multiplying by $Y_{2\nu}(\theta', \phi') \sin\theta' d\theta' d\phi'$, integrating over the full range of θ' and ϕ' , and invoking the orthonormality of the $Y_{2\mu}$ leads to

$$a_{\nu} = \sum_{\mu} \alpha_{\mu} D_{\nu\mu}^{2*}(b^{-1}) = \sum_{\mu} \alpha_{\mu} D_{\mu\nu}^2(b)$$

This result appears in the main text as Equation (2.3).

E. Clebsch-Gordon Coefficients

Let us suppose that S_1 and S_2 are independent physical systems [or independent aspects of a single system] described by LAB generalized coordinate sets q^1 and q^2 respectively. Operators effecting the active rotation b [about $\hat{n}$ through the angle θ] will be written as

$$R_1(b) = e^{-i\theta\hat{n}\cdot\mathbf{J}_1}$$

and

$$R_2(b) = e^{-i\theta\hat{n}\cdot\mathbf{J}_2}$$

(F.56)

respectively for the two systems. The pseudo-spherical components of $\mathbf{J}_k$ [$k = 1, 2$] will be denoted as $J_{k,\mu}$ ($\mu = 0, \pm 1$). They satisfy

Equations (F.36) for each of $k = 1, 2$:

$$[J_{k,+1}, J_{k,-1}] = -J_{k,0}, \quad [J_{k,0}, J_{k,\pm 1}] = \pm J_{k,\pm 1} \quad (F.57)$$

Since q^1 and q^2 are independent, we also have

$$[J_{1,\mu}, J_{2,\nu}] = 0, \quad \text{all } \mu, \nu \quad (F.58)$$

Let $\{\psi_{j_1 m_1}(q^1); m_1 = j_1, j_1-1, \dots, -j_1\}$ and $\{\chi_{j_2 m_2}(q^2); m_2 = j_2, j_2-1, \dots, -j_2\}$ be sets of normalized functions of the generalized coordinates which are basis sets for the $(2j_1+1)$ and $(2j_2+1)$ -dimensional IR of $R(3)$ respectively. That is, each set is assumed to consist of eigenfunctions of the appropriate $(J_k)^2$ and $J_{k,0}$, and to satisfy Equations (F.40) and (F.41). In the preceding section, the $D_{mm'}^j(\theta_i)$ were constructed such that the finite [Equations (F.42b) and (F.45)] and infinitesimal [Equations (F.41)] forms for the rotation matrix elements were equivalent. Consequently we have

$$\begin{aligned} R_1(b) \psi_{j_1 m_1}(q^1) &= \sum_{m'_1} D_{m'_1 m_1}^{j_1}(\theta_i) \psi_{j_1 m'_1}(q^1) \\ R_2(b) \chi_{j_2 m_2}(q^2) &= \sum_{m'_2} D_{m'_2 m_2}^{j_2}(\theta_i) \chi_{j_2 m'_2}(q^2) \end{aligned} \quad (F.59)$$

The problem arises of finding linear combinations of the product functions $\psi_{j_1 m_1} \chi_{j_2 m_2}$ which belong to a specific IR of $R(3)$. In particular we seek normalized functions

$$\phi_{jm}(q^1, q^2) = \sum_{m_1 m_2} C(j_1 j_2 j; m_1 m_2 m) \psi_{j_1 m_1} \chi_{j_2 m_2} \quad (F.60)$$

which transform according to

$$R(b)\phi_{jm} = \sum_{m'} D_{m',m}^j(\theta_i)\phi_{jm'} \quad . \quad (F.61)$$

In Equation (F.61), the appropriate operator for effecting active rotations of the product functions is simply

$$R(b) = R_1(b)R_2(b) = e^{-i\theta\hat{n}\cdot\mathbf{J}_1} e^{-i\theta\hat{n}\cdot\mathbf{J}_2} = e^{-i\theta\hat{n}\cdot(\mathbf{J}_1+\mathbf{J}_2)} \quad .$$

The angular momentum operator for the product space is thus identified as

$$\mathbf{J} \equiv \mathbf{J}_1 + \mathbf{J}_2 \quad .$$

By virtue of Equations (F.57) and (F.58), the components

$$J_\mu = J_{1,\mu} + J_{2,\mu}$$

satisfy the expected commutation relations, Equations (F.36). The coupled product we seek, ϕ_{jm} [or more properly $\phi_{j_1 j_2 jm}$], is a simultaneous eigenfunction of four mutually commuting operators:

$$\begin{aligned} (J_1)^2 \phi_{jm} &= j_1(j_1 + 1)\phi_{jm} \quad , \quad (J_2)^2 \phi_{jm} = j_2(j_2 + 1)\phi_{jm} \quad , \\ J^2 \phi_{jm} &= j(j + 1)\phi_{jm} \quad , \quad J_o \phi_{jm} = m\phi_{jm} \quad . \end{aligned} \quad (F.62)$$

Furthermore we assume that the phases of the ϕ_{jm} are chosen such that Equations (F.41) [and consequently Equation (F.61)] hold. The uncoupled product $\psi_{j_1 m_1} \chi_{j_2 m_2}$, on the other hand, is a simultaneous eigenfunction of $(J_1)^2$, $J_{1,o}$, $(J_2)^2$, and $J_{2,o}$.

