Statistical shape fluctuations in ^{166}Er

Alan L. Goodman
Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118
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Statistical shape fluctuations are calculated for ^{166}Er at spins 0 and 40$\hbar$. The fluctuations produce an average shape, which is distinct from the most probable (i.e., mean field) shape. At low temperatures the average shape is similar to the most probable shape, and the shape fluctuations are small. With increasing temperature the shape fluctuations increase, as does the difference between the average shape and the most probable shape. The fluctuations smooth out the sharp shape transitions predicted by mean field theories. Although the most probable phase at spin 40$\hbar$ and critical temperature 1.64 MeV is oblate noncollective rotation, the fluctuations create a high probability for prolate collective, prolate noncollective, and oblate collective rotations as well.

I. INTRODUCTION

The collective properties of hot nuclei can be characterized by appropriate order parameters. For example, the order parameters for the spherical-deformed transition are the shape multipole moments Q_{LM}. For the normal fluid-superfluid transition, the order parameter is the pair gap Δ. For the liquid-gas transition it is $\rho-\rho_c$, where ρ_c is the density at the critical point.

Consider a macroscopic system which is in an equilibrium state. Assume that the system is not at a critical point and not undergoing a first-order phase transition. Then the order parameters have specific well-defined values. These are the equilibrium, or most probable values which are determined by minimizing the appropriate free energy. There are statistical fluctuations in the order parameters, but they are negligible in the thermodynamic limit of large N. For example, the fractional fluctuation in the density is proportional to $1/\sqrt{N}$.

Next consider hot nuclei, which have finite N. The statistical fluctuations in the order parameters can create large deviations from the most probable state. It should be emphasized that these fluctuations would exist even if the exact density operator were known.

Hot nuclei are often described by mean field theories, such as the finite-temperature Hartree-Fock-Bogoliubov (HFB) cranking (FTHFBC) theory[1-3] or the Landau theory of phase transitions.[4-8] Since these theories are derived from variational principles, they approximate the equilibrium, or most probable values of the order parameters. For given temperature and angular momentum, the FTHFBC theory predicts specific well-defined values for Q_{LM} and Δ. For given temperature and pressure, the Landau theory predicts a specific value for $\rho-\rho_c$. (If the nucleus is in the transition region of a first-order phase transition, the order parameter can be multivalued.)

The mean field theories ignore the statistical fluctuations in the order parameter. Since N is finite, the fluctuations can be large. They can produce an average value for an order parameter which is qualitatively different from the equilibrium or mean field value.

For example, the Landau theory predicts a sharp first-order liquid-gas phase transition in nuclei for any temperature below a critical value T_c. However, when statistical density fluctuations are included, the transition is washed out for temperatures within several MeV of T_c.[6]

The FTHFB theory predicts that raising the temperature induces a sharp second-order transition from superfluid to normal fluid. However, when statistical fluctuations in Δ are included, this transition is smoothed out.[9,10] Similarly, the FTHFBC theory predicts that rotation can induce a sharp first-order transition from superfluid to normal fluid for any temperature below a critical value T_c. When statistical fluctuations in Δ are included, the transition is smoothed out for temperatures between $\sim\frac{1}{2}T_c$ and T_c.[10]

Next consider the shapes of hot nonrotating nuclei. The FTHFB theory[11-13] and the Landau theory[7] predict that a deformed nucleus will become spherical when the temperature is raised to a critical value T_c. Egido *et al.*[14] have studied the effects of statistical shape fluctuations in hot ^{158}Er nuclei at spin 0. When the shape fluctuations are included, the average shape of ^{158}Er retains a significant deformation even for temperatures above T_c.

Finally, we consider the shapes of hot rotating nuclei. The FTHFBC theory[15] and the Landau theory[8] predict that for ^{166}Er, increasing the temperature at fixed angular momentum produces a transition from a prolate shape rotating collectively to an oblate shape "rotating" noncollectively. The purpose of this article is to extend the calculations of Egido *et al.*[14] to include rotations. We will calculate the statistical shape fluctuations in hot rotating ^{166}Er nuclei. The resulting average shape will be compared with the FTHFBC shape.

There are several experimental techniques for investigating the shapes of hot rotating nuclei. These include measurements of the giant dipole resonance (GDR) built upon excited states,[16-18] alpha-gamma angular correlations,[19] and rotational damping.[20] Statistical shape fluctuations are important for interpreting GDR experiments.[18,21] Large fluctuations wash out the structure of the GDR and increase the GDR width. The shape of the GDR is a highly sensitive probe of the deformation energy surface. For example, experiments can discriminate between a shallow minimum for a spherical shape and a shallow minimum for a prolate shape.[22] This suggests that a fruitful interaction between theory and experiment can inform us about the shapes of hot rotating nuclei, even when the shapes are not sharply defined. Shape fluctuations may also cause the damping of nuclear rotational motion at modest temperatures ($\sim$0.5 MeV).[20,23]

