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# Temperature-induced deformation in $^{148}$Sm

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The finite-temperature Hartree-Fock-Bogoliubov equations are solved for $^{148}$Sm with the pairing-plus-quadrupole interaction. Although the static shape is spherical at zero temperature, raising the temperature induces a second-order phase transition to a prolate deformed shape. The onset of deformation is related to the thermal destruction of the pairing gap.

Many nuclei exhibit a static deformation. This departure from a spherical shape is attributed to shell effects. A nucleus in its ground state has a temperature of zero. If the temperature is increased sufficiently, then the thermal excitations wash out the shell effects,[1] and the static nuclear deformation vanishes.[2] Raising the temperature eliminates the deformation. This is the normal scenario.

In this article we give an example of the inverse effect: Although $^{148}$Sm is spherical at zero temperature, it acquires a deformation when the temperature is increased. This effect is described with the finite-temperature Hartree-Fock-Bogoliubov (FTHFB) equation.[3] This is a mean field theory in which the Hartree-Fock field $\mathscr{H}$ and the pair correlation field $\Delta$ are treated simultaneously and self-consistently. The FTHFB equation is

$$\begin{pmatrix} \mathscr{H} & \Delta \\ -\Delta^* & -\mathscr{H}^* \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix} , \tag{1}$$

where the eigenvalues $E_i$ are the quasiparticle energies. At finite temperature there is a statistical mixture of quasiparticle excitations. The quasiparticle occupation probability is

$$f_i = \frac{1}{1+e^{E_i/kT}} . \tag{2}$$

The mean fields $\mathscr{H}$ and $\Delta$ are temperature dependent. They are functions of $U$, $V$, and $f$.

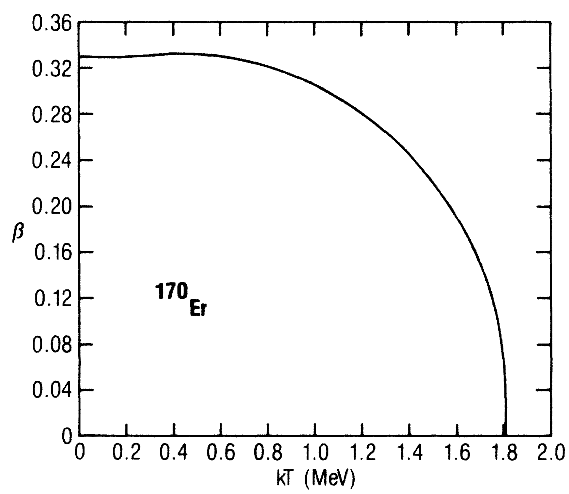


FIG. 1. The quadrupole deformation vs the temperature for $^{170}$Er.

The Hamiltonian is chosen as the pairing-plus-quadrupole (PPQ) Hamiltonian, as defined by Kumar and Baranger.[4] For axially symmetric shapes, the FTHFB potential in Eq. (1) has three degrees of freedom: the quadrupole deformation $\beta$, the proton pair gap $\Delta_p$, and the neutron pair gap $\Delta_n$. At each temperature Eq. (1) determines the values of $\beta$, $\Delta_p$, and $\Delta_n$ which minimize the free energy, $F=E-TS$, where $S$ is the entropy. The cranking term, $-\omega J_x$, is not included in Eq. (1), so these calculations are restricted to zero spin. The active valence space contains the $N=4, 5$ shells for protons and the $N=5, 6$ shells for neutrons.

For rare earth nuclei with $150 < A < 190$, the ground states have a static quadrupole deformation. For example, the shape of $^{170}$Er is prolate and axially symmetric. The FTHFB equations have been solved for $^{170}$Er. Figure 1 shows how $\beta$ varies with temperature. At zero-temperature $\beta = 0.33$. When $kT = 1.81$ MeV the deformation disappears in a second-order phase transition. Thermal quasiparticle excitations wash out the shell effects. This is the normal scenario mentioned above.

The nucleus $^{148}$Sm is a transitional nucleus. The ground state static shape is spherical. Figure 2 shows the FTHFB quadrupole deformation versus the temperature. The shape is spherical for temperatures below 0.40 MeV. When the temperature is raised above 0.40 MeV, the nucleus suddenly acquires a prolate deformation. This is a dramatic example of how increasing the temperature can turn a spherical shape into a prolate shape. When the temperature is 0.91 MeV, the thermal excitations overwhelm the shell effects. The deformation disappears, and the shape is once again spherical.