The Clebsch-Gordan coefficient [CGC] $C(j_1 j_2 i; m_1 m_2 m)$ appears in

Equation (F.60) as an element of a unitary transformation connecting the coupled and uncoupled functions. From the orthogonality properties of the S_1 , S_2 , and product¹ functions

$$\begin{aligned}\langle \psi_{j_1 m_1} | \psi_{j_1 m'_1} \rangle &= \delta_{m_1, m'_1} \\ \langle \chi_{j_2 m_2} | \chi_{j_2 m'_2} \rangle &= \delta_{m_2, m'_2} \\ \langle \phi_{j m} | \phi_{j' m'} \rangle &= \delta_{j, j'} \delta_{m, m'}\end{aligned}\quad (F.63)$$

we may use Equation (F.60) to deduce

$$\sum_{m_1 m_2} C^*(j_1 j_2 j; m_1 m_2 m) C(j_1 j_2 j'; m_1 m_2 m') = \delta_{j, j'} \delta_{m, m'} \quad (F.64a)$$

A second orthogonality relationship,

$$\sum_{j m} C^*(j_1 j_2 j; m_1 m_2 m) C(j_1 j_2 j; m'_1 m'_2 m) = \delta_{m_1, m'_1} \delta_{m_2, m'_2} \quad (F.64b)$$

may be deduced from the inverse expansion

$$\psi_{j_1 m_1} \chi_{j_2 m_2} = \sum_{j m} C^*(j_1 j_2 j; m_1 m_2 m) \phi_{j m} \quad (F.65)$$

Other CGC relationships may be found by using Equation (F.60) together with Equations (F.40)-(F.41). For example,

¹ If $\int_{\Omega_1} d\Omega^1(\tilde{q}^1)$ and $\int_{\Omega_2} d\Omega^2(\tilde{q}^2)$ are used in the computation of inner products for S_1 and S_2 functions respectively, then $\int_{\Omega_1} \int_{\Omega_2} d\Omega^1(\tilde{q}^1) d\Omega^2(\tilde{q}^2)$ is used for the product functions.

$$m\phi_{jm} = J_0\phi_{jm} = (J_{1,0} + J_{2,0})\phi_{jm}$$

leads one to

$$\sum_{m_1 m_2} C(j_1 j_2 j; m_1 m_2 m) \psi_{j_1 m_1} \chi_{j_2 m_2} = \sum_{m_1 m_2} C(j_1 j_2 j; m_1 m_2 m) \\ \times (m_1 + m_2) \psi_{j_1 m_1} \chi_{j_2 m_2}.$$

Consequently,

$$C(j_1 j_2 j; m_1 m_2 m) = 0 \quad \text{unless } m = m_1 + m_2. \quad (\text{F.66a})$$

One may also deduce that

$$C(j_1 j_2 j; m_1 m_2 m) = 0 \quad \text{unless } j \text{ is one of } (j_1 + j_2), (j_1 + j_2) - 1, \dots \\ |j_1 - j_2|. \quad (\text{F.66b})$$

Furthermore every value of j in the above list is found to be realized exactly once [i.e., if ϕ_{jm} is a linear combination of the $\psi_{j_1 m_1} \chi_{j_2 m_2}$ having the four eigenvalues indicated by Equations (F.62), then no other linearly independent combination has the same four eigenvalues].

Equations (F.60) and (F.41) serve to determine each CGC to within a phase. A specific choice of phases¹, compatible with these equations, leads to Racah's (73) closed form which is employed in this thesis:

¹In particular the CGC's are all chosen to be real, and $C(j_1 j_2, j_1 + j_2; j_1 j_2, j_1 + j_2)$ is taken as +1. Other phase choices imposed during the development of Equation (F.67) are discussed in Appendix A of Reference (31).

