ALGEBRAIC APPROACH TO THE THEORY OF
COLLECTIVE MOTION: SPHERICAL TO DEFORMED
TRANSITION IN THE SINGLE- j SHELL[†]

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ABSTRACT

The program of the algebraic approach to nuclear collective motion is summarized. In essence, it should permit an accurate solution of the many-body problem within a subspace of the many particle space if the conditions defining collective motion are present. The formulation, containing both dynamical and kinematical aspects, leads to coupled non-linear algebraic equations for the matrix elements between collective states of fermion pair operators. An explicit set of ^{equations} /... is given for the problem of N (even) particles confined to a single- j -shell and described by the conventional pairing plus quadrupole-quadrupole interaction Hamiltonian. This formulation is designed to be nearly exact in the pairing dominant (seniority) limit and to be accurate enough (based on plausibility arguments) to describe the transition from spherical to deformed shape. That this is so is verified for configurations - the largest being $j^N = (21/2)^6$ - for which exact solutions are available. The present method can be viewed as an angular momentum conserving alternative to the description of the transition based on the Hartree-Bogoliubov-BCS method. Qualitative and detailed comparisons of the two methods are carried out. In particular, it is shown from approximate analytic results that the two theories predict the transition to occur for almost identical values of the parameters. Overall agreement with exact

results is much better for the algebraic method, however, confirming its status as an approximate method of variation after projection.

I. INTRODUCTION

A. The Program of the Algebraic Method.

The algebraic approach to the derivation of theories of collective motion starting from a shell model Hamiltonian will be described first in quite general terms: We are given a set of single particle levels α and a spherical shell model Hamiltonian of conventional type,

$$H = \sum_{\alpha\beta} h_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \quad (1.1)$$

i.e. a sum of one particle and two-particle operators, where a_{α} , $a_{\alpha}^{\dagger}$ are the usual shell model destruction and creation operators. Consider now only even nuclei and some specified part of the low-lying spectrum of each nucleus, which we term "collective states". Can we then find a closed set of equations which will characterize all the observables associated with this subspace and, by implication, allow us to decouple in a reasonable approximation from the remainder of the states? This requires that the set of equations involves only matrix elements of the operator pairs $(a_{\alpha}^{\dagger} a_{\beta})$, $(a_{\alpha} a_{\beta})$, and $(a_{\alpha}^{\dagger} a_{\beta}^{\dagger})$ among the chosen states. For then we can compute all

transition matrix elements among the states in question and, a fortiori, from the manner in which the scheme will be developed, also the energies. We consider how this aim can be realized. [¶] Let X_ρ be the above set of fermion pair operators which either conserve the number of fermions or change the number by two. H can be considered a polynomial in the X_ρ , in general in many ways. We assume that this choice has been made: For simple models with separable interactions such as the pairing plus quadrupole-quadrupole interaction model it is the obvious one. We then wish to diagonalize the Hamiltonian within the subspace of collective states and find its eigenvalues and "eigenvectors". But we do not follow the conventional road of setting up a basis of antisymmetric states and then diagonalizing the Hamiltonian within this basis.

To see how to avoid this step, let $|K\rangle$ be the set of even states in question. By collective band we mean that for the matrix element of a sufficient set of products X_ρ, X_σ , we can write

$$\langle K | X_\rho X_\sigma | K' \rangle \cong \sum_{K''} \langle K | X_\rho | K'' \rangle \langle K'' | X_\sigma | K' \rangle, \quad (1.2)$$

that is, sum rules are effectively saturated within the band. This cannot be true in general for all choices of generators X_ρ since if it were, the entire space spanned by the X_ρ and the collective space would be synonymous. The latter is true only for certain extremely simplified models such as that of MGL^(1,2); but we are

precisely desirous in this paper of moving beyond such simplifications toward real problems where to attempt a solution, subspaces and subalgebras have somehow to be singled out. We shall assume, in what follows, that the Hamiltonian has been expressed in terms of a subset of the X_p which permit the straightforward application of (1.2). We are then ready to list the basic assumptions of the method. Readers who find the following account too abstract should consult ref. 2 or simply proceed to Part B of this section.

As the first dynamical condition, we require that

$$\langle K | H | K' \rangle = 0, \quad K \neq K', \quad (\text{D.I})$$

namely that the Hamiltonian be diagonal. If this equation is not trivially satisfied because of invariance considerations, - angular momentum, parity, etc., - it becomes, with the help of the sum rule (1.2) a non-linear relation among the amplitudes $\langle K | X_p | K' \rangle$.

The second dynamical condition is that the eigenvalues of H be correctly given in the collective subspace. We have found that there are three convenient more or less equivalent expressions of this condition. For example, let S be any polynomial in the generators X_p which commutes with all the operators (other than H) specifying $|K\rangle$. The relation

$$\langle K | [S, H] | K \rangle = 0 \quad (\text{D.II})$$

leads, upon utilization of (1.2), to a further sum rule which may be viewed as our version of the Schrodinger equation. On the other hand if S is of the form

$$S = \sum_i T_i^i T_i, \quad (1.3)$$

where i is an appropriate tensor index, we may use instead of (D.II), the "equations of motion"

$$\langle K | [T_i, H] | K' \rangle = [W(K') - W(K)] \langle K | T_i | K' \rangle. \quad (D.II')$$

It is not difficult to show that (D.II) is a consequence of the set (D.II'). That (D.II') brings in new variables, the energy differences $[W(K') - W(K)]$, is not necessarily a disadvantage, since we want these numbers anyway.

The third form of this condition and the form to be used in the present work consists in the computation of the eigenvalue $W(K)$ in the obvious manner, by use of (1.2),

$$W(K) = \langle K | H | K \rangle = W(K; \langle K' | X_\rho | K'' \rangle). \quad (1.4)$$

The Rayleigh-Ritz principle is then applied under the assumption that the $\langle K | X_\rho | K' \rangle$ may be considered variational parameters. We thus use the condition

$$\delta W[K; \langle K' | X_\rho | K'' \rangle] = 0 \quad (D.II'')$$

The dynamical conditions are however not sufficient to characterize the matrix element set $\langle K | X_\rho | K' \rangle$. This should surprise no one, since we have not fully imposed the equivalent of the conditions that the set of states $|K\rangle$ be an orthonormal one and impose satisfy the Pauli principle. We must/the condition that the set

$|K\rangle$ constitute a subspace of a specified representation of the algebra satisfied by X_ρ . We have first to satisfy the commutation relations

$$[X_\rho, X_\sigma] = \sum_\tau C_{\rho\sigma\tau} X_\tau, \quad (1.5)$$

from which we derive the first set of kinematical conditions

$$\sum_{K''} \langle K | X_\rho | K'' \rangle \langle K'' | X_\sigma | K' \rangle - (\rho \leftrightarrow \sigma) = \sum_\tau C_{\rho\sigma\tau} \langle K | X_\tau | K' \rangle. \quad (K.I)$$

But conditions (K.I) hold for any representation of the algebra, and so finally we must add the conditions that the states describe fermions. The most general way of specifying this information is to give the eigenvalues of all the algebraically independent Casimir invariants of the algebra (1.5). If $\hat{C}$ is any of these polynomials in the X_ρ , we have

$$\langle K | \hat{C} | K' \rangle = \delta_{KK'} \lambda, \quad (K.II)$$

where the eigenvalue λ is known from group theory and is independent of K . In place of (K.II), one can then derive directly from the Fermion anticommutators special algebraic relations among the X_ρ which are true only for the representation of interest and from which sum rules may be formed containing the same information as (K.II).

The general method described in this introduction has been applied successfully so far to a few highly simplified models^(2,3) to a discussion of ground state correlations at closed shells^(4,5,6)

and to some preliminary work on the model utilized in this paper.⁽⁷⁻¹³⁾ This previous work suggests strongly that the theoretical framework is complete, the physics of each problem representing a new challenge, however, as to the best choice of subalgebraic framework.

B. The Single-j Model, with Pairing Plus Quadrupole Interaction Hamiltonian.

In this paper we shall attempt a first implementation of the program outlined above for the problem of N particles (N even) confined to a single- j shell and interacting according to the pairing plus quadrupole-quadrupole interaction Hamiltonian described in Sec. II. It is now well-established from exact diagonalization studies⁽¹⁴⁻¹⁷⁾ that this system undergoes a transition from a spherical to a deformed shape if one artificially increases the strength of the quadrupole-quadrupole interaction relative to the pairing interaction. It is the purpose of this investigation to show how the algebraic method may be used to illuminate the properties of this transition. We have taken great pains in Sec. II to explain fully and carefully how we have given substance to the abstract formulation described in this introduction, leading to a well-defined, albeit approximate, calculational scheme.