II. STATISTICAL FLUCTUATIONS

For a nucleus with a given temperature T and angular momentum I, the equilibrium state is the state which minimizes the free energy

$$F=E-TS \ , \tag{1}$$

where S is the entropy. If the FTHFBC approximation is used with the pairing-plus-quadrupole (PPQ) Hamiltonian, then each state is characterized by the quadrupole deformation parameters β and γ and the pair gaps Δ_p and Δ_n. The FTHFBC approximation provides the free energy function $F(\beta,\gamma,\Delta_p,\Delta_n;I,T)$. For given I and T, the minimum in F defines the equilibrium or most probable state of the nucleus. This state is also determined by the self-consistent solution of the FTHFBC equation. If we are interested in shape fluctuations, but not fluctuations of the pair gap, we can consider the function $F(\beta,\gamma;I,T)$. For each combination of β and γ, it is implied that one chooses the values of Δ_p and Δ_n which minimize F for the given shape. In addition, for each combination of β and γ, the angular velocity ω is adjusted to yield the desired spin I, and the chemical potentials μ_p and μ_n are adjusted to give the correct proton and neutron numbers. It is assumed that the core nucleons are inert and have a spherical shape.

Statistical fluctuations can produce shapes which deviate from the equilibrium shape. The probability that a given shape occurs is

$$P(\beta,\gamma;I,T)\propto \exp[-F(\beta,\gamma;I,T)/T] \ . \tag{2}$$

For given I and T, consider an ensemble of nuclei with this distribution of deformations. The quadrupole deformation can also be characterized by the coordinates

$$a_0=\beta\cos\gamma \ , \tag{3}$$

$$a_2=\beta\sin\gamma \ . \tag{4}$$

The ensemble average of a_k is

$$\bar{a}_k=\langle a_k\rangle=\frac{\int a_k P(\beta,\gamma)\beta d\beta d\gamma}{\int P(\beta,\gamma)\beta d\beta d\gamma} \ . \tag{5}$$

The mean square fluctuation in a_k is

$$(\Delta a_k)^2=\langle a_k^2\rangle-\langle a_k\rangle^2 \ . \tag{6}$$

The volume element $\beta d\beta d\gamma$ is the infinitesimal area for the polar coordinates β,γ. Reference 21 uses this volume element. Reference 14 uses da_0da_2, which is equivalent to $\beta d\beta d\gamma$. Another choice for the volume element will be discussed in Sec. III.

The coordinates a_0 and a_2 refer to the deformation of the Hartree-Fock potential in the FTHFBC equation. The mass distribution is characterized by $\tilde{a}_0$ and $\tilde{a}_2$, which are proportional to the multipole moments $\langle Q_{20}\rangle$ and $\langle Q_{22}+Q_{2-2}\rangle$. The values of a_k and $\tilde{a}_k$ are equal only at the minimum of $F(\beta,\gamma;I,T)$. All figures are shown for a_k.

III. HOT NONROTATING NUCLEI

Shape fluctuations are calculated for ^{166}Er. In this section we consider nuclei which are heated but not rotating. Then one 60° sector of the β,γ plane describes all quadrupole shapes. The FTHFBC free energy $F(\beta,\gamma;I=0,T)$ is evaluated for mesh points with β ranging from 0 to 0.6 in steps of 0.05, and γ varying from 0° to 60° in steps of 10°. Sixteen temperatures are selected, varying from 0 to 1.4 MeV. For each combination of β, γ, and T, self-consistent pair gaps Δ_p and Δ_n are determined, and the chemical potentials μ_p and μ_n are adjusted to give the correct particle numbers Z and N.

The free energy $F(\beta,\gamma)$ is shown in Fig. 1 for various temperatures. The shape is prolate at $\gamma=0°$, and oblate at $\gamma=60°$. The dot in the center of the shaded region marks the state of minimum free energy which is the equilibrium, or most probable shape, i.e., $\beta_{\rm HFB},\gamma_{\rm HFB}$. The equilibrium shape is prolate for all temperatures below $T_c=1.74$ MeV. At $T=0$ the shape is very stiff in both the β and γ coordinates. For $T=1.0$ MeV the shape is softer in β and γ. At the critical temperature $T_c=1.74$ MeV, $\beta_{\rm HFB}=0$ and the equilibrium shape is spherical. The thermal excitations have almost eliminated the shell effects. The free energy contours are starting to resemble concentric arcs centered on the origin. This is the signature of a classical liquid drop.

Since $\gamma_{\rm HFB}=0°$ at all temperatures, then $a_0^{\rm HFB}=\beta_{\rm HFB}$. The function $a_0^{\rm HFB}(T)$ is shown in Fig. 2. The FTHFB theory predicts a sharp phase transition from a prolate shape to a spherical shape at T_c.