$$\begin{aligned}
C(j_1 j_2 j; m_1 m_2 m) &= \delta_{m, m_1 + m_2} \left[(2j+1) \frac{(j_1 + j_2 - j)! (j + j_1 - j_2)! (j + j_2 - j_1)!}{(j_1 + j_2 + j + 1)!} \right]^{\frac{1}{2}} \\
&\times [(j_1 + m_1)! (j_1 - m_1)! (j_2 + m_2)! (j_2 - m_2)! (j + m)! (j - m)!]^{\frac{1}{2}} \\
&\times \sum_v \frac{(-1)^v}{v!} [(j_1 + j_2 - j - v)! (j_1 - m_1 - v)! (j_2 + m_2 - v)! \\
&\times (j - j_2 + m_1 + v)! (j - j_1 - m_2 + v)!]^{-1} \quad (F.67)
\end{aligned}$$

In the sum, v extends over those values for which all factorial arguments are simultaneously non-zero. An examination of Equation (F.67) leads to the symmetry relationships

$$\begin{aligned}
C(j_1 j_2 j; m_1 m_2 m) &= (-1)^{j_1 + j_2 - j} C(j_1 j_2 j; -m_1, -m_2, -m) \\
&= (-1)^{j_1 + j_2 - j} C(j_2 j_1 j; m_2 m_1 m) \quad (F.68) \\
&= (-1)^{j_1 - m_1} \left[\frac{(2j+1)}{(2j_2+1)} \right]^{\frac{1}{2}} C(j_1 j j_2; m_1, -m, -m_2)
\end{aligned}$$

Evaluation of Equation (F.67) for $j_2 = 0$ results in

$$C(j_1 \ 0 \ j; m_1 \ 0 \ m) = \delta_{j_1, j} \delta_{m_1, m} \quad (F.69)$$

Simpler expressions for $C(j_1 \ 2 \ j; m_1 \ 2 \ m)$, involving no summation, may be found in Chapter XIV of Reference (74). These [with j_1 and j integral] were used in computation of the right-hand side of Equation (D.9b).

Equations (F.59)-(F.61) provide a connection between the CGC's and

the rotation matrix elements. One may easily deduce the Clebsch-Gordon series

$$D_{\mu_1 m_1}^{j_1}(\theta_i) D_{\mu_2 m_2}^{j_2}(\theta_i) = \sum_{j m \mu} C(j_1 j_2 j; m_1 m_2 m) C(j_1 j_2 j; \mu_1 \mu_2 \mu) D_{\mu m}^j(\theta_i) \quad , (F.70a)$$

and its inverse

$$D_{\mu m}^j(\theta_i) = \sum_{\substack{m_1 m_2 \\ \mu_1 \mu_2}} C(j_1 j_2 j; \mu_1 \mu_2 \mu) C(j_1 j_2 j; m_1 m_2 m) D_{\mu_1 m_1}^{j_1}(\theta_i) D_{\mu_2 m_2}^{j_2}(\theta_i) \quad . (F.70b)$$

Equations (F.47) and (F.70a) permit the ready evaluation of the integral of three rotation matrices:

$$\int_{\theta_1=0}^{2\pi} \int_{\theta_2=0}^{\pi} \int_{\theta_3=0}^{2\pi} D_{\mu_3 m_3}^{j_3*}(\theta_i) D_{\mu_2 m_2}^{j_2}(\theta_i) D_{\mu_1 m_1}^{j_1}(\theta_i) \sin \theta_2 d\theta_1 d\theta_2 d\theta_3 =$$

$$\frac{8\pi^2}{2j_3+1} \delta_{\mu_1+\mu_2, \mu_3} \delta_{m_1+m_2, m_3} C(j_1 j_2 j_3; \mu_1 \mu_2 \mu_3) C(j_1 j_2 j_3; m_1 m_2 m_3) \quad . (F.71)$$

F. Irreducible Tensor Operators

Let ϕ and ψ be two functions of the generalized coordinates $\underline{q}$, and let ϕ' and ψ' denote their actively rotated counterparts under b :

$$\begin{aligned} \phi'(\underline{q}) &= R(b)\phi(\underline{q}) \\ \psi'(\underline{q}) &= R(b)\psi(\underline{q}) \end{aligned} .$$

If $\mathcal{O}$ is an arbitrary operator on the space of functions of $\underline{q}$, we may define its actively rotated counterpart $\mathcal{O}'$ by

$$b: \mathcal{Q} \rightarrow \mathcal{Q}', \quad \mathcal{Q}' \equiv R(b)\mathcal{Q}R(b^{-1}) \quad (F.72)$$

This definition is chosen to insure that¹

$$\begin{aligned} \langle \phi' | \mathcal{Q}' | \psi' \rangle &= \int_{\Omega(q)} \phi'^* \mathcal{Q}' \psi' d\Omega(q) \\ &= \langle \phi | \mathcal{Q} | \psi \rangle \end{aligned}$$