Although this scheme (and certainly any future generalizations of it) has to be dealt with numerically in general, as

described in Sec. III, we are also able to derive in that section an approximate analytic expression for the critical ratio of coupling strengths at which an idealized sharp phase transition occurs as a function of particle number. In Sec. IV, our solution is compared, favorably on the whole, with exact diagonalizations⁽¹⁷⁾, but some sense of its limitations are also imparted. Calculations are also presented for large j and N in order to emphasize the increasing sharpness of the transition as these parameters increase, to testify to the transition as a band property, and to verify the validity of the analytic criterion. The description of the transition inherent in the Hartree-Bogolubov method is reviewed in Sec. V and compared with the algebraic method. The final section contains a critique of our work and suggestions for future improvements.

Besides the spherical to deformed transition considered in this paper, the model is also suitable for a study of the Coriolis anti-pairing transition as we plan to show in the next paper of this sequence (see also (13)). As is well-known⁽⁸⁾, it also exhibits an oblate to prolate transition in the deformed region as we pass through the mid-shell value of N . This property is derived briefly in the appendix following some details of the algebraic method.

II. THE MODEL: STATEMENT AND ANALYSIS OF APPROXIMATIONS

We turn then to the study of an even number N of identical fermions confined to a single j -shell. We utilize a conventional model Hamiltonian which contains a pairing interaction with force constant G and a quadrupole interaction with force constant χ , namely ($\Omega = j + \frac{1}{2}$)

$$H = - G\Omega A_0^{o\dagger} A_0^o - \frac{1}{2}\chi \sum_q B_q^2 B_q^2. \quad (2.1)$$

The operators $A_0^{o\dagger}$, A_0^o , and B_q^2 are special cases of the general two-particle transfer operators and multipole operators that can be constructed from the single-shell creation and destruction operators,

$$A_q^{k\dagger} = (2)^{-\frac{1}{2}} \sum_m \begin{bmatrix} j & j & k \\ m & q-m & q \end{bmatrix} a_m^\dagger a_{q-m}^\dagger, \quad (2.2)$$

$$B_q^k = (2k+1)^{-\frac{1}{2}} \sum_m \begin{bmatrix} j & j & k \\ m & q-m & q \end{bmatrix} (-)^{j-m+q} a_m^\dagger a_{m-q}, \quad (2.3)$$

where the square brackets are Clebsch-Gordan coefficients. These operators span the Lie Algebra $O(4j+2)$ (see the Appendix), characterized by the commutators

$$[B_q^k, A_{q'}^{k'\dagger}] = \sum_{k''} 2(2k'+1)^{\frac{1}{2}} (-)^{2j-k''} \begin{bmatrix} k & k' & k'' \\ q & q' & q+q' \end{bmatrix} \left\{ \begin{matrix} k & k' & k'' \\ j & j & j \end{matrix} \right\} A_{q+q'}^{k''\dagger}, \quad (2.4)$$

$$[A_q^k, A_{q'}^{k'\dagger}] = \delta_{qq'} \delta_{kk'} - 2 \sum_{k''} (-)^{2j+q} [(2k+1)(2k'+1)(2k''+1)]^{\frac{1}{2}} \\ \left[\begin{matrix} k & k' & k'' \\ -q & q' & q'-q \end{matrix} \right] \left\{ \begin{matrix} k & k' & k'' \\ j & j & j \end{matrix} \right\} B_{q'-q}^{k''}, \quad (2.5)$$

$$[B_q^k, B_{q'}^{k'}] = \sum_{k''} (-)^{2j-k''} [1 - (-)^{k+k'+k''}] \\ (2k''+1)^{\frac{1}{2}} \left[\begin{matrix} k & k' & k'' \\ q & q' & q'+q \end{matrix} \right] \left\{ \begin{matrix} k & k' & k'' \\ j & j & j \end{matrix} \right\} B_{q+q'}^{k''}, \quad (2.6)$$

where the curly brackets are 6-j symbols.

We wish to apply to the Hamiltonian (2.1) and to the commutators (2.4) - (2.6) the algebraic method described in general terms in the introduction. Since the equations do not in any way specify the representation of the algebra, we shall require additional statements in terms of the operators A and B which perform this function; these will be discussed below because their justification is a matter of some delicacy. But first we shall discuss the physical dimensions of the problem to be tackled.

We define the ground state band of the Hamiltonian (2.1) as the sequence of states of angular momentum $I = 0, 2, 4, \dots$, each being the state of lowest energy for the given angular momentum. In the limit $(X/G\Omega) \rightarrow \infty$, this is precisely the sequence which forms the ground state rotational band. In that limit the conventional picture of a deformed intrinsic state has habituated us to the view that this band has in some reasonable approximation an existence isolated from the remaining states of the system. In our language,

this means precisely that sum rules based on selected members of the algebra (2.4) - (2.6) and other algebraic relations (see below) are largely exhausted within the ground state band.

In the present paper we shall suppose that in a similar quantitative sense, a ground state band also exists in the spherical region. We shall consequently assume that a sufficient number of sum rules can be given, all of them exhausted within the ground state band, so as to determine the dynamical characteristics of such a band. The average reader will certainly be surprised by such an assertion. Therefore we consider it advisable to interject at this point our a posteriori understanding of its justification and limitations. For this explanation, seniority conservation is a vital ingredient.

First, it is by no means implied that the same set of sum rules accurately characterizes both the spherical and the deformed regions. In another paper based on the same model we shall show that distinct algebraic schemes are preferable in each region, as long as one restricts oneself to a single band. In this paper we shall utilize a scheme which is essentially exact in the limit of good seniority $(X/GQ) \rightarrow 0$. The algebraic scheme, in this limit, is, in fact, redundant. The choice actually made was based in part on (a possibly false) analogy with the behavior of real nuclei and in part on a semi-quantitative analysis of relationships in the deformed region. For values of $j \leq (21/2)$ and $I \leq 6$, it is possible

to check our scheme against the exact solutions of the model⁽¹⁷⁾, and, as we show in Section IV, no gross inadequacies are uncovered. Indications are, however, that a deterioration sets in for higher angular momentum. In order to carry the model of this paper accurately into the transition region, therefore, a minimal amount of band mixing will be required. We hope to present such a scheme in a further development of the model. The present scheme does, however, accurately predict the transition from spherical to deformed, and, quite remarkably, allows us to explore the full range of values of $(X/G\Omega)$ without suffering any discontinuity in choice of solution or any mathematical breakdown.

We must now translate the above verbiage into action. Let us denote the states of the band by $|(N)IM\rangle$, where M is the magnetic quantum number and the designation of N will henceforth be suppressed. We define reduced matrix elements in the usual way,

$$\langle IM|B_q^k|I'M'\rangle = (2I+1)^{-\frac{1}{2}} [I' \begin{smallmatrix} k & I \\ M' & q & M \end{smallmatrix}] B^k(I, I') \quad , \quad (2.7)$$

$$\langle IM|A_q^k|I'M'\rangle = (2I+1)^{-\frac{1}{2}} [I' \begin{smallmatrix} k & I \\ M' & q & M \end{smallmatrix}] A^k(I, I') \quad . \quad (2.8)$$

In terms of these quantities and our basic assumption concerning saturation within a single band, the energy of the state $|IM\rangle$ is given by

$$\begin{aligned} (2I+1) \langle IM|\hat{H}|IM\rangle &= (2I+1)W(I) \\ &= -G\Omega A^0(I, I)^2 - \frac{1}{2}X [B^2(I, I-2)^2 + B^2(I, I)^2 + B^2(I, I+2)^2] \quad . \end{aligned} \quad (2.9)$$

Since $\hat{H}$ is guaranteed, by angular momentum conservation, to be diagonal within the band, the dynamical content of our theory is completely expressed by the requirement that $W(I)$ be stationary for variation of all the matrix elements upon which it depends. In the present paper we shall show that it suffices to consider a restricted scheme in which the matrix elements connecting to the states of lower angular momentum, - in (2.9) the quantity $B^2(I, I-2)$ - can be considered to be known from a previous calculation, relating to the states $|I-2, M\rangle$.