Statistical fluctuations create shapes which deviate from the equilibrium shape. Equation (2) gives the relative probability $P(\beta,\gamma)$ that the nucleus has a given shape. The probability distribution is shown in Fig. 3 for different temperatures. The normalization is chosen so that $P=1.0$ for the most probable state, i.e., $\beta_{\rm HFB},\gamma_{\rm HFB}$. At zero temperature there are no statistical fluctuations. For $T=1.0$ MeV the shape can deviate significantly from the equilibrium shape, fluctuating over a broad range in β and γ. Although the HFB shape is axially symmetric, fluctuations create triaxial shapes. At the critical temperature, $T_c=1.74$ MeV, the fluctuations extend over all values of γ and a wide range in β. Although the HFB shape is spherical, fluctuations create prolate, triaxial, and oblate shapes of varying degrees of deformation.

The statistical shape fluctuations create an average shape, defined by Eq. (5). Figure 2 gives the average quadrupole deformation $\bar{a}_0$. The solid line for $\bar{a}_0$ is calculated with the volume element $\beta d\beta d\gamma$. For $T<1.6$ MeV, $\bar{a}_0$ is very similar to $a_0^{\rm HFB}$. However, at higher temperatures $\bar{a}_0$ retains about one-half the ground state value, whereas $a_0^{\rm HFB}$ vanishes. The conclusion is that statistical shape fluctuations wash out the phase transition predicted by the FTHFB theory.

Since $\gamma_{\rm HFB}=0°$ at all temperatures, so does $a_2^{\rm HFB}=0$. The solid line in Fig. 4 shows the average $\bar{a}_2$. Gamma fluctuations are important even at low temperatures. When the temperature is 2.3 MeV, the average $\bar{\gamma}$ is 30°, which denotes the most triaxial shape.

It should be noted that the shape has been averaged over the $\gamma=0°$ to $\gamma=60°$ sector. However, for spin zero, $F(\beta,\gamma)=F(\beta,-\gamma)$ at all temperatures. Therefore, if the average shape would be calculated over the $\gamma=-60°$ to $\gamma=60°$ sector, then the average values $\bar{\gamma}$ and $\bar{a}_2$ would be zero at all temperatures.

The fluctuations Δa_0 and Δa_2 are given by the solid curves in Figs. 5 and 6. They increase rapidly as the temperature is raised to 1.4 MeV. At higher temperatures the fluctuations are relatively constant or decrease slightly.

Egido *et al.*[14] have applied the same analysis to ^{158}Er at zero spin. Their conclusions for ^{158}Er are essentially the same as ours for ^{166}Er. Statistical shape fluctuations create large deviations from mean field shapes at high temperatures. One difference is that ^{166}Er is more deformed than ^{158}Er at zero temperature. Consequently, the critical temperature for ^{166}Er, $T_c=1.74$ MeV, is higher than for ^{158}Er, $T_c=1.4$ MeV.

