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SHAPE ISOMERS: MEAN-FIELD DESCRIPTION AND BEYOND⁺

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INTRODUCTION

Nuclear Hartree-Fock (HF) + BCS calculations have led to predictions of shape isomerism in isotopes of Pt, Hg and Os nuclei¹⁾. These have been confirmed through the observation of superdeformed rotational bands in ^{190, ..., 194}Hg. Encouraged by these measurements and similar observations in ¹⁹⁴Pb, we have extended these calculations to a wide range of contiguous nuclei. These HF results, for ^{192, 194}Pt, ^{190, ..., 198}Hg and ¹⁹⁴Pb, have been employed in a Generator Coordinate Method (GCM) calculation utilizing the quadrupole deformation as the generating variable²⁾. The resulting spectra confirm the conclusions drawn from the HF results and agree with those experiments which have been performed.

Adding a phenomenological assumption for the moments of inertia of our GCM states, we can construct the radiative transitions within and out of the superdeformed band. The results are in good agreement with the observed de-population of the superdeformed band built upon the shape isomer both in minimum angular momentum and in rapidity of de-population. Inferences for the existence of shape isomers will be drawn.

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MEAN FIELD CALCULATIONS

Our description is based upon the Hartree Fock (HF) mean field theory which can be derived from a variational principle where the energy

$$E = \langle \Psi | \hat{H} | \Psi \rangle / \langle \Psi | \Psi \rangle \quad (1)$$

is minimized for a given set of trial many-body wave-functions $|\Psi\rangle$. When all possible wave-functions are allowed, the exact many body Schödinger equation is recovered. To get the HF approximation, the variations are restricted to the Hilbert space built on Slater determinants only.

From an effective two-body force V_{ij} , which includes among other terms a spin-orbit force, a pairing interaction and the coulomb repulsion between the protons, the HF approximation constructs the mean one-body potential which averages the interactions of a given nucleon with all the others. The full many-body problem is reduced to the solution of the one-body HF equations,

$$h \varphi^\lambda = e^\lambda \varphi^\lambda \quad (2)$$

The HF hamiltomian, $h = t + U$, is the sum of a kinetic energy term and a mean field,

$$U(\mathbf{r}) = \int d^3r' v(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}') \quad , \quad (3)$$

which depends upon the solution of the HF equations through the density ρ . Due to this dependence the HF equations are non-linear. In addition, the mean field may be non local, depending upon the choice of the effective interaction. The solution of these equations yields both the single particle spectrum $\{e^\lambda, \varphi^\lambda\}$, and the total energy of the nucleus, $E = \sum_\lambda e^\lambda - \frac{1}{2} \sum_{\lambda\mu} V_{\lambda\mu}$, where the sum runs over occupied states only. The density matrix, $\rho_{\lambda\mu}$, built from the single particle spectrum, is used to calculate expectation values of one-body observables: $\langle \hat{A} \rangle = A_{\lambda\mu} \rho_{\mu\lambda}$. Finally, the many-body wave function representing the nucleus is a Slater determinant constructed on the occupied single particle orbitals φ_λ .

The HF energy being variational is guaranteed to be an extremum. However it may be only a local minimum. As the HF equations are non linear, they are solved iteratively from a suitable "first guess" of the converged solution. Depending on the starting point, it is a matter of experience that besides the absolute minimum, it is often possible to generate secondary local minima corresponding for instance to collective excitations of the nucleus.

To explore a given collective degree of freedom, such as the quadrupole deformation, it is convenient to generate a sequence of shapes evolving continuously from the ground state to an eventual secondary local minimum. For that purpose the two-body Hamiltonian $\hat{H}$ is replaced in the variational principal by the operator sometimes called the routhian $\hat{H} - \lambda \hat{Q}$, where $\hat{Q}$ is a collective operator

which generates the different shapes and λ the corresponding Lagrange multiplier. In general we choose for $\hat{Q}$ the quadrupole operator $\hat{Q} = (3z^2 - r^2)$. The resulting new HF equations read as:

$$(\hbar - \lambda \hat{Q}) \varphi^\lambda = e^\lambda \varphi^\lambda \quad (4)$$

The value of λ is adjusted so that the expectation value of the collective operator $\hat{Q}$ is equal to a desired value $q = \langle \hat{Q} \rangle$. For each choice of q , one obtains a Slater determinant which minimizes the energy. In particular, the energy is minimal with respect to any other unconstrained degrees of freedom, at least locally. This implies that no parametrization of higher multipoles of the nuclear shape has to be done.

