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Shape coexistence in ^{151}Gd

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A microscopic justification of the experimental observation of shape coexistence in ^{151}Gd is given. The potential energy as a function of nuclear deformation in β-γ space is calculated. The Hartree-Bogoliubov method is used with the usual pairing-plus-quadrupole schematic interaction. The location of the potential minimum is strongly dependent on which single particle state the odd neutron occupies. Three distinct nuclear shapes are predicted in agreement with the data. The stability of these shapes is tested by a dynamic calculation.

[NUCLEAR STRUCTURE ^{151}Gd; calculated potential energy of shape; calculated shape stability.]

I. INTRODUCTION

The heavy rare earth nuclei appear to undergo a gentle shape transition from prolate to triaxial to oblate to spherical as their mass is increased from $A \approx 184$ to $A \approx 202$.[1] In contrast, the shape transition in the lighter mass ($N = 88$) region is believed to involve a sudden change from spherical to prolate.[1] However, a recent experiment[2] suggests that an odd nucleus in this region, ^{151}Gd (for which $N = 87$), has rotational bands built on intrinsic states with very different shapes. According to this experiment, a strongly deformed prolate shape is obtained when there is a neutron hole in the $0h_{11/2}$ configuration. However, a triaxial shape is obtained when the odd neutron is in the $0i_{13/2}$ configuration. Intrinsic states in which the odd neutron is in other configurations did not form rotational bands. The moments of inertia of the band built on the $i_{13/2}$ particle and the $h_{11/2}$ hole differ by approximately a factor of 2. This interesting phenomenon has been called[3,4] "shape coexistence."

It is the purpose of this paper to give a microscopic justification of the experimental results. An investigation is made of intrinsic states in ^{151}Gd for which the extra neutron is allowed to occupy the 8 Nilsson orbitals nearest in energy to the Fermi level. For each of these intrinsic states, the corresponding shape is determined by calculating the corresponding static potential energy surface using the pairing-plus-quadrupole force. In Sec. II, some details of this model are given. In Sec. III, the static potential surface for each of the intrinsic states is given. In Sec. IV, the role of collective dynamics is investigated. Finally, a summary and discussion follows in Sec. V.

II. THE MODEL

The usual pairing-plus-quadrupole model is extended to handle odd nuclei. For definiteness, only the case of an odd number of neutrons is described. The values of the spherical single particle energies e_s, the quadrupole-quadrupole force strength χ, and the pairing force strengths G_p and G_n are the same as those used by Kumar and Baranger.[1] The odd neutron is allowed to occupy any of the 8 Nilsson orbitals closest to the Fermi level, thereby blocking that level from the pairing correlations. For each blocked state, the Bardeen-Cooper-Schrieffer (BCS) equations are then solved for the (even) N-1 neutrons occupying the remaining unblocked states.

The Coriolis force will strongly mix the different Nilsson orbitals, especially at small deformations. For this reason the potential energies obtained by this method must be interpreted as the *diagonal* matrix elements of the potential of the coupling of an odd neutron to an even-even core of the Bohr-Mottelson type. A calculation involving this coupling is feasible. This point will be discussed in more detail later.

To map the potential energy surface, we first solve the one-body problem for a triaxial quadrupole field of arbitrary shape specified by parameters βc and γc. The Nilsson orbitals $|i\rangle$ are defined in a spherical harmonic oscillator basis $|s)$ by $|i\rangle = \sum_s c_s^{(i)} |s)$. The coefficients $c_s^{(i)}$ and the single particle energies ϵ_i are determined by solving

$$\sum_t [e_s\delta_{st} - \alpha\hbar\omega(\beta_c \cos\gamma_c \langle s|r^2Y_{20}|t\rangle + \beta_c \sin\gamma_c \langle s|r^2(Y_{22}+Y_{2-2})/\sqrt{2}\,|t\rangle)]\,c_t^{(i)} = \epsilon_i c_s^{(i)}, \quad (1)$$

where, following Kumar and Baranger,[1]

$\alpha \to \alpha_p = (2Z/A)^{1/3}$, for protons

$\alpha \to \alpha_n = (2N/A)^{1/3}$, for neutrons.

All units of length are expressed in terms of the oscillator length $(\hbar/m\omega)^{1/2}$.