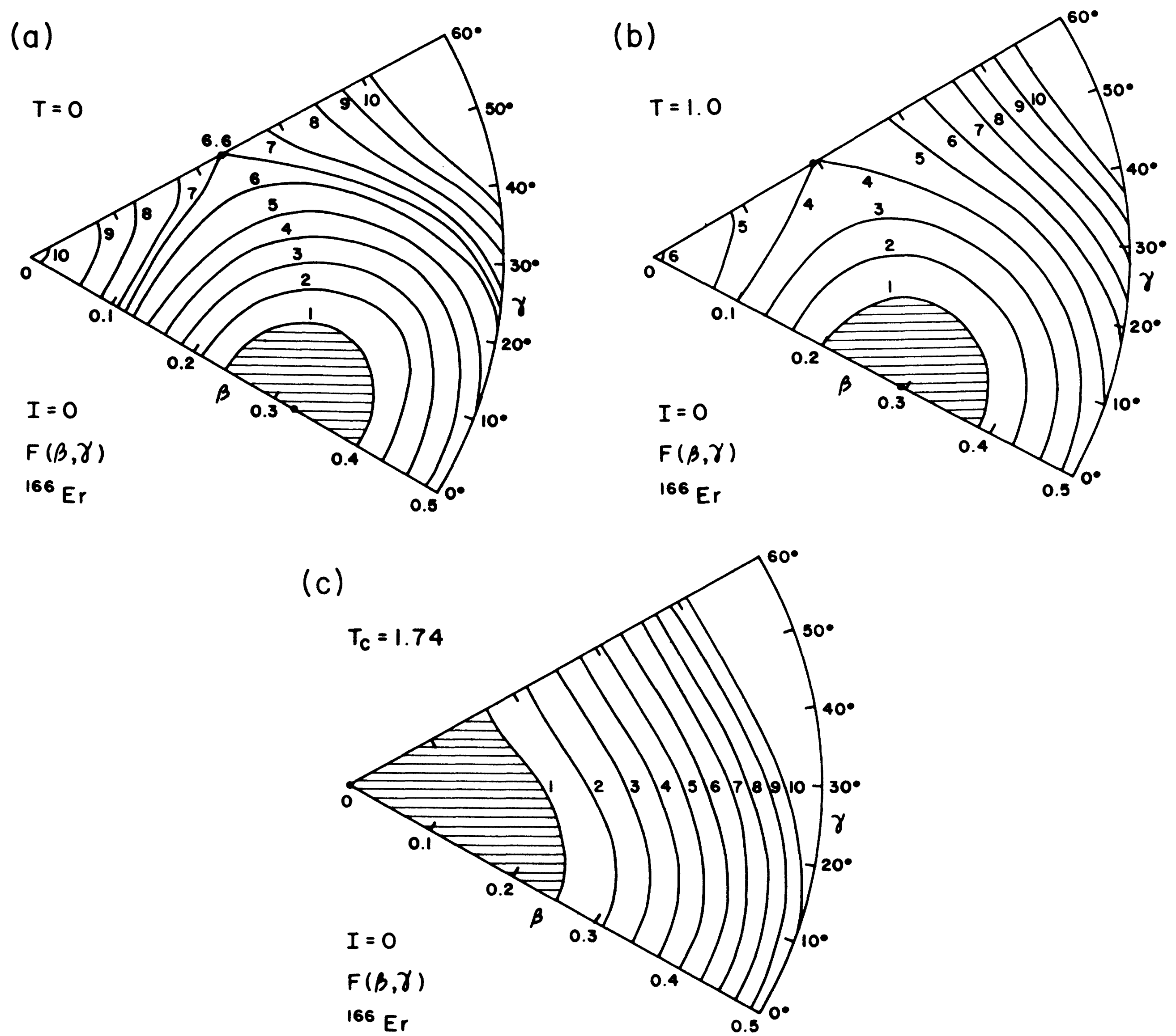

FIG. 1. Contour map of the free energy in the β,γ plane. The lines have constant values of F in units of MeV. Each map corresponds to a different temperature which has units of MeV. The nucleus is ^{166}Er. The angular momentum is zero.

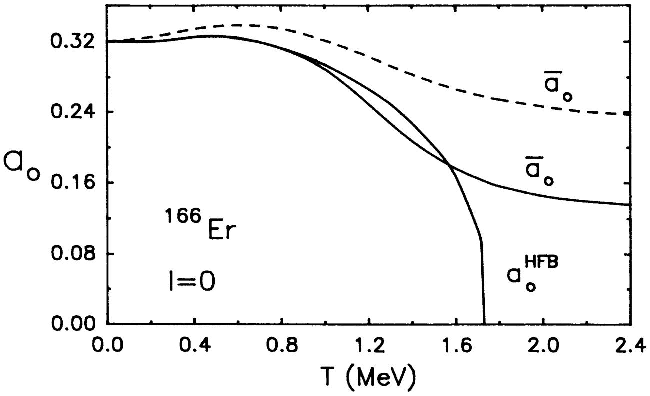

FIG. 2. The quadrupole deformation a_0 vs the temperature T at spin zero.

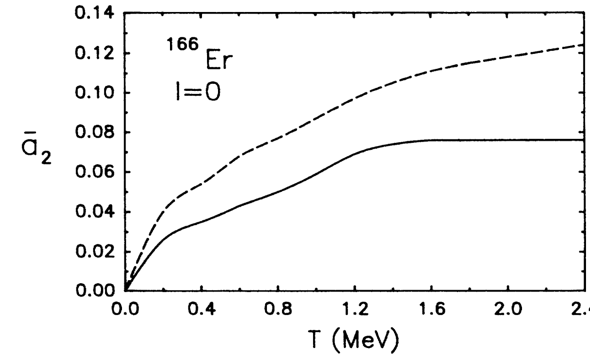

FIG. 4. The average quadrupole deformation $\bar{a}_2$ vs the temperature T at spin zero.

The average shape $\bar{a}_k$ has been calculated with the volume element $\beta d\beta d\gamma$, or equivalently $da_0 da_2$. The Bohr rotation-vibration model uses the volume element $\beta^4 \,|\sin 3\gamma\,|\, d\beta d\gamma$. We have also calculated the average shape produced by substituting this volume element into Eq. (5). The values of $\bar{a}_k$ and Δa_k are given by the dashed curves in Figs. 2 , 4 , 5, and 6. Observe that for all temperatures, this change in volume element barely affects the fluctuations Δa_0 and Δa_2. It causes an increase in $\bar{a}_0$ at high temperatures, and an increase in $\bar{a}_2$ at all temperatures. However, the essential conclusion remains the same. Statistical shape fluctuations wash out the shape transition predicted by the mean field theory.

IV. HOT ROTATING NUCLEI

The FTHFBC equation has been solved for ^{166}Er.[15] For any fixed positive spin, increasing the temperature causes a transition from prolate collective rotation to oblate noncollective rotation. In a collective rotation, the rotation axis is perpendicular to the symmetry axis. For a noncollective rotation, the axes coincide. The critical temperature for this transition is spin dependent. If $I=40\hbar$, then $T_c=1.64$ MeV. It should be emphasized that this shape transition refers to the most probable shape. The question addressed in this section is whether the statistical shape fluctuations affect this phase transition.