In the calculations presented below, we have used Skyrme-type two-body effective interactions³⁾. This particular choice of interaction leads to a local mean field. In addition, we include in the Hamiltonian a term which describes the pairing correlations since they are known to be crucial for a description of nuclear collective motion. We choose the standard constant G pairing matrix element ansatz.

We solve the HF equations in coordinate space according to the discretization procedure described in Ref. 4. The collective space is mapped through doubly constrained HF calculations defined by the quadrupole deformation q and the asymmetry angle γ . These two parameters are adapted to the description of any axial and non-axial ellipsoidal nuclear shape.

In fig. 1, we have drawn the quadrupole deformation energy curve for ^{194}Hg with the Skyrme interaction SkM*⁵⁾. Only the axial degree of freedom is investigated so that $\gamma = 0^\circ$ for the prolate deformations ($q > 0$) and $\gamma = -180^\circ$ for oblate ones ($q < 0$). The curve exhibits three local minima. The absolute minimum is oblate and slightly deformed ($q \approx -10$ b). On the prolate side ($q \approx 8$ b) there is a second minimum whose excitation energy is about 1.0 MeV. At a much larger deformation ($q \approx 44$ b), there is a third minimum 5.0 MeV above the absolute minimum and separated from the main well by a barrier of 2.2 MeV (see Ref. 6).

These predictions have been verified through the observation of superdeformed (SD) bands extending to low angular momentum in the Hg nuclei^{7,8)}. They are qualitatively consistent with the model calculation of Pashkevitch in 1969 (Ref 9), with more recent calculations^{10,11)} and with the mean field calculations of the Gogny group¹²⁾.

Fig. 2a,e displays a more complete survey of the Hg isotopes. The deformation energy curves (solid lines) are obtained from our HF+BCS calculations using the axial quadrupole constraint described above and the same SkM* interaction⁵⁾. The ground state configuration is associated with the absolute minimum. For each five isotopes, a secondary minimum occurs at a rather large deformation corresponding to a mass quadrupole moment of approximately 44 b. This deformation corresponds to a typical value of the β_2 parameter of 0.5,

or equivalently to a 1.6 to 1 axis ratio of the ellipsoidal shape of the nuclear density. On the basis of these static calculations, one can identify these nuclei whose second minimum corresponds to an isomeric state which will ultimately decay electromagnetically.

The indirect confirmation of this assumption^{7,8)} through the experimental observation of the SD decay has led us to make an extensive study of the mass region ranging from Gadolinium nuclei up to Radium. The choice of this mass region is twofold. First these nuclei are heavy enough so that shape isomerism will occur at low spin: no additional centrifugal force is required to stabilize them as in the case of those Dysprosium isotopes which exhibit SD rotational bands which terminate at angular momentum above $20\hbar$. On the other hand, they must not be too heavy otherwise spontaneous fission will take over and we would enter the known region of fission isomers. The occurrence of a second well deformed minimum for many nuclei in this mass region is a theoretical common pattern: fig. 3 presents our results for the region which we call the isthmus of shape isomerism. It may be used as an indication of candidate nuclei for the experimental observation of shape isomerism.

BEYOND THE MEAN FIELD

The generator coordinate method (GCM) is the next term of the Hartree-Fock theory which incorporates collective and single-particle dynamics into a coherent quantum mechanical formulation. Given a family of N-body wave functions $|\Phi(q)\rangle$, depending on a collective continuous variable q , the GCM determines approximate eigenstates of the Hamiltonian $\hat{H}$ having the form:

$$|\Psi_k\rangle = \int dq f_k(q) |\Phi(q)\rangle \quad . \quad (5)$$

The weight functions f_k are found by requiring that the mean energy (1) calculated with $|\Psi_k\rangle$ is stationary with respect to arbitrary variations δf_k . This prescription leads to the Hill-Wheeler (HW) integral equation¹³⁾

$$\int (\mathcal{H}(q, q') - E_k \mathcal{J}(q, q')) f_k(q') dq' = 0 \quad , \quad (6)$$

in which the Hamiltonian ($\mathcal{H}$) and the overlap kernel ($\mathcal{J}$) are:

$$\mathcal{H}(q, q') = \langle \Phi(q) | \hat{H} | \Phi(q') \rangle \quad , \quad \mathcal{J}(q, q') = \langle \Phi(q) | \Phi(q') \rangle \quad . \quad (7)$$

The HW equation is solved by using the generating states $|\Phi(q)\rangle$ defined for a finite set of deformations q_i ⁶⁾, and discretizing the integrals in (5) and (6). One

obtains a discrete approximation to the GCM, where kernels become matrices, and the integral equation (6) a matrix equation.