In Section B, sets of functions were classified under the IR of $R(3)$ by their transformation properties [Equations (F.22a), (F.42a)]. A similar classification procedure may be adopted for operators. By definition, the set of operators $\{T_{LM}; M = L, L-1, \dots, -L\}$ is an irreducible tensor operator of rank L if

$$R(\theta_i) T_{LM} R(\theta_i)^{-1} = \sum_{M'} D_{M'M}^L(\theta_i) T_{LM'} \quad (F.73)$$

When infinitesimal rotations about the three LAB axes are considered, the content of Equation (F.73) may be expressed by the commutation relations

$$\begin{aligned} [J_0, T_{LM}] &= M T_{LM}, \quad \text{and} \\ [J_{\pm 1}, T_{LM}] &= \mp 2^{-\frac{1}{2}} [(L \mp M)(L \pm M + 1)]^{\frac{1}{2}} T_{L, M \pm 1} \end{aligned} \quad (F.74a)$$

or equivalently

$$[J_{\mu}, T_{LM}] = -[L(L+1)]^{\frac{1}{2}} \sum_{M'} C(1LL; \mu MM') T_{LM'} \quad (F.74b)$$

¹The proof of this statement assumes that J is Hermitian with respect to the inner product in question, i.e., that

$$\langle J_i \phi' | (\mathcal{Q}\psi) \rangle = \langle \phi' | J_i (\mathcal{Q}\psi) \rangle \quad i = 1, 2, 3$$

From two irreducible tensors¹, $\{T_{L_1 M_1}\}$ and $\{V_{L_2 M_2}\}$, of ranks L_1 and L_2 respectively, we can construct product tensors with ranks of

$$L = (L_1 + L_2), (L_1 + L_2 - 1), \dots, |L_1 - L_2|$$

In particular the set $\{W_{LM}\}$, whose members are defined by

$$W_{LM} \equiv \sum_{M_1 M_2} C(L_1 L_2 L; M_1 M_2 M) T_{L_1 M_1} V_{L_2 M_2}, \quad (F.75)$$

may be shown to satisfy Equation (F.73) if $\{T_{L_1 M_1}\}$ and $\{V_{L_2 M_2}\}$ do. Similarly, if a set of functions $\{\phi_{j' m'}\}$ transforms according to

$$R(\theta_i) \phi_{j' m'} = \sum_{m''} D_{m'' m'}^{j'}(\theta_i) \phi_{j' m''}, \quad (F.76)$$

and if $\{T_{LM}\}$ transforms according to Equation (F.73), then $\{\psi_{jm}\}$ defined by

$$\psi_{jm} \equiv \sum_{M m'} C(L j' j; M m' m) T_{LM} \phi_{j' m'} \quad (F.77)$$

$$j = \text{one of } (L+j'), (L+j'-1), \dots, |L-j'|$$

may be shown to be a basis for the $(2j+1)$ -dimensional IR of $R(3)$:

$$R(\theta_i) \psi_{jm} = \sum_{m'} D_{m' m}^j(\theta_i) \psi_{j m'} \quad (F.78)$$

When functions and operators are classified according to IR of $R(3)$, the Wigner-Eckart theorem may be used to speed the evaluation of matrix

¹ $\{A_{jm}\}$ denotes the set $\{A_{j,j}, A_{j,j-1}, \dots, A_{j,-j}\}$ for an operator or function A .

elements. This theorem¹ states that if $\{\phi_{j'm'}\}$, $\{T_{LM}\}$ and $\{\psi_{jm}\}$ transform according to Equations (F.76), (F.73), and (F.78) respectively, then

$$\langle \phi_{j'm'} | T_{LM} | \psi_{jm} \rangle = C(jLj'; m M m') \langle \phi_{j'} || T_L || \psi_j \rangle, \quad (\text{F.79})$$

where the reduced matrix element $\langle \phi_{j'} || T_L || \psi_j \rangle$ is independent of m , M , and m' . The set of operators

$$T_{L\mu} = J_{\mu}, \quad \mu = 1, 0, -1$$

satisfy Equations (F.74) for $L = 1$, and $\{J_{\mu}\}$ is thus identified as a first rank tensor. The matrix elements of J_{μ} , given in Equations (F.41), may be written in a form which makes the Wigner-Eckart theorem manifest:

$$\langle \phi_{jm} | J_{\mu} | \phi_{j'm'} \rangle = C(j' \ 1 \ j; m' \ \mu \ m) \{ [j(j+1)]^{\frac{1}{2}} \delta_{jj'} \}. \quad (\text{F.80})$$

¹A proof may be found in Chapter V of Reference (31).

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The horse is made ready for the day of battle,
but the victory belongs to the Lord.

Pro 21:31