When the cranking model is used to describe rotating nuclei, three 60° sectors of the β,γ plane are required in order to specify the orientation of the rotation axis relative to the symmetry axis. The Hill-Wheeler convention for γ is chosen.[24] The angles $\gamma=-60°$, 0°, 60°, and 120° correspond, respectively, to oblate noncollective rotation, prolate collective rotation, oblate collective rotation, and prolate noncollective rotation.

Consider the spin $40\hbar$. The FTHFBC free energy $F(\beta,\gamma;I=40\hbar,T)$ is calculated for mesh points with β varying from 0 to 0.6 in steps of 0.05, γ varying from $-60°$ to 120° in steps of 10°, and 13 temperatures ranging from 0 to 2.4 MeV. At each mesh point the angular ve-

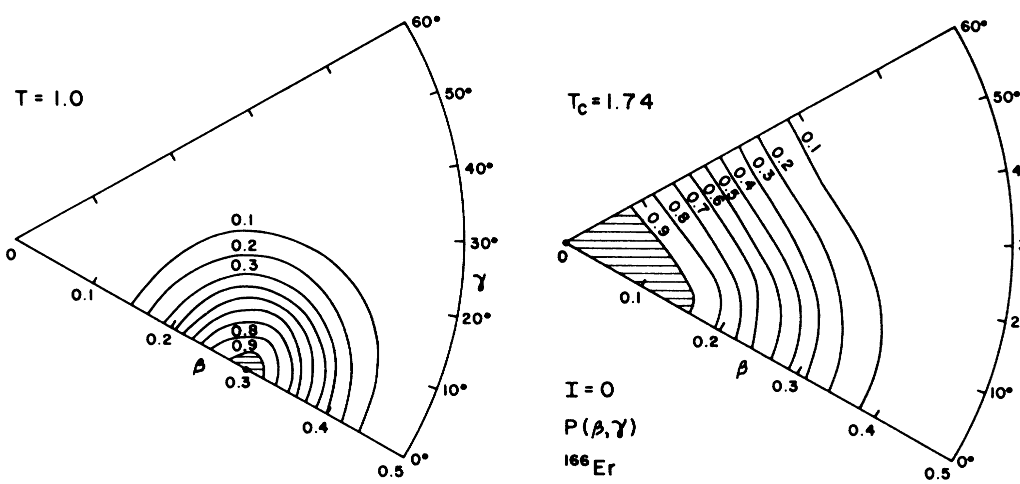

FIG. 3. Contour map of the shape probability distribution in the β,γ plane. The lines have constant values of probability. Each map corresponds to a different temperature, which has units of MeV. The angular momentum is zero.

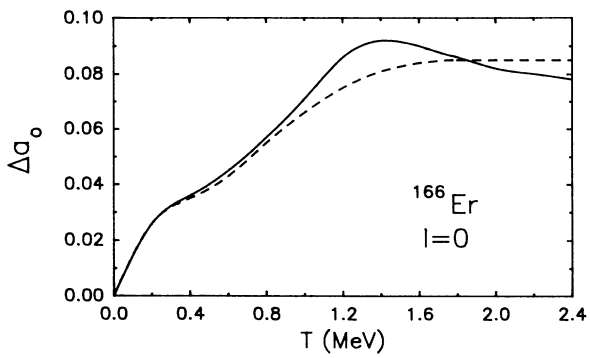

FIG. 5. The fluctuation in a_0 vs the temperature T at spin zero.

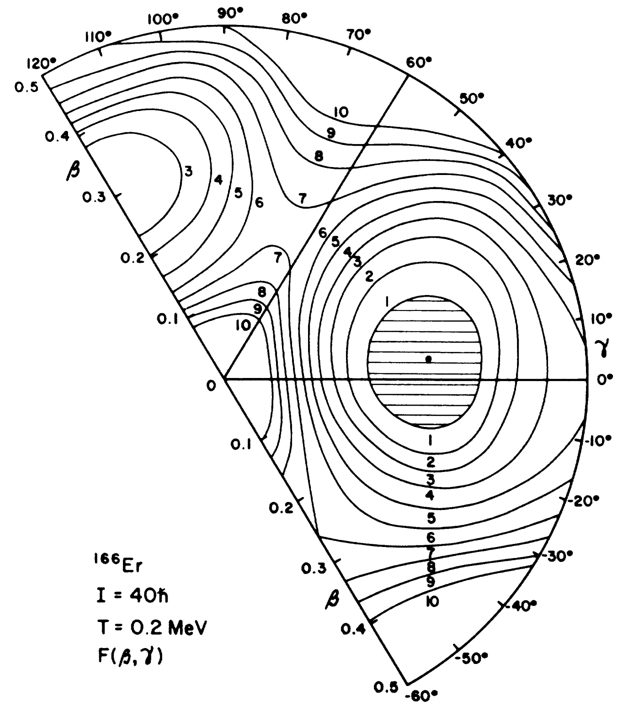

FIG. 7. See Fig. 1. The spin is $40\hbar$. The temperature is 0.2 MeV.

locity ω is adjusted to give the spin $I=40\hbar$, and the chemical potentials μ_p and μ_n are adjusted to give the correct Z and N.