The major questions in the application of the variational principle concerns the total number of variables and the number of independent ones. To investigate these points, we turn first to the algebra (2.4) - (2.6). We shall have to utilize the commutators containing number non-conserving pairing operators. It is then easy to see that, strictly, it is impossible to close the system of equations with respect to particle number. In order to simplify our discussion we shall therefore introduce the assumption

$$|2[d\Theta(I, I')/dN]| \ll |\Theta(I, I')|, \quad (2.10)$$

where $\Theta(I, I')$ is any reduced matrix element defined in (2.7), (2.8). This will allow us to decouple the problems for various N . Once the decoupled problems have been solved, one can reintroduce number conservation, since the derivatives previously ignored can now

be retained and computed with successively increasing accuracy. This has been done, in part, and the results will be quoted appropriately. It has been verified that number conservation results only in a quantitative not a qualitative change in our results. Below, we shall record equations only in the approximate form following from (2.10).

Our assumption of number non-conservation also puts into sharp focus that certain commutators are obviously inconsistent in the number non-conserving limit, and should not be used to define the scheme. In such relations, one side (but not the other) contains only derivatives with respect to number. An example is the commutator

$$[A_0^0, A_0^{0\dagger}] = 1 - (N/\Omega) \quad (2.11)$$

which becomes, in leading order, in the ground state

$$2 \frac{d}{dN} A^0(0,0)^2 = 1 - (N/\Omega) \quad (2.12)$$

This relation doesn't contradict (2.10), since $A^0(0,0)^2 \sim N$, but means that (2.12) will not be utilized in the present formulation.

Following this line of thought and proceeding from the lowest available multipoles, the first useful equations we encounter are (2.4) and (2.5) for $k = k' = 2$. We shall not utilize (2.6) at all in the present considerations, and this too requires some comment. It is not difficult to prove, though we shall not present the demonstration here^(8,9) that for $k = k' = 2$, the right hand side

of (2.6) is always small for the low-lying members of the ground state band. As shown by a number of authors ^(8,9,18), the resulting commutativity of the operators B_q^2 implies, under restriction to intermediate states of the same band, that the nucleus has a rigid shape. Since this result is neither acceptable intuitively in the spherical region, nor does it agree with the exact diagonalization, we thereby gain two insights: Band mixing must be more important in the spherical than in the deformed region. When this is so, either the simplest scheme is vitiated or else one must be very careful to choose sum rules which are less sensitive to this mixing. Our results will be seen to substantiate our choices in the latter regard.

It should be remarked that the above discussion represents largely hindsight and that our original reason for not considering (2.6) was simply that in the ground state it is identically satisfied and therefore not useful, in contradistinction to (2.4) and (2.5). When we turned to excited states we continued to ignore it mainly because we were able, as will be seen below, to fully define without it a scheme acceptable in the seniority limit. On the other hand, our best simple scheme for the deformed region relies quite naturally on (2.6).

The commutators (2.4) and (2.5) are conveniently viewed as separate equations for each spherical tensor component, namely for

$$L = 0, 2, 4,$$

$$\sum_q \begin{bmatrix} 2 & 2 & L \\ q & Q-q & Q \end{bmatrix} [A_q^2, B_{Q-q}^2] = (-)^L (5)^{\frac{1}{2}} \left\{ \begin{matrix} 2 & 2 & L \\ j & j & j \end{matrix} \right\} A_Q^{L\dagger}, \quad (2.13)$$

$$\begin{aligned} \sum_q (-)^q \begin{bmatrix} 2 & 2 & L \\ -q & Q+q & Q \end{bmatrix} [A_q^2, A_{Q+q}^{2\dagger}] &= \delta_{L,0} (5)^{\frac{1}{2}} \\ &+ 10 (2L+1)^{\frac{1}{2}} \left\{ \begin{matrix} 2 & 2 & L \\ j & j & j \end{matrix} \right\} B_Q^L. \end{aligned} \quad (2.14)$$

From diagonal matrix elements of (2.13), (2.14) applied to the $L = 0$ relations in the number non-conserving approximation within the ground state band, we easily derive the following two equations:

$$\begin{aligned} B^2(I, I+2) [A^2(I, I+2) - A^2(I+2, I)] + [10(2I+1)/\Omega]^{\frac{1}{2}} A^0(I, I) \\ = B^2(I, I-2) [A^2(I-2, I) - A^2(I, I-2)], \end{aligned} \quad (2.15)$$

$$\begin{aligned} [A^2(I, I+2)]^2 - [A^2(I+2, I)]^2 &= A^2(I-2, I)^2 - A^2(I, I-2)^2 \\ &+ 5(2I+1)(N-\Omega)/\Omega. \end{aligned} \quad (2.16)$$

The $L = 2$ components of (2.13) and (2.14) suggest a number of sum rules both diagonal and off-diagonal and like (2.15) and (2.16) essentially exact in the seniority limit. Of these we chose only one, namely the average of the two sum rules obtained from (2.13) when considering in turn matrix elements going from $I \rightarrow I+2$ and from $I+2 \rightarrow I$. This yields the equation

$$\begin{aligned}
& \left\{ \begin{smallmatrix} 2 & 2 & 2 \\ I & I & I-2 \end{smallmatrix} \right\} \left\{ 2A^2(I, I)B^2(I, I-2) - B^2(I, I)[A^2(I, I-2) + A^2(I-2, I)] \right\} \\
& = \left\{ \begin{smallmatrix} 2 & 2 & 2 \\ I & I-2 & I-2 \end{smallmatrix} \right\} \left\{ 2A^2(I-2, I-2)B^2(I, I-2) - B^2(I-2, I-2)[A^2(I, I-2) \right. \\
& \quad \left. + A^2(I-2, I)] \right\} + 2 \left\{ \begin{smallmatrix} 2 & 2 & 2 \\ j & j & j \end{smallmatrix} \right\} [A^2(I-2, I) - A^2(I, I-2)] . \quad (2.17)
\end{aligned}$$

We have averaged simply because, as will be seen in Sec. III, in the deformed region $A^2(I, I+2) \cong A^{(2)}(I+2, I)$ (for small I) and the two matrix elements become almost identical and of the order $N^{\frac{1}{2}}$. Equation (2.14) leads to a relation less accurate in the deformed region.

In partial reprise the choice of the set (2.15) - (2.17) was guided by the desire to have equations which could be relied on both in the seniority limit $(\chi/G\Omega) \rightarrow 0$, and in the strong coupling region $(\chi/G\Omega) \rightarrow \infty$. Our original aims were thus quite ambitious. Assuming that the reduced matrix elements involving at least one index $(I-2)$ are known, we see that the four expressions (2.9), (2.15) - (2.17) involve six unknowns: $A^0(I, I)$, $B^2(I, I)$, $B^2(I, I+2) = B^2(I+2, I)$, $A^2(I, I)$, $A^2(I, I+2)$, $A^2(I+2, I)$. Since we shall require $\delta W(I) = 0$, we must then imagine that there are three independent variables or else add further supplementary conditions.

The former view is completely untenable since so far, none of the equations specify the representation of the Lie Algebra. In order to fix the latter, additional equations should be chosen

from among the Casimir invariants of $O(4j+2)$ since the eigenvalues of these operators uniquely specify the representation. In practice we shall utilize only approximate versions of a subset of these, which suffice, hopefully, to characterize the very particular subspace - the band - to which we confine ourselves. To illustrate the considerations involved in this part of the argument, consider the quadratic invariant $\hat{C}^{(2)}$,

$$\begin{aligned} \hat{C}^{(2)} = \sum_{k,q} \{A_q^{k\dagger}, A_q^k\} + \sum_{k \neq 0,q} (2k+1) B_q^k (-)^q B_q^k \\ + \frac{1}{2}\Omega [1 - (N/\Omega)^2] = \frac{1}{2}\Omega + \sum_{k(\text{even})} (2k+1) \end{aligned} \quad (2.18)$$

where the eigenvalue, given by the last equality, is obtained by computation of the expectation value of $\hat{C}^{(2)}$ in the vacuum state. The matrix elements of (2.18) within the band would appear, however, to pose a dilemma, insofar as all the multipoles apparently contribute, and our implicit effort, successful thus far, to confine the problem to the computation of low order multipoles appears to have failed.

In the seniority limit at least, the difficulty is more apparent than real. There we have the quasi-spin subgroup generated by $A^0, A^{0\dagger}$, and N with its invariant

$$\hat{C}_s^{(2)} = \{A^{0\dagger}, A^0\} + \frac{1}{2}\Omega [1 - (N/\Omega)^2] = \frac{1}{2}\Omega + 1. \quad (2.19)$$

Furthermore from the exact matrix elements in the seniority limit

given in the Appendix, we can show, $k = \text{even} \neq 0$,

$$\begin{aligned} \sum_q \langle N, 0 | \{ A_q^{k\dagger}, A_q^k \} | N, 0 \rangle + (2k+1) \sum_q \langle N, 0 | B_q^k(-)^q B_{-q}^b | N, 0 \rangle \\ = 2[A^k(0, k)]^2 + (2k+1)[B^k(k, 0)]^2 + (2k+1) [(1 - (N/\Omega))] = (2k+1) \end{aligned} \quad (2.20)$$

where in $A^k(0, k)$, etc. the state $I = k$ is a unique state of seniority two, and, of course, the expectation value of the terms in (2.18) involving odd-multipole invariants vanishes.