All the numerical problems related to the solution of the HW equations have been addressed to in Ref. 6. The same two-body Hamiltonian is used in the HF+BCS calculations and in the construction of the kernel (7). Since HF+BCS wave functions are not eigenstates of the particle number operator, the GCM states may not have the correct particle number. To restore it, one introduces additional constraints on the neutron and proton particle number operators in the GCM Hamiltonian kernel, with appropriate Lagrange multipliers.

Let us note that the GCM incorporates automatically the effects of ingredients of the Bohr collective Hamiltonian^{14,4)} method such as the zero point motion energy and the effective collective masses. Moreover, it does not rely on assumptions such as the gaussian overlap approximation nor on the validity of quadratic expansions of the kernels¹⁵⁾ which are often used to derive microscopically these ingredients¹²⁾.

The short horizontal bars in fig. 2a,e show the results of the diagonalization of the HW equations for five Hg isotopes ($N = 110 - 118$). The ordinate is the total energy of the states (where the GCM ground state is taken as zero) and the abscissa of the center of the bar the average of the quadrupole moment for that particular state. The energy shifts of the two HF minima relative to their corresponding GCM states are nearly equal. This means that the excitation energy of the shape isomer as predicted from static HF calculations is not significantly modified by the collective correlations induced by configuration mixing.

The modifications of the deformation energy curves as a function of N strongly affect the shape isomeric state. In fig. 2a,e the vertical dotted lines point to the mass quadrupole moment of the second well minima. One notes that the mean value $\langle \hat{Q} \rangle$ of the best superdeformed candidate amongst the GCM eigenstates (vertical arrow on the Q axis) is close to that of the HF+BCS minima at large N and slowly moves toward lower Q as neutrons are removed. This phenomenon can be understood by the changes as a function of N in the thickness and height of the barrier separating the first and second well. The smaller of either of these quantities, the more likely the GCM will mix HF states of comparable energy in the first and second well, shifting the shape isomer toward smaller deformations.

Assuming that the moment of inertia of the shape isomer is given by the rigid body value, our calculations reproduce the band head moment of inertia inferred from the recent measurements on $^{190-194}\text{Hg}$. Moreover, our results are compatible with the observation of ^{192}Hg and ^{194}Hg having the same moment of inertia while that measured in ^{190}Hg is slightly smaller¹⁶⁾. Concomitantly, we predict that the moment of inertia for the SD band in ^{196}Hg and ^{198}Hg should be the same as observed in ^{192}Hg and ^{194}Hg .

DEPOPULATION OF THE SUPERDEFORMED BANDS

From this study, it is possible to make predictions on the de-excitation rates in and out of the superdeformed band. A necessary ingredient for that purpose is the set of matrix elements of the charge quadrupole operator. It can be calculated within the GCM, assuming that the rotational states can be described as a product of a collective rotor times an intrinsic state.

In addition, we introduce phenomenological estimates of the moments of inertia of the bands in order to allow an extrapolation of the GCM results to non-zero spin states. For the SD band, we choose the rigid body moment of inertia^{17,18)}. We then assume that the collective GCM states at smaller values of the quadrupole moment are band heads for rotational bands which function as doorways at the appropriate values of the angular momentum. From the choice of the moment of inertia for each band, one constructs a rotational spectrum based on GCM states in the first well. The moment of inertia $\mathcal{J}_k$ of a given band k is chosen phenomenologically²⁾ according to:

$$\mathcal{J}_k = \sqrt{a^2 + b^2(Q_k/Q_{SD})^2} \quad , \quad (8)$$

where $Q_k = \langle \Psi_k | \hat{Q} | \Psi_k \rangle$ is the quadrupole moment of the corresponding band head. The coefficients $a = 12.5\hbar^2/\text{MeV}$ and $b = 100\hbar^2/\text{MeV}$ have been selected to reproduce the rigid body moment of inertia at large Q and to have the order of magnitude suggested by experiment¹⁹⁾ at small Q . The last ingredient of the model is the energy E_k^{0+} of the first state of each band. It has been determined from the corresponding GCM intrinsic state energy E_k by subtracting the rotational energy:

$$E_k^{0+} = E_k - \frac{\hbar^2}{2\mathcal{J}_k} \langle \hat{J}^2 \rangle \quad . \quad (9)$$

In this formula $\langle \hat{J}^2 \rangle$ denotes the HF+BCS expectation value total angular momentum for quadrupole moment value of the band head.