At spin $40\hbar$ the neutron pair gap Δ_n is zero even at zero temperature, and the proton gap Δ_p vanishes at the very low temperature of 0.13 MeV. Although this statement refers to the pair gaps associated with the most probable shape, it is reasonable to neglect the pair correlations for all shapes at spin $40\hbar$. This substantially reduces the computation time.

The free energy $F(\beta,\gamma)$ for $I=40\hbar$ and $T=0.2$ MeV is shown in Fig. 7. The absolute minimum in F describes a nearly prolate shape rotating collectively. There is also a relative minimum for prolate noncollective rotation. Observe that the energy surface is very stiff in β and γ. Figure 8 is the shape probability distribution $P(\beta,\gamma)$. Because the temperature is low and the shape is stiff, the shape fluctuations are small. They deviate very little from the most probable shape.

Keep the spin fixed at $40\hbar$ and raise the temperature to 1.0 MeV. Figure 9 shows $F(\beta,\gamma)$. The equilibrium state still describes prolate collective rotation. However, the increased temperature has made the shape much softer with respect to γ fluctuations. The shape is also softer for decreases in β. Figure 10 is $P(\beta,\gamma)$. The shape fluctuations now extend over a considerably larger range in β and γ. Nevertheless, the fluctuations remain centered on the most probable shape.

For spin $40\hbar$ the critical temperature T_c is 1.64 MeV. Figures 11 and 12 display $F(\beta,\gamma)$ and $P(\beta,\gamma)$ for this temperature. The equilibrium state is an oblate shape rotating noncollectively. The thermal excitations of quasi-

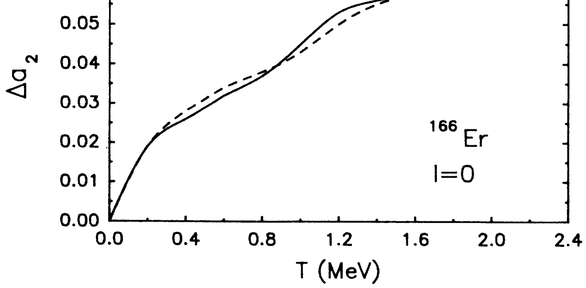

FIG. 6. The fluctuation in a_2 vs the temperature T at spin zero.

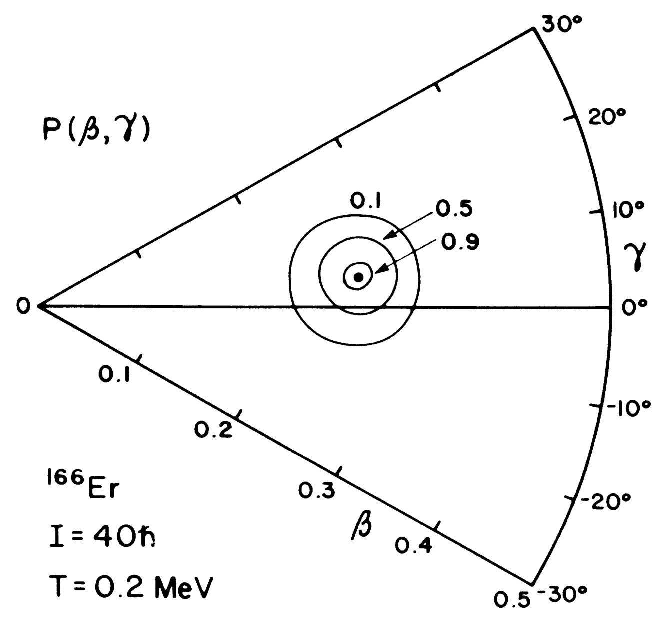

FIG. 8. See Fig. 3. The spin is $40\hbar$. The temperature is 0.2 MeV.

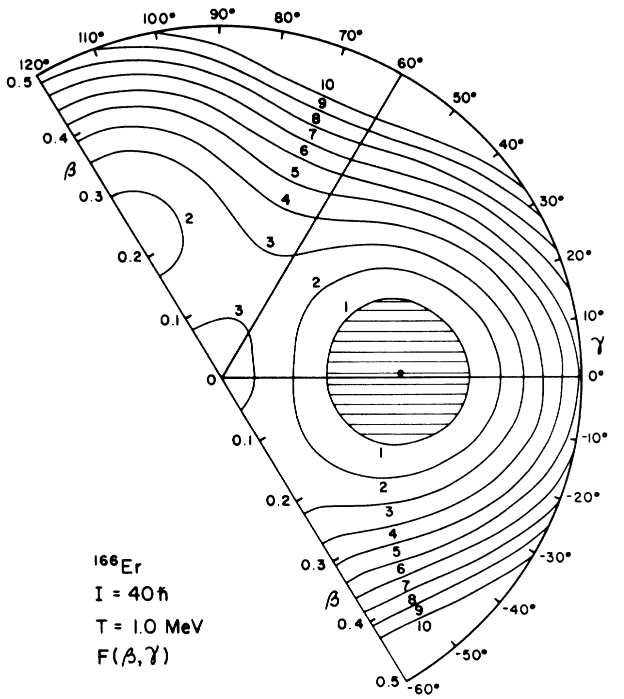

FIG. 9. See Fig. 1. The spin is 40ħ. The temperature is 1.0 MeV.