(Evaluation of (2.20) and of analogous expressions below also utilize the commutation relations.) Notice that (2.20) becomes

$$2[A^k(0, k)]^2 + (2k+1)[B^k(k, 0)]^2 = (2k+1)N/\Omega, \quad (2.21)$$

whereas the ground state expectation value of (2.19) yields

$$[A^0(0, 0)]^2 = \frac{1}{2}N - (N^2/4\Omega) + (N/2\Omega). \quad (2.22)$$

These last two relations plus the simplest ideas concerning the character of a phase transition suggest a viable approximation procedure. Thus (2.22) tells us that $A^0(00) = 0(N^{\frac{1}{2}})$ in the seniority limit whereas (for $k \sim 1$), $A^k(0, k)$ and $B^k(k, 0)$ are $O(1)$. The nature of a phase transition - here we must imagine that $N \gg 1$ - is that one or more of the matrix elements for higher multipoles rises from $O(1)$ to $O(N^{\frac{1}{2}})$ over a relatively small range of values of (x/Ω) . (Since we are dealing with a model we feel free to vary the coupling strengths continuously.) In view of the interaction chosen, we are prejudiced in favor of the quadrupole

amplitudes undergoing the phase transition. Though we have no rigorous basis for it, we shall assume that no other multipole undergoes the transition in the sense that its matrix elements within the ground state band increase from $O(1)$ to $O(N^{\frac{1}{2}})$.

Further remarks concerning this assumption are reserved for the final discussion.

Finally, in quantitative terms, we shall assume that at least the low-lying states of the band admit an approximate Casimir operator, which is obtained from (2.18) by equating separately those parts of the two sides for which $k \leq 2$. This amounts to assuming that the generalization of the sum of (2.21) and (2.22) remains valid. This has the two virtues: It is exact in the seniority limit and it permits the quadrupole mode to rob "strength" from the monopole pairing mode. The diagonal matrix element of this relation yields the equation

$$\begin{aligned}
 & 2(2I+1)^{-1} [A^0(I,I)^2 + A^2(I,I+2)^2 + A^2(I,I)^2 + \frac{5}{2} B^2(I,I+2)^2 \\
 & + \frac{5}{2} B^2(I,I)^2] = N - (N^2/2\Omega) + (6N/\Omega) - [3I(I+1)/j(j+1)(2j+1)] \\
 & - 2(2I+1)^{-1} [A^2(I,I-2)^2 + \frac{5}{2} B^2(I,I-2)^2] \quad . \quad (2.23)
 \end{aligned}$$

This relation was tested⁽¹⁷⁾ using the exact solution for $I = 0$ and $j^N = (\frac{21}{2})^6$ and found to be almost exact up to the transition region and correct to about 50% even for $(\chi/G\Omega) = \infty$.

We shall finally pull one more kinematical constraint from

the algebraic hat and thus reduce the number of independent variables to one. For this we could go to the quartic Casimir operator (the orthogonal groups possess only even order invariants). An alternative is to construct among the generators tensor relations which are a direct consequence of the Pauli Principle. The straight-forward procedure for doing this is described in the Appendix leading to the set of Eq. (A.7). The monopole member of this set yields the Casimir invariant $\hat{C}_2$. The quadrupole member as given in Eq. (A.16) again contains all multipoles. But once more we are able to show that for the lowest (in angular momentum) non-vanishing matrix elements the terms with $k \leq 2$ yield a relation correct in the seniority limit and indeed a sum of two terms each separately satisfied. We adopt this relation as our final kinematical constraint. From the obvious off-diagonal matrix element there emerges the equation (see Appendix for further details of the above arguments)

$$\begin{aligned}
 & \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} \left\{ \begin{matrix} 2 & 2 & 2 \\ I & I & I-2 \end{matrix} \right\} [25B^2(I, I)B^2(I, I-2) + 10 A^2(I, I)A^2(I-2, I)] \\
 & - \sqrt{2} [5\Omega(2I+1)]^{-\frac{1}{2}} A^0(I, I)A^2(I-2, I) + [(\Omega+2-N)\Omega^{-1} + 50 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\}^2] \\
 & B^2(I, I-2) = \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} \left\{ \begin{matrix} 2 & 2 & 2 \\ I-2 & I & I-2 \end{matrix} \right\} [25B^2(I, I-2)B^2(I-2, I-2) \\
 & + 10 A^2(I, I-2)A^2(I-2, I-2)] + \sqrt{2} [5\Omega(2I-3)]^{-\frac{1}{2}} A^0(I-2, I-2) \\
 & A^2(I, I-2) . \quad (2.24)
 \end{aligned}$$

To summarize, we have derived five subsidiary conditions from kinematical constraints, the dynamics entering solely through the variation of the energy expression. Further we remark that up to number non-conservation the subsidiary conditions when referring to the ground state and to the state $I = 2$ are satisfied by the exact solution in the seniority limit. We then assume that they will keep their validity away from the seniority limit and higher in the spectrum.

III. THE GENERAL CALCULATION AND SOME SPECIAL ANALYTIC RESULTS:

PREDICTION OF A PHASE TRANSITION.

In consequence of the arguments developed in the previous section, we have emerged with a well-defined problem. To determine the six variables $A^0(I,I)$, $A^2(I,I+2)$, $A^2(I+2,2)$, $B^2(I,I+2)$, $B^2(I,I)$, and $A^2(I,I)$ we shall use the condition

$$\delta W(I) = 0, \quad (3.1)$$

where $W(I)$ is given by (2.9) and all variables other than $B^2(I,I-2)$ are to be varied; this variation is carried out subject to five supplementary conditions, Eqs. (2.15), (2.16), (2.17), (2.23), and (2.24). These are utilized conventionally by the introduction of Lagrange multipliers. For numerical purposes a convenient alternative is as follows: Let us relabel the variables X_i , $i = 1, \dots, 6$ (not to be confused with the generators) and the five supplementary conditions $S_\alpha(X_i) = 0$, $\alpha = 1, \dots, 5$. Then the five variations

$$\delta S_\alpha(X_i) = 0 \quad (3.2)$$

together with (3.1) yield six homogeneous equations for the δX_i . The compatibility of these equations requires that the determinant, D , of the coefficients of the δX_i vanish,

$$D(X_i) = 0 \quad (3.3)$$

This equation is equivalent to the condition that is obtained by introduction and then elimination of Lagrange multipliers, but

avoids much of the intermediate algebra. Equation (3.3) is now viewed as replacing (3.1). Thus in conjunction with the five equations

$$S_{\alpha}(X_i) = 0 \quad (3.4)$$

constitute six non-linear equations for the variables X_i .

These equations were solved by the Newton-Raphson technique described in a previous publication⁽²⁾ for all values of the ratio $(\lambda/\Omega G)$ starting with the seniority limit and systematically varying this ratio. Some of the results will be described in the next section. For the ground state problem, simplifications occur which permit us to obtain limited analytic results which provide essential insights. We devote the remainder of this section to these aspects.

For $I = 0$, the variables are reduced to four in number, since $B^2(I, I)$ and $A^2(I, I)$ vanish. Correspondingly Eqs. (2.17) and (2.24) of our set are only defined for $I \geq 2$. In this case the most transparent procedure is to eliminate $A^2(20)$ and $A^2(02)$ from the problem using (2.14) and (2.15). With the definitions

$$z = A^0(0,0)^2, \quad y = B^2(20)^2, \quad (3.5)$$

The Casimir relation (2.23) takes the form

$$S = 0 = -z^2 y + [b + (5/2)]zy - (5/2)zy^2 - (5/8)(\Omega - N)^2 \Omega^{-1} y^2 - (5/2)(z^2/\Omega), \quad (3.6)$$

$$b = \frac{1}{2}N - (N^2/4\Omega) + (N/2\Omega) \quad (3.7)$$

The equations which follow from the variational principle

$$\delta[W_0 + 2ES] = 0, \quad (3.8)$$

become, upon elimination of E, the Lagrange multiplier,

$$(5\Omega G/\chi) = \left\{ z^2 y^2 - (5/8)(\Omega-N)^2 \Omega^{-1} y^3 + (5/2) \Omega^{-1} z^2 y \right\} \\ \left\{ z^2 y^2 + \frac{1}{4}(\Omega-N)^2 \Omega^{-1} zy^2 - \Omega^{-1} z^3 \right\}^{-1}, \quad (3.9)$$

which is to be solved in conjunction with (3.6) for z and y.