If the exchange part of the interaction is neglected, the total energy can be written as

$$E_a(\beta_c,\gamma_c) = \sum_i v_{pi}^2\epsilon_{pi} + \sum_{i\neq a} v_{ni}^2\epsilon_{ni} + \epsilon_{na} - \Delta_p^2/G_p - \Delta_n^2/G_n + (\hbar\omega\beta_c\cos\gamma_c - \tfrac{1}{2}\chi Q_0)Q_0 + (\hbar\omega\beta_c\sin\gamma_c - \tfrac{1}{2}\chi Q_2)Q_2 . \quad (2)$$

In the above equation, a labels the blocked Nilsson orbital. The quantities ϵ_{pi} and ϵ_{ni} represent the Nilsson single particle energies for protons and neutrons respectively. The quantities v_{pi} and v_{ni} are the familiar single particle occupation amplitudes resulting from the solution of the BCS equations for protons and neutrons. The expectation values in the BCS state of the quadrupole operators are given by Q_0 and Q_2. More specifically,

$$Q_\mu = 2\alpha_p \sum_{i>0} v_{pi}^2 q_{pi}^{(\mu)} + 2\alpha_n \sum_{\substack{i>0\\ i\neq a}} v_{ni}^2 q_{ni}^{(\mu)} + \alpha_n q_{na}^{(\mu)}, \quad \mu = 0, 2 \quad (3)$$

where for the protons, for example,

$$q_{pi}^{(0)} = \langle i|r^2 Y_{20}|i\rangle \quad (4a)$$

and

$$q_{pi}^{(2)} = \langle i|r^2(Y_{22}+Y_{2-2})/\sqrt{2}\,|i\rangle \quad (4b)$$

and $i\rangle$ represents a proton Nilsson orbital. The notation $i>0$ refers to states of one time sense only.

We define the deformation parameters β and γ of the matter density by

$$\beta = \chi(Q_0^2 + Q_2^2)^{1/2}/\hbar\omega , \quad (5a)$$

$$\gamma = \tan^{-1}(Q_2/Q_0), \quad -\pi/2 \leq \gamma \leq \pi/2 . \quad (5b)$$

Then the energy defined by Eq. (2) can be expressed in terms of β and γ instead of in terms of the *field* parameters β_c and γ_c. The energy surface is stationary at a point of self-consistency:

$$\beta_c = \beta , \quad (6a)$$

$$\gamma_c = \gamma . \quad (6b)$$

In particular, this condition can be used to determine the location of the Hartree-Bogoliubov minimum.

III. RESULTS: STATIC POTENTIAL ENERGY SURFACES

Contour diagrams of the energy surface $E_a(\beta,\gamma)$ will be given for a representing one of the 8 neutron Nilsson orbitals near the Fermi level. The traditional scheme for labeling Nilsson orbitals cannot be used because the potential well is, in general, axially asymmetrical. We will consider a hole in the highest energy orbital arising from the spherical $0h_{11/2}$ configuration. We will also consider the lowest two orbitals from the $0i_{13/2}$ spherical configuration. These orbitals, in order of increasing energy, will be labeled $i_{13/2}\ \nu=1$ and $i_{13/2}\ \nu=2$. The spherical configurations $0h_{9/2}$ and $1f_{7/2}$ are strongly mixed by the quadrupole force. We will consider the 5 lowest energy orbitals arising from those spherical states. These orbitals will be labeled, in order of increasing energy, fh_ν, $\nu = 1, 2, 3, 4, 5$.

The contour diagrams are given in Fig. 1 and Fig. 2. The contour lines are labeled by absolute energies so that the different surfaces may be compared. The orbital having the minimum with the lowest energy is the fh_3 orbital. In all cases the energy minimum occurs for axially symmetric prolate deformation. But here the similarity ends. The $h_{11/2}$ state is much more strongly deformed than all the other states. This is in agreement with the data. Coriolis effects are expected to be small for a rotational band built on a prolate hole.[5] Hence a well formed $\Delta J = 1$ band is expected to be built on this state.

Table I contains the deformation energies and the prolate-oblate energy differences of the different intrinsic states. It can be seen that the $i_{13/2}\ \nu=1$ state has unique features. It is the only orbital which combines reasonable deformation energy (1.45 MeV) with considerable γ softness. This is in agreement with the suggestion of Smith *et al.*[2] They were able to obtain a good fit to their measured positive parity spectra by using