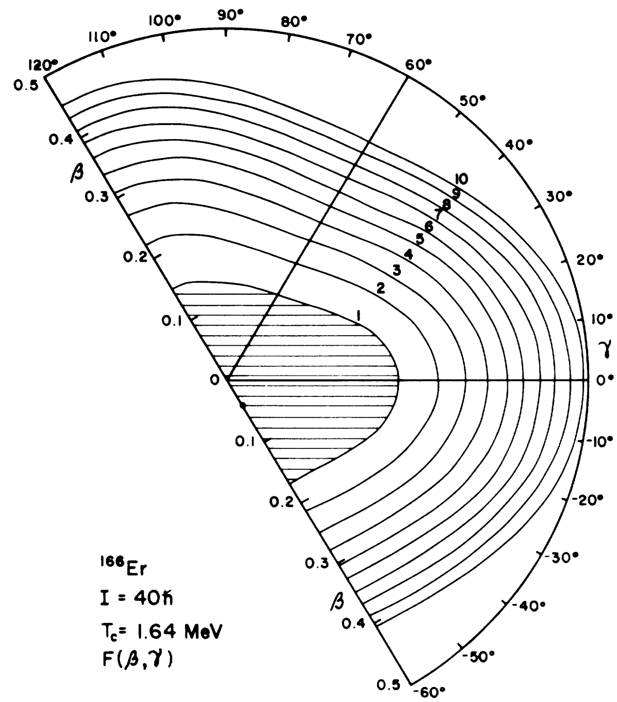

FIG. 11. See Fig. 1. The spin is 40ħ. The temperature is 1.64 MeV.

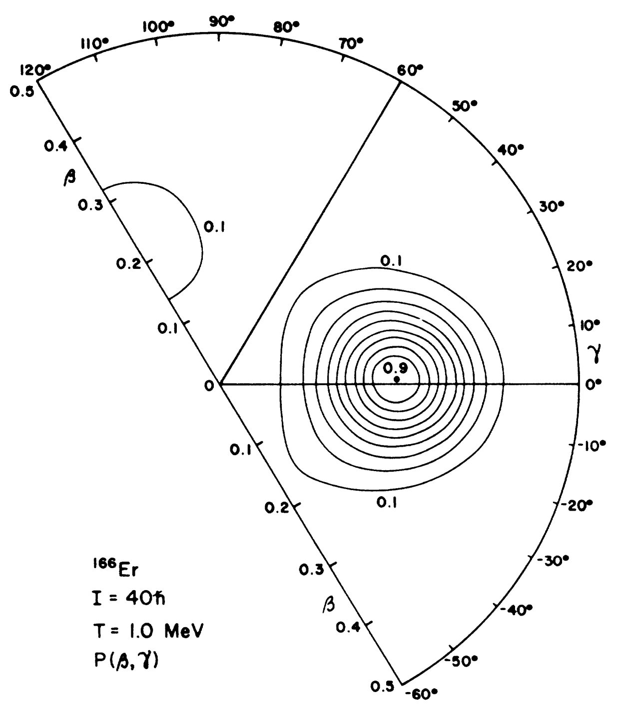

FIG. 10. See Fig. 3. The spin is 40ħ. The temperature is 1.0 MeV.

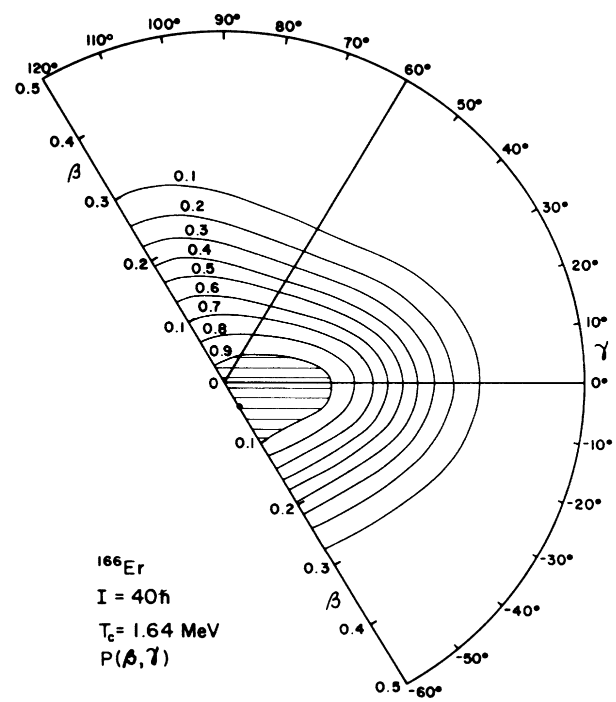

FIG. 12. See Fig. 3. The spin is 40ħ. The temperature is 1.64 MeV.