It is not difficult to see that there is algebraic simplification at the points (i) $\chi = 0$, (ii) $G = 0$, and (iii) $\chi = 5\Omega G$.

We shall quote the results of solving (3.6) and (3.9) for these cases.

(i) $\chi = 0$:

$$A^0(0,0) = \sqrt{b} \\ B^2(2,0) = (2b/\Omega)^{\frac{1}{2}}, \\ A^2(2,0) = (5)^{\frac{1}{2}} (2\Omega-N)/2\Omega, \\ A^2(0,2) = -(5)^{\frac{1}{2}} N/2\Omega. \quad (3.10)$$

(ii) $G = 0$; ($N < \Omega$):

$$A^{(0)}(0,0) = [(\Omega-N)N(N+10)/4\Omega(N+5)]^{\frac{1}{2}}, \\ B^2(2,0) = [N(N+10)/10\Omega]^{\frac{1}{2}}, \\ A^2(20) = \frac{1}{2}(N+10) [(\Omega-N)/\Omega(N+5)]^{\frac{1}{2}}, \\ A^2(02) = \frac{1}{2}N [(\Omega-N)/\Omega(N+5)]^{\frac{1}{2}}. \quad (3.11)$$

(III) $x = 5\Omega G$:

$$\begin{aligned} A^0(0,0) &= [N(\Omega-N)(2\Omega-N+10)/4\Omega(\Omega-N+5)]^{\frac{1}{2}}, \\ B^2(2,0) &= [N(2\Omega-N+10)/2\Omega(\Omega-N+5)]^{\frac{1}{2}}, \\ A^2(2,0) &= [5(\Omega-N)/\Omega]^{\frac{1}{2}}, \\ A^2(0,2) &= 0. \end{aligned} \quad (3.12)$$

These results are first of all of interest either as starting values for numerical procedures or as partial checks of the latter. They are of basic qualitative interest if we contrast solutions (i) and (iii) with (ii), and especially consider the limit $\Omega \rightarrow \infty$, (N/Ω) finite. We then see that for $(x/5\Omega G) < 1$

$$\begin{aligned} A^0(0,0) &= O(N^{\frac{1}{2}}), \\ B^2(2,0) \sim A^2(2,0) \sim A^2(0,2) &= O(1), \end{aligned} \quad (3.13)$$

whereas for $(x/5\Omega G) \gg 1$, we have

$$A^{(0)}(0,0) \sim B^2(2,0) \sim A^2(2,0) \sim A^2(0,2) = O(N^{\frac{1}{2}}). \quad (3.14)$$

These results have the obvious interpretation of a phase transition from a spherical to a quadrupole deformed "shape". This conclusion will be equally clear from the detailed results to be presented in the next section, where it will be seen that the conclusions are applicable to the excited states as well.

In the limit $\Omega \rightarrow \infty$, (N/Ω) finite, it is possible to speak of the phase transition occurring at a specific value of $(x/5\Omega G)$. This value can be deduced from (3.6) and (3.9) by the following argument. Let us suppose that we are in the deformed

regime. Then both z and y are $O(N)$. If we examine (3.9), it is straightforward to see that under the assumptions of this paragraph, keeping only the leading term, it reduces to the expression

$$(5\Omega G/x) = \left\{ z^2 - (5/8)(\Omega-N)^2 \Omega^{-1} y \right\} \left\{ z^2 + \frac{1}{4} (\Omega-N)^2 \Omega^{-1} z \right\}^{-1}. \quad (3.15)$$

We see that by increasing the coupling strength ratio on the left hand side this equality ultimately becomes untenable. The limiting value is clearly obtained by setting $y = 0$ and inserting for z^2 its maximum value, which is precisely its value in the seniority limit, given by (3.10). In leading order, we then obtain for the transition point

$$(5\Omega G/x)_{\text{transition}} = N(2\Omega-N)/\Omega^2. \quad (3.16)$$

It is, of course, more orthodox (and physical) to view Eq. (3.16) as a condition on the number of particles for fixed coupling strength. In Section V, we shall compare this result with that given by the classical argument which compares energies of the aligned and pairing coupling schemes.

We note that in the limit of large N and Ω , the two amplitudes $A^2(2,0)$ and $A^2(02)$ become equal. Therefore there are strictly only three large amplitudes in the strong coupling limit, rather than four. This observation could have formed the basis for equivalent reasoning leading to (3.16) and was the basis for the choice of (2.17) as one of our equations, namely we sought a

condition which was exact in the seniority limit and in the strong coupling limit reduced to a non-trivial relation among large amplitudes, which are the best-determined by our procedures.

IV. NUMERICAL RESULTS. COMPARISON WITH EXACT SOLUTIONS AND STUDY OF PHASE TRANSITIONS.

We first present selected comparisons between the results of the algebraic calculations and the exact diagonalizations.⁽¹⁷⁾ In Fig. 1 that comparison is made for the matrix elements $A^0(0,0)$ and $B^2(2,0)$. We have actually presented, in this case, the results of a number-conserving calculation, but the results for the approximation actually described in Section II are quite similar. For these matrix elements the results of the ground state calculation are completely satisfactory. For this state, further detailed comparisons of which Fig. 1 is a prototype have been carried out in previous work to which we refer the reader.⁽¹⁷⁾

All algebraic results for higher states have been obtained since the previous work was reported. In general, the overall quality of agreement becomes less satisfactory as we move up the band. This is a consequence not only of the chain character of our method of computation, and of number non-conservation, but also, as the results will show, the increasing importance, in the transition region of band coupling. This is clearly shown by Fig. 5.

2 and 3. In Fig. 2, the energy difference $W(4) - W(2)$ of the variational calculation is in good agreement with an appropriately chosen difference at the two coupling extremes, but in between makes the best of a bad situation by averaging. As shown in Fig. 3, in the transition region, there are two states with substantial values of $B^2(4,2)$, one emanating from a seniority four, the other from a seniority two limiting state. The variational value of $B^2(4,2)$ is never far from the sum of the values contributed by each state. It is clear that for an accurate treatment of the transition region band mixing will have to be included. In the seniority limit, the calculation picks up the state with $I = s$ and in the strong coupling limit the member of the ground state rotational band.

For sufficiently large Ω and N , the problem formulated in this paper continues to give answers in the sense just described up to rather large angular momenta. These are quite accurate, as we should expect, in the seniority limit. In the deformed region we have formulated a superior one band approximation which will be presented in a later publication (see Ref. (13), however).

Turning away from the comparison with the exact solution which has required our keeping to "small" systems, we shall next turn to the further study of the phase transition. Here we present results for $\Omega = 200$, $N = 104$. For such a case the

inaccuracies due to number non-conservation should be a few per cent at most. In Fig. 4, we show two types of matrix elements, $A^0(I,I)/(2I+1)^{\frac{1}{2}}$ and $B^2(I,I+2)$ plotted vs. the interaction strength. For comparison the value of the critical strength predicted analytically in Section III is indicated. We also wish to look at the transition as a function of N for fixed coupling strength. This property is seen most clearly in the matrix element of the pairing correlation as shown in Fig. 5. If we naturally identify the transition point with the maxima in the curves, we see that there is very little shift with angular momentum and that the position agrees well with ^{the} value predicted by the analytic formula.

This is as far as we can reasonably go with the present approach. We defer further discussion to Section VI.

V. COMPARISON WITH PREVIOUS CRITERION FOR PHASE TRANSITION.

HARTREE-BOGOLIUBOV RESULTS.