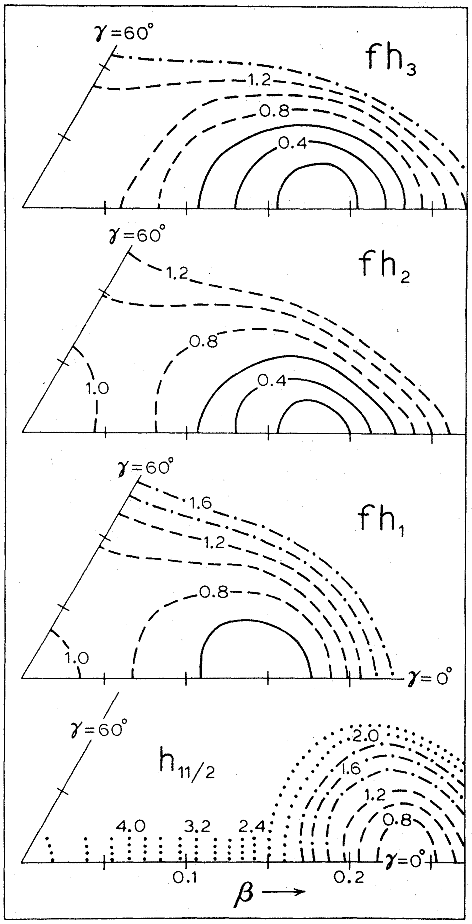

FIG. 1. Contour plot of absolute potential energy surface in β-γ space for 4 neutron orbitals. Labels on contours are in units of MeV.

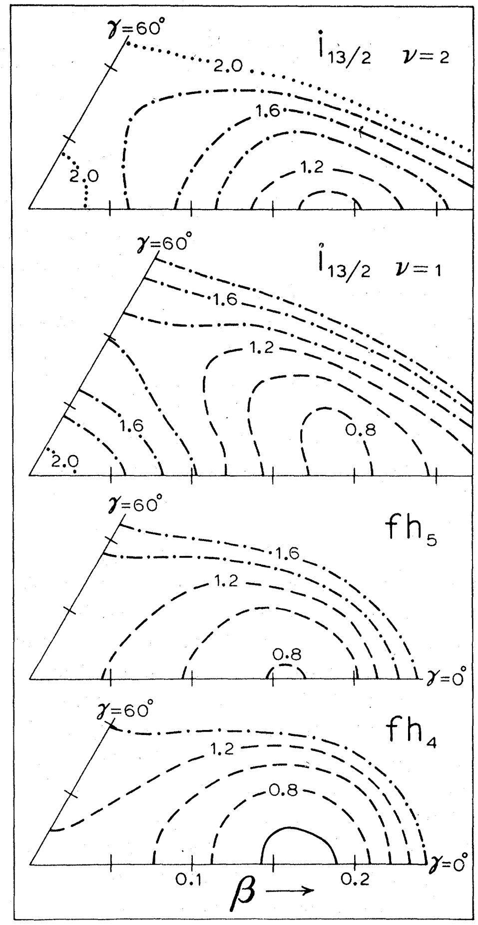

FIG. 2. See caption to Fig. 1.

TABLE I. Potential energy surfaces corresponding to the different neutron orbitals. E_{exc} gives the energy of the minimum of each energy surface relative to the minimum of the fh_3 surface. E_{def} is the energy difference between the stable prolate shape with $\beta = \beta_{pr}$ and a spherical shape. The prolate-oblate energy difference is $E_{op} - E_{pr}$.

Level	E_{exc} (MeV)	β_{pr}	E_{def} (MeV)	$E_{ob}-E_{pr}$ (MeV)
$h_{11/2}$	0.59	0.238	4.13	3.44
fh_1	0.40	0.148	0.68	0.47
fh_2	0.04	0.181	1.05	0.86
fh_3	0	0.187	1.10	1.06
fh_4	0.47	0.166	0.62	0.74
fh_5	0.73	0.155	0.57	0.57
$i_{13/2}$ $\nu=1$	0.66	0.192	1.45	0.67
$i_{13/2}$ $\nu=2$	0.89	0.185	1.23	0.92
^{151}Sm	...	0.242	3.54	2.38
^{153}Gd	...	0.245	3.75	2.47

the model of Meyer-ter-Vehn.[6] This involves coupling an $i_{13/2}$ neutron quasiparticle to a rigid triaxial rotor. The best fit in this calculation was obtained for $\gamma = 34°$ and $\hbar^2/2\mathcal{I}_0 = 0.0573$ MeV. Using a semiempirical expression for the inertial parameters,[7] this corresponds to a prolate deformation parameter $\beta_{pr} = 0.17$.