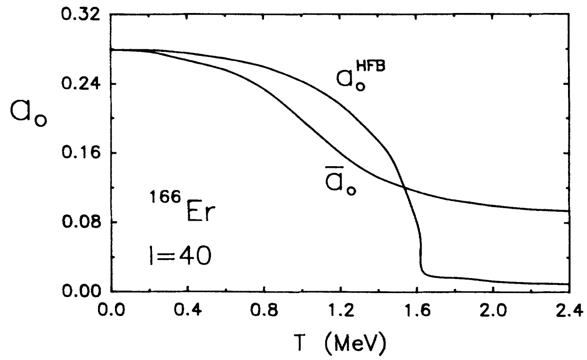

FIG. 13. The quadrupole deformation a_0 vs the temperature T at spin $40\hbar$.

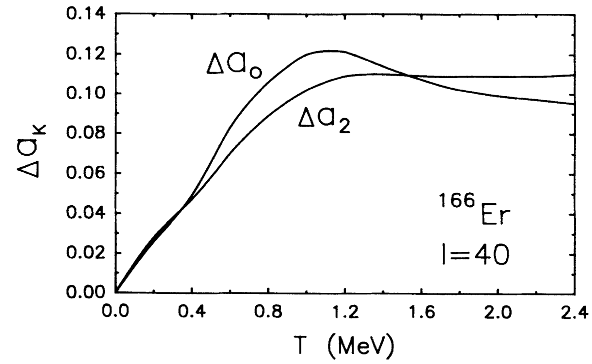

FIG. 15. The fluctuation in a_0 and a_2 vs the temperature T at spin $40\hbar$.

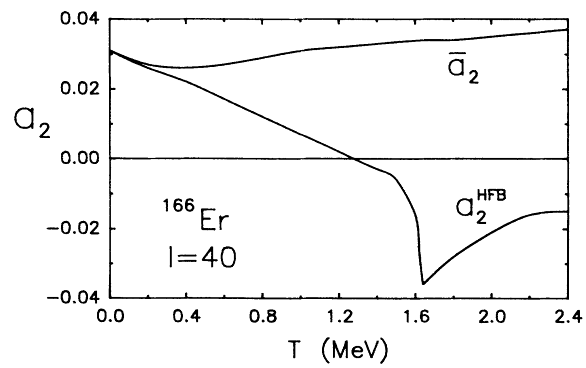

FIG. 14. The quadrupole deformation a_2 vs the temperature T at spin $40\hbar$.

particles have almost eliminated the shell structure. The free energy contours resemble those of a rotating liquid drop. Observe that the shape is extremely soft in γ, and very soft in β for $\beta<0.2$. Although the most probable phase is oblate noncollective rotation, the statistical fluctuations produce a high probability for also observing prolate collective, oblate collective, and prolate noncollective rotations.

The average quadrupole deformation $(\bar{a}_0,\bar{a}_2)$ is defined by Eq. (5). The range of integration in β is 0–0.6. The range in γ is $-60°-120°$. Figure 13 compares the average shape $\bar{a}_0$ to the most probable shape $a_0^{\rm HFB}$. They are similar for $T<1.6$ MeV. However, at higher temperatures the average value is much larger than the most probable value. Figure 14 gives the comparison for a_2. The most probable value $a_2^{\rm HFB}$ changes from positive to negative at high temperatures, with a cusp at $T_c=1.64$ MeV. This marks the transition from prolate collective rotation to oblate noncollective rotation. Because of the large shape fluctuations at high temperatures, the average value $\bar{a}_2$ does not change sign. The average shape produced by the statistical fluctuations does not pass through the phase transition which is displayed by the most probable shape.

The fluctuations Δa_0 and Δa_2 are given in Fig. 15. They increase with temperature up to $T\simeq 1.2$ MeV. At higher temperatures they show little change.

V. CONCLUSIONS

Because nuclei have finite particle numbers, statistical fluctuations in collective order parameters can be significant. For ^{166}Er the most probable shape at spin zero changes from prolate to spherical at a critical temperature $T_c=1.74$ MeV. However, statistical shape fluctuations create an average shape which does not become spherical at high temperatures. Similarly, at spin $40\hbar$ the most probable phase changes from prolate collective rotation to oblate noncollective rotation at $T_c=1.64$ MeV. However, statistical shape fluctuations lead to an average shape which does not pass through this transition.

These calculations do not include angular momentum projection. Investigations at zero temperature show that if the unprojected energy surface is gamma unstable, then spin projection leads to well-defined energy minima and stiffer shapes.[25] If this also occurs at finite temperature, then spin projection would considerably reduce the shape fluctuations.

The statistical fluctuations have been calculated for nuclei assuming a given temperature in the grand canonical ensemble. Before drawing final conclusions about the importance of these fluctuations, one should also calculate the fluctuations for nuclei with a given energy in the microcanonical ensemble.[26–28]

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