A. The Classical Argument

It is amusing to compare the value given in Eq. (3.16) for the transition coupling strength ratio with that which emerges from a careful application of the textbook argument.⁽¹⁹⁾ We consider the case of an oblate deformation, $N < \Omega$. We then compare the ground state energy in the seniority scheme

$$W_0^s = - G\Omega A^0(0,0)^2 = - G\Omega N(2\Omega - N + 2)/4\Omega, \quad (5.1)$$

with the energy obtained from an aligned wave function. In this case we have

$$W_o^d = -\frac{1}{2}\chi \langle B_o^2 \rangle^2 . \quad (5.2)$$

By a straightforward calculation, we find⁽⁸⁾

$$\begin{aligned} \langle B_o^2 \rangle &= \langle \text{aligned} | B_o^2 | \text{aligned} \rangle \\ &= (5)^{-\frac{1}{2}} \sum_{m=\pm j}^{\pm(j-\frac{1}{2}N)} (-)^{j-m} \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix} \\ &= \frac{N(2N-N)(4N-N)}{4[2N(2N^2-1)(4N^2-1)]^{\frac{1}{2}}} . \end{aligned} \quad (5.3)$$

The point of transition is taken to be defined by the condition

$$W_o^s = W_o^d . \quad (5.4)$$

With the use of (5.1) - (5.3) this yields

$$(5G\Omega/\chi) = (5/16) [(4N-N)^2/4N^2] [N(2N-N)/N^2] , \quad (5.5)$$

neglecting $O(1)$, compared to $O(N)$. Comparing with Eq. (3.16), we see that

$$(5G\Omega/\chi)|_{\text{classical}} = (5/16) [(4N-N)^2/4N^2] (5G\Omega/\chi)|_{\text{algebraic}} . \quad (5.6)$$

For $N = \frac{1}{2}\Omega$, where maximum deformation is expected, we have

$$(5G\Omega/\chi)|_{\text{classical}} \cong (15/16) (5G\Omega/\chi)|_{\text{algebraic}} , \quad (5.7)$$

a quite remarkable degree of concordance.

B. Hartree-Bogoliubov-BCS Method.

We shall briefly review the elements of the Hartree-Bogoliubov (or deformed BCS) method for the study of the phase transition⁽²⁰⁾ and then present a comparison with the results of the algebraic method. We thus compute the expectation value of H in the state

$$|BCS\rangle = \prod_{m>0} (u_m + s_m v_m a_m^\dagger a_{-m}^\dagger) |vac\rangle, \quad (5.8)$$

where

$$u_m^2 + v_m^2 = 1, \quad s_m = -s_{-m}. \quad (5.9)$$

Calling this expectation value W_0 , we have

$$\begin{aligned} W_0 = & -\frac{1}{4}G \left[\left(\sum_m u_m v_m \right)^2 + \sum_m v_m^4 \right] \\ & - \frac{1}{10} \times \left\{ \left[\sum_m \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix} s_m v_m^2 \right]^2 \right. \\ & \left. - \frac{1}{10} \times \sum_m \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix}^2 u_m^2 v_m^2 \right\}. \end{aligned} \quad (5.10)$$

If we compare this with the definition

$$W_0 = -G\Omega \langle A_0^0 \rangle_{\text{eff}}^2 - \frac{1}{2} \times \langle B_0^2 \rangle_{\text{eff}}^2, \quad (5.11)$$

we arrive at the identifications

$$\langle A_0^0 \rangle_{\text{eff}} = \frac{1}{2} \Omega^{-\frac{1}{2}} \left[\left(\sum_m u_m v_m \right)^2 + \sum_m v_m^4 \right]^{\frac{1}{2}}, \quad (5.12)$$

$$\begin{aligned} \langle B_0^2 \rangle_{\text{eff}} = & (5)^{-\frac{1}{2}} \left[\left(\sum_m \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix} s_m v_m^2 \right)^2 \right. \\ & \left. + \sum_m \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix}^2 u_m^2 v_m^2 \right]^{\frac{1}{2}}. \end{aligned} \quad (5.13)$$

We now vary (5.10) subject to the constraints (5.9) (Lagrange multipliers $\frac{1}{2} E_m$) and

$$N = \sum_m v_m^2, \quad (5.14)$$

(Lagrange multiplier λ); we thus derive the well-known equations of the BCS method,

$$\begin{aligned} [E_m - (\epsilon_m - \lambda)] v_m &= -\Delta u_m, \\ [E_m + (\epsilon_m - \lambda)] u_m &= -\Delta v_m, \end{aligned} \quad (5.15)$$

$$\Delta = \frac{1}{2} G \sum_m u_m v_m, \quad (5.16)$$

$$\begin{aligned} \epsilon_m &= - (5)^{-\frac{1}{2}} \times \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix} s_m \langle B_0^2 \rangle \\ &\quad - \frac{1}{4} G (1 + v_m^2 - u_m^2) + \frac{1}{10} \times \begin{bmatrix} j & j & 2 \\ m & -m & 0 \end{bmatrix}^2 (v_m^2 - u_m^2), \end{aligned} \quad (5.17)$$

where $\langle B_0^2 \rangle$ means the expectation value of the operator in the BCS state. We then obtain the solution

$$E_m = [(\epsilon_m - \lambda)^2 + \Delta^2]^{\frac{1}{2}}, \quad (5.18)$$

with Δ and λ determined from the equations

$$\frac{1}{4} G \sum_m E_m^{-1} = 1 \quad (5.19)$$

$$\sum_m v_m^2 = N, \quad (5.20)$$

$$v_m^2 = \frac{1}{2} \left[1 - \frac{\epsilon_m - \lambda}{E_m} \right] \quad (5.21)$$

For our purposes the transition occurs when λ is large enough to give a solution $\langle B_0^2 \rangle \neq 0$. (Because of our definition,

it turns out that $\langle B_0^2 \rangle_{\text{eff}} \neq 0$ everywhere.)

In Fig. 6 some results of the BCS calculation are compared both with the exact results and with the results of the algebraic treatment. In carrying out this comparison, the concept of effective matrix element introduced in Eqs. (5.11) - (5.13) is utilized. We see that the pairing correlations are in agreement in the spherical region, whereas the quadrupole matrix element agrees in the deformed region. The transition occurs where expected. The superiority of the relatively simple algebraic procedure developed in this paper is manifest, however. In Fig. 7, a similar comparison is made for a very large configuration, where exact calculations are, of course, out of the question. Also noted on the figure is the position of the transition point as predicted by the approximate analytic treatments.

It should be remarked that $\langle B_0^2 \rangle$ vanishes in the spherical region and Δ vanishes in the strong coupling limit in the BCS method. The failure of our curves to reflect these facts is only apparent, expressing only difference in definition between the above quantities and those plotted, namely the effective matrix elements (5.12), (5.13).

VI. DISCUSSION

It remains only to be skeptical concerning the foundations of the method of this paper. The most serious logical deficiency is that we have not proved that higher multipoles can be neglected.

There is at least one claim in the literature that they cannot be neglected in the single (large) j model in the strong coupling limit.⁽⁹⁾ That claim, cogent but not rigorous, does not per se vitiate our particular method for decoupling the higher multipoles in the spherical and transition region and in particular, our results for low-angular momentum.

To attempt to shore up foundations, we hope to carry out further work along the following lines: (i) The inclusion of up to hexadecupole moments in a single band approximation. (ii) Band mixing in the transition region, starting with the monopole-quadrupole limitations of the present paper. (iii) comparison of the results of this paper with a calculation based on the generalized Hartree-Fock approximation.⁽²¹⁾ (iv) a reinvestigation of the strong coupling limit to which most attention has been paid in previous work, but where, in the writers' opinion serious questions remain unresolved.

APPENDIXA. THE ALGEBRA AND PAULI PRINCIPLE RELATIONS.

Our main aim here is to derive the algebraic relations from which the subsidiary conditions (2.24), (2.25) were obtained and to add some remarks on the approximations involved. Define the operators - $j \leq m \leq j$.

$$g_{mm'} = a_m^\dagger a_{m'} - \frac{1}{2} \delta_{mm'} \equiv G_{mm'} - \frac{1}{2} \delta_{mm'} \quad (A.1)$$

$$F_{mm'} = a_m a_{m'} = (F_{mm'}^\dagger)^\dagger \quad (A.2)$$

From the anticommutators follows the algebra

$$[g_{mm'}, g_{m''m'''}] = \delta_{m'm''} g_{mm'''} - \delta_{mm'''} g_{m''m'} , \quad (A.3)$$

$$\begin{aligned} [F_{mm'}, F_{m''m'''}] &= \delta_{mm''} g_{m''m'} - \delta_{m'm'''} g_{m''m} \\ &+ \delta_{mm'''} g_{m''m'} - \delta_{m'm''} g_{m''m'} , \end{aligned} \quad (A.4)$$

$$[F_{mm'}, g_{m''m'''}] = \delta_{mm''} F_{m''m'} - \delta_{m'm'''} F_{m''m} , \quad (A.5)$$

$$[F_{mm'}^\dagger, g_{m''m'''}] = \delta_{m'm'''} F_{m''m}^\dagger - \delta_{mm'''} F_{m''m'}^\dagger \quad (A.6)$$

This can be shown to be the Lie Algebra of $O(4j+2)$.