From the calculated spectrum and using standard formulae for transition rates¹⁵⁾, we can follow the population of the SD band as a function of angular momentum, assuming it to be unity at $30\hbar$. Our results are shown on the right side of fig. 4 for the five Hg isotopes. A nearly complete depopulation of the SD bands occurs in two to three transitions and begins at about 8 to $14\hbar$. Both results appear qualitatively consistent with experiments in the Hg isotopes. The left side of fig. 4 displays the spectrum of depopulating γ -rays expected from our calculated transitions. The pattern changes systematically as a function of neutron number, with the predicted spectrum hardening with increasing N . If this is the correct mechanism for the emptying of the SD rotational band, then perhaps these γ -rays could be observed. However, the actual γ -ray spectrum may be more complicated since we expect the states in the first well to dilute their strength within states of the non-collective continuum. The resulting spreading will render more difficult the identification of the depopulating γ -rays.

The mechanism responsible for the sudden depopulation of the SD bands has its origin in the structure of the transition rates which are proportional to the square of the quadrupole transition matrix element and to the fifth power of the energy of the transition. The former dependence favors in band transitions whereas the second is responsible for the depopulation as soon as the energy of an out of band transition is large enough to overcome the smallness of the off-diagonal matrix elements of $\hat{Q}$.

It is relevant to be concerned that other than quadrupole transitions will alter our conclusions. However we believe that direct out of band $E1$ transitions will not be important as most of the observed dipole strength lies at too high an excitation energy to affect this process in the Hg isotopes. The situation might be quite different for the SD bands observed in the Dysprosium region since they have been observed to disappear at a much higher angular momentum and absolute energy.

CONCLUSION

Microscopic mean field theory calculations have been performed for nuclei ranging from Gadolinium to Radon and a large number of these isotopes are predicted to exhibit shape isomerism. Where experiments have been performed within this isthmus of isomerism through observation of superdeformed bands built upon these predicted shape isomers, they are completely consistent with the measurements. We have compared the energy and position in collective space of the GCM eigenstates with those obtained in static HF+BCS calculation. We conclude from this study that the excitation energy of the SD band head or shape isomer predicted from HF+BCS methods is almost unaltered by the introduction of quadrupole correlations. The next step in this theory, GCM, yields subtle variation in the moment of inertia of the observed SD rotational bands in the Hg isotopes which are consistent with experiment and correctly reproduces the observed rapid de-population and limiting angular momentum. This explanation of the sudden de-population of the SD band makes it unlikely that the SD band head can be reached through the direct feeding of high lying rotational states at high angular momentum. Alternative experiments involving a direct feeding of SD states at low spin will have to be implemented.

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HG194 - SKM*

Fig. 1. HF+BCS deformation energy curve of ^{194}Hg as a function of the quadrupole moment (b) with the SkM* interaction.

Fig. 2. HF+BCS deformation energy curves as a function of the quadrupole moment (b). The ordinate of the horizontal bars are the energies of the GCM states. The mid-segment abscissae give the GCM mean values of the quadrupole moment. The dashed vertical lines point to the HF+BCS SD minimum and the arrows to the GCM SD state. The interaction is SkM*.

2 MeV
3 MeV

Fig. 3. Isthmus of shape ismerism: excitation energies and well depths of secondary minima for various isotopes of even nuclei ranging from Gadolinium to Radium. Some isotopes of Thorium and Uranium are also shown for comparison. The lower (upper) part of each bar diagram corresponds to the excitation energy (well depth).

Fig. 4. Decay of the SD band for five Hg isotopes. Left side: relative intensities of the depopulating E2 gamma rays as a function of their energies. Right side: evolution of the population of the SD band as a function of angular momentum. The vertical arrow indicates the spin below which the SD band is excited with respect to at least one positive parity band.

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