It would be nice to generalize the Meyer-ter-Vehn model to allow β and γ dynamics instead of using a rigid rotor. In fact such a calculation has been done by Leander[8] and applied to nuclei in the gold region of the periodic table. A class of potentials with an axially symmetric minimum but with differing γ softness was used in that calculation. It is interesting to compare Fig. 1(b) of that paper with Fig. 6(a) in the Meyer-ter-Vehn paper.[6] The similarity of the two energy level diagrams is remarkable. It seems reasonable to expect that a good fit to the sequence of positive parity levels in ^{151}Gd can be obtained by using the method of Leander[8] with the $i_{13/2}$ $\nu = 1$ potential in Fig. 2 of this paper. We repeat that an "asymmetric like" spectrum can be obtained from a particle coupled by a potential with an axially *symmetric* minimum provided that the potential is sufficiently γ soft.

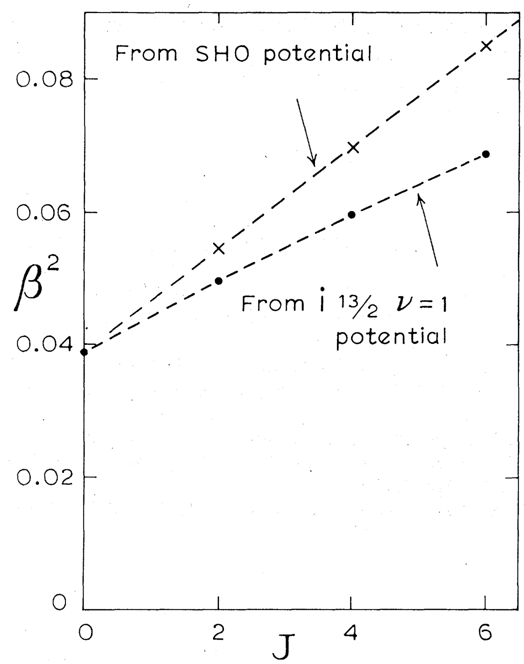

FIG. 3. Centrifugal deformation as a function of nuclear spin for an even-even nucleus with the $i_{13/2}$ $\nu = 1$ potential shown in Fig. 2.

IV. RESULTS: SHAPE DYNAMICS

The $i_{13/2}$ $\nu = 1$ potential has a static deformation energy of only 1.45 MeV. For this reason, the role of collective dynamics should be investigated. The rough calculation described below indicates that the collective vibrations will not alter the results of the previous section. The $i_{13/2}$ $\nu = 1$ potential was inserted into the Bohr-Mottelson[9,10] Hamiltonian appropriate to an even-even nucleus. The usual Bohr[9] inertial parameters were used with $B = 102/(\hbar^2 \text{ MeV})$. The resultant Schrödinger equation was solved numerically[11] to obtain the lowest few eigenstates. If the minimum of the potential is taken to have zero energy, the energy of the $J = 0$ state (i.e., the zero-point energy) is 1.64 MeV. This is slightly more than the deformation energy but not enough to "wash it out." For this potential, $(E_{J=4} - E_{J=0})/(E_{J=2} - E_{J=0}) = 2.14$. This is to be compared with $\frac{5}{2}$ which is the corresponding value for a potential which is β rigid and γ independent[12] and 2 which is the value for a spherical harmonic vibrator.[9]

There is considerable centrifugal stretching from the $J = 0$ to the $J = 4$ state. However, it is less than that for a simple harmonic oscillator as shown in Fig. 3. Actually the data of Smith *et al.*[2] indicate that a certain amount of centrifugal stretching takes place.

Aside from the $i_{13/2}$ $\nu = 1$ potential, there are other γ soft potentials shown in Figs. 1 and 2, especially the fh_1 potential. However, these potentials have such small deformations that a weak coupling scheme (not investigated in this work) would be more appropriate. The $i_{13/2}$ $\nu = 1$ state is the only one which displays both γ softness and reasonable deformation. The role of the orbital was investigated in the neighboring odd N nuclei ^{151}Sm and ^{153}Gd. The relevant parameters are given in the last two lines of Table I. It can be seen that in both cases, the potential is fairly γ hard. As a result, an "asymmetric like" positive parity band is not expected in these nuclei.

V. SUMMARY AND CONCLUSIONS

The transition from a spherical to a prolate shape in the light rare earth nuclei is more interesting than originally believed. This microscopic calculation supports the hypothesis that the odd transitional nucleus ^{151}Gd can exist in several different shapes. These shapes may be weakly deformed, strongly prolate, or reasonably triaxial. Which shape is taken depends on which orbital is occupied by the odd neutron.

If the odd neutron is in the lowest $i_{13/2}$ orbital (and only this orbital) the nucleus has a tendency to become triaxial. This interesting effect is not expected in neighboring nuclei differing by 2 neutrons. It would be interesting to ascertain if these peculiar effects are obtained with more realistic forces.

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