We are, of course, interested only in representations which satisfy the Pauli Principle. These can be characterized by additional algebraic relations in whose derivation Fermi-Dirac statistics plays the essential role. This is true of the identity

$$\begin{aligned}
& \frac{1}{2} \left\{ G_{mm'}, G_{m''m'''} \right\} + \frac{1}{2} \left\{ F_{mm''}^\dagger, F_{m'''m'} \right\} \\
& - \frac{1}{2} \delta_{m'm} G_{m''m'''} - \frac{1}{2} \delta_{m'''m''} G_{mm'} \\
& = \frac{1}{2} (\delta_{mm'''} \delta_{m'm''} - \delta_{mm'} \delta_{m''m'''}) , \tag{A.7}
\end{aligned}$$

whose verification requires the detailed definitions (A.1), (A.2), and the anticommutation relations. Since the right hand side of (A.7) is a constant, the quadratic functions of the generators on the left hand side commute with all the generators.

We next show that the quadratic Casimir operator is a linear combination of these quadratic forms. We first substitute the relations inverse to Eqs. (2.2) and (2.3) of the main text, namely,

$$G_{mm'} = (-)^{j-m} \sum_k (2k+1)^{\frac{1}{2}} \begin{bmatrix} j & j & k \\ m & -m' & m-m' \end{bmatrix} B_{m-m'}^k , \tag{A.8}$$

$$F_{mm'}^\dagger = \sqrt{2} \sum_k \begin{bmatrix} j & j & k \\ m & m' & m+m' \end{bmatrix} A_{m+m'}^{k\dagger} \tag{A.9}$$

We then set $m = m'''$, $m' = m''$, and sum over m and m' . We thereby obtain the following operator relation:

$$\begin{aligned}
& \frac{1}{2} \sum_{k,q} (2k+1) (-)^q \left\{ B_q^k, B_{-q}^k \right\} + k \sum_q \left\{ A_q^{k\dagger}, A_q^k \right\} - \hat{N} \\
& = \Omega (2\Omega-1) , \tag{A.10}
\end{aligned}$$

where

$$\hat{N} = \sum_m a_m^\dagger a_m . \tag{A.11}$$

We have also

$$N = 2\Omega \quad B_0^0 . \tag{A.12}$$

With the help of (A.12) and of the sum

$$\sum_{k(\text{even})}^{2j-1} (2k+1) = \Omega(2\Omega-1) \quad , \quad (\text{A.13})$$

(A.10) can be rewritten as

$$\begin{aligned} \frac{1}{2} \sum_{k \neq 0, q} (2k+1) (-)^q \{ B_q^k, B_{-q}^k \} + \sum_{k, q} \{ A_q^{k\dagger}, A_q^k \} \\ + \frac{1}{2} \Omega [1 - (\hat{N}/\Omega)]^2 = \frac{1}{2} \Omega + \sum_{k(\text{even})}^{2j-1} (2k+1) \quad . \end{aligned} \quad (\text{A.14})$$

This is the quadratic Casimir operator, since to show directly that the left hand side commutes with all generators, one needs only the commutation relations. The right hand side then represents its eigenvalue for the representation of interest to us.

The approximation to this equation has been adequately discussed in the text.

To obtain consequences of (A.7) which are independent of (A.14), we again substitute (A.8) and (A.9), but this time we set $m' = m''$, and then project out a spherical tensor of rank (k'', q'') by multiplying by $(-)^{j-m''} \begin{bmatrix} j & j & j'' \\ m & -m'' & q'' \end{bmatrix}$ and summing over m , m' , and m'' . We thus obtain the relation

$$\begin{aligned} \frac{1}{2} \sum_{kk'q} (-)^{k''} (2k+1)(2k'+1) \left\{ \begin{matrix} k & k' & k'' \\ j & j & j \end{matrix} \right\} \begin{bmatrix} k & k' & k'' \\ q & q''-q & q'' \end{bmatrix} \{ B_q^k, B_{q''-q}^{k'} \} \\ + \sum_{kk'q} (-)^{k''+q+q''} [(2k+1)(2k'+1)]^{\frac{1}{2}} \left\{ \begin{matrix} k & k' & k'' \\ j & j & j \end{matrix} \right\} \begin{bmatrix} k & k' & k'' \\ q & q''-q & q'' \end{bmatrix} \{ A_q^{k\dagger}, A_{q-q''}^{k'} \} \\ + (2k''+1)^{\frac{1}{2}} B_{q''}^{k''} + \frac{1}{2} (2\Omega-1)(2\Omega)^{\frac{1}{2}} \delta_{k'',0} \delta_{q'',0} = 0 \quad . \end{aligned} \quad (\text{A.15})$$

The Casimir invariant is regained for $k'' = 0$. An independent relation is obtained by using $k'' = 2$, namely

$$\begin{aligned} & \frac{1}{2} \sum_{k,k',q} (2k+1)(2k'+1) \left\{ \begin{matrix} k & k' & 2 \\ j & j & j \end{matrix} \right\} \left[\begin{matrix} k & k' & 2 \\ q & -q & 0 \end{matrix} \right] \left\{ B_q^k, B_{-q}^{k'} \right\} \\ & + \sum_{k,k',q} (-)^q (2k+1)^{\frac{1}{2}} (2k'+1)^{\frac{1}{2}} \left\{ \begin{matrix} k & k' & 2 \\ j & j & j \end{matrix} \right\} \left[\begin{matrix} k & k' & 2 \\ q & -q & 0 \end{matrix} \right] \left\{ A_q^{k+}, A_q^{k'} \right\} \\ & + (5)^{\frac{1}{2}} B_0^2 = 0 \end{aligned} \quad (A.16)$$

The usefulness of this equation to us depends upon the approximate validity of the identity when restricted to the values $k, k' \leq 2$. Our justification for this approximation stems from the consideration of Eq. (2.24) for the case $I = 0$ when it becomes

$$\begin{aligned} & 2 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} A^2(0,2) A^2(2,2) + 5 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} B^2(2,0) B^2(2,2) \\ & = (2/5\Omega)^{\frac{1}{2}} A^0(0,0) [A^2(2,0) + A^2(0,2)] - \left[\frac{(\Omega-N)}{\Omega} + 50 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} \right] B^2(2,0). \end{aligned} \quad (A.17)$$

The validity of this relation in the seniority limit is now readily established by considering it as the sum of two parts.

One part, of the form

$$(2/5\Omega)^{\frac{1}{2}} A^0(0,0) [A^2(2,0) + A^2(0,2)] - [(\Omega-N)/\Omega] B^2(2,0) = 0 \quad (A.18)$$

can be derived from (2.14) and (2.15) for $I = 0$ and remains approximately valid for all regimes of coupling strength. The remaining relation

$$\begin{aligned}
& 2 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} A^2(0,2) A^2(2,2) + 5 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} B^2(2,0) B^2(2,2) \\
& = - 50 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\}^2 B^2(2,0) .
\end{aligned} \tag{A.19}$$

is exactly satisfied in the seniority limit, as one verifies from the results quoted in Sec. B of this appendix.

This demonstration, which for one thing, is valid only for the ground state, implies strongly that the tensor relation will be useful at most up to the phase transition and is not to be trusted beyond. As will be shown in our next paper in this series, it is incompatible with the expression of a well-defined and rigid quadrupole deformation.

B. MATRIX ELEMENTS IN THE SENIORITY LIMIT.

Matrix elements in the seniority limit connecting the ground state of seniority, $s = 0$ to states with $s = 2$ can be obtained directly from a chain calculation based on the algebra. Confining ourselves to the matrix elements of interest to us in the present paper, we used equations obtained from the commutators for $k \leq 2$. These are listed below:

$$A^0(0,0)^2 - A_{<}^0(0,0)^2 = \frac{(\Omega - N + 2)}{\Omega} , \tag{A.20}$$

$$A^2(2,0)^2 - A_{<}^2(0,2)^2 = \frac{5(\Omega - N + 2)}{\Omega} , \tag{A.21}$$

$$\frac{A^0(2,2)}{\sqrt{5}} A^2(2,0) - A_{<}^0(0,0) A_{<}^2(2,0) = -\sqrt{\frac{10}{\Omega}} B_{<}^2(2,0) , \tag{A.22}$$

$$B^2(2,0) A^0(0,0) - \frac{A_{<}^0(2,2)}{\sqrt{5}} B_{<}^2(2,0) = \sqrt{\frac{2}{5\Omega}} A^2(2,0) , \quad (\text{A.23})$$

$$A^0(0,0) A^2(0,2) - \frac{A_{<}^0(2,2)}{\sqrt{5}} A_{<}^2(0,2) = -\sqrt{\frac{10}{\Omega}} B_{<}^2(2,0) , \quad (\text{A.24})$$

$$A^2(0,2) B_{<}^2(2,2) - B^2(2,0) A^2(2,2) = 10 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} A^2(0,2) , \quad (\text{A.25})$$

and

$$A^2(2,0) B^2(2,2) - B_{<}^2(2,0) A^2(2,2) = -10 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} A^2(2,0) .$$

The lesser sign (<) attached to some of the reduced matrix elements means that these refer to the (N-2) particle system rather than to the N particle system.

The operators $A_o^{0\dagger}$ and A_o^0 cannot change the seniority of the states. On the other hand $A_q^{2\dagger}$, A_q^2 and B_q^2 can change the seniority or the angular momentum of the states by as much as two units.

Because of these seniority selection rules, and because of angular momentum coupling, we see that all the sums over intermediate states in the equations above are reduced to one term. This makes the equations exact in the seniority scheme.

We solve this system of equations by induction. We first solve the equations for the $N = 2$ system; in this case we know the lesser quantities are zero. Then we solve successively the equations for the systems with 4 and 6 particles. From these partial results we can induce the general form of the solution for an arbitrary system with an even number of particles. This finally

yields the following expressions:

$$A^0(0,0) = \left[\frac{N(2\Omega - N + 2)}{4\Omega} \right]^{\frac{1}{2}}, \quad (A.27)$$

$$B^2(2,0) = \left[\frac{N(2\Omega - N)}{2\Omega(\Omega - 1)} \right]^{\frac{1}{2}}, \quad (A.28)$$

$$A^2(2,0) = \left[\frac{5}{4} \cdot \frac{(2\Omega - N + 2)(2\Omega - N)}{\Omega(\Omega - 1)} \right]^{\frac{1}{2}}, \quad (A.29)$$

$$A^2(0,2) = - \left[\frac{5}{4} \cdot \frac{N(N-2)}{\Omega(\Omega-1)} \right]^{\frac{1}{2}}, \quad (A.30)$$

$$A^0(2,2) = \left[\frac{5(N-2)(2\Omega - N)}{4\Omega} \right]^{\frac{1}{2}}, \quad (A.31)$$

$$A^2(2,2) = 10 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} \frac{1}{\Omega - 2} \left[\frac{5(N-2)(2\Omega - N)}{2} \right]^{\frac{1}{2}}, \quad (A.32)$$

and

$$B^2(2,2) = - 10 \left\{ \begin{matrix} 2 & 2 & 2 \\ j & j & j \end{matrix} \right\} \frac{\Omega - N}{\Omega - 2}. \quad (A.33)$$

These results are of use to us as starting values in the numerical procedures. Prior to that, however, they serve to verify our assertions in Section II and in Sec. A of this appendix concerning the validity of Eqs. (2.23) and (2.24) of our scheme.

C. OBLATE-PROLATE DEFORMATION

In this section we shall show that our algebraic solutions exhibit an oblate or a prolate shape depending on whether $N < (2j+1)/2$ or $N > (2j+1)/2$. The transition from oblate to prolate shape is usually associated with a change of sign in the intrinsic quadrupole moment. We shall demonstrate that in general

all the matrix elements of the even multipole operators have a different sign, depending on whether the particle number is below or above the mid-shell point.

The solution for the second half of the shell is obtained from the solution in the first half using particle-hole conjugation. Let the operators $b_m^\dagger$ and b_m be the creation and annihilation operators for holes in a j -shell. They are related, through particle-hole conjugation, to the fermion operators of creation and annihilation of particles $a_m^\dagger$ and a_m by the equivalences

$$\begin{aligned} a_m^\dagger &\rightarrow (-)^{j-m} b_{-m} \quad , \\ a_m &\rightarrow (-)^{j-m} b_{-m}^\dagger \quad , \end{aligned} \quad (\text{A.34})$$

Applying these rules to the operators $A_q^{k\dagger}$, A_q^k and B_q^k yields the following transformation rules

$$\begin{aligned} A_q^{k\dagger} &\rightarrow (-)^{k+q} \sigma_{-q}^k \quad , \\ A_q^k &\rightarrow (-)^{k+q} \sigma_{-q}^{k\dagger} \quad , \end{aligned} \quad (\text{A.35})$$

and

$$B_q^k \rightarrow 2\Omega \delta_{k,0} - (-)^k \beta_q^k \quad . \quad (\text{A.36})$$

Here the script operators $\sigma_q^{k\dagger}$, σ_q^k and β_q^k have the following definitions

$$\begin{aligned} \sigma_q^{k\dagger} &= \frac{1}{\sqrt{2}} \sum_m \begin{bmatrix} j & j & k \\ m & q-m & q \end{bmatrix} b_m^\dagger b_{q-m}^\dagger \quad , \\ \sigma_q^k &= \frac{1}{\sqrt{2}} \sum_m \begin{bmatrix} j & j & k \\ m & q-m & q \end{bmatrix} b_m b_{q-m} \end{aligned} \quad (\text{A.37})$$

According to (A.36) the particle-number operator $\hat{N}$ is related to the hole-number operator $\hat{N}_h$ by the transformation rule

$$\hat{N} = 2\Omega - \hat{N}_h. \quad (\text{A.39})$$

Equation (A.36) has an obvious interpretation: The odd multipole operators and the even multipole operators with $k \neq 0$ transform respectively without and with a change of sign into the odd and even hole-multipole operators. Thus, any matrix element of an even multipole operator will undergo a change of sign under particle-hole conjugation.

To complete the proof that this change of sign of the matrix element of the even multipole operator is the only observable consequence of particle-hole conjugation, we need to show that the algebra is invariant and that the Hamiltonian is invariant up to a multiple of N . That the algebra is invariant follows from the fact that the fermion anticommutation relations are invariant under (A.34) (but, of course, can be proved directly). For the Hamiltonian we obtain (including a single-particle term)

$$\begin{aligned} H &= \epsilon \hat{N} - G\Omega A_0^{o\dagger} A_0^o - \frac{1}{2} \times \sum_q (-)^q B_q^2 B_{-q}^2 \\ &= \epsilon (2\Omega - \hat{N}_h) + 6(\Omega - \hat{N}_h) - 6\Omega a_0^{o\dagger} a_0^o \\ &\quad - \frac{1}{2} \times \sum_q (-)^q B_q^2 B_{-q}^2, \end{aligned} \quad (\text{A.40})$$

which has the required property.

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Figure Captions

- Fig. 1. Comparison between the reduced matrix elements $A^0(0,0)$ and $B^2(2,0)$ as calculated exactly and by the variational approach. The configuration is $(21/2)^6$.
- Fig. 2. The energy difference between the $I = 4$ and the $I = 2$ states as calculated by the variational approach compared with the results of the exact calculation. Curves 1 and 3 correspond respectively to the energy difference between the $I = 2$ state and the states evolving from the $I = 4, S = 4$ and $I = 4, S = 2$ states in the pairing limit. Curve 2 is the variational result. The configuration is $(17/2)^4$.
- Fig. 3. Comparison of values of the reduced matrix element $B^2(2,4)$ as calculated exactly and by the variational approach. Curve 1 is the variational result. Curves 2 and 3 represent respectively the transition between the $I = 2$ state and the states evolving between the $I = 4, S = 2$ and the $I = 4, S = 4$ states in the pairing limit. The configuration is $(17/2)^4$.
- Fig. 4. The reduced matrix elements $A^0(0,0)$, $A^0(2,2)/(5)^{\frac{1}{2}}$, $B^2(4,2)$ plotted versus the relative interaction strength. The transition from the spherical to the deformed nuclear shape is apparent. For comparison we illustrate the analytical result of Section III for the critical interaction strength at which the transition takes place. The configuration is $\Omega = 200$, $N = 104$.
- Fig. 5. Some of the normalized reduced matrix elements $A^0(I,I)/(2I+1)^{\frac{1}{2}}$ plotted versus the number of particles. The shell is $\Omega = 200$ and the relative interaction strength is $50\% = 0.76$. The analytical results of Section III predict that the transition from a spherical to a deformed nuclear shape takes place at $N = 102$.
- Fig. 6. Comparison between exact, algebraic, and BCS approximations to the matrix elements $A^0(0,0)$ and $B^2(2,0)$. The configuration is $(21/2)^6$.
- Fig. 7. Comparison between algebraic and BCS approximations to the matrix elements $A^0(0,0)$ and $B^2(2,0)$ for the configuration $\Omega = 200$, $N = 104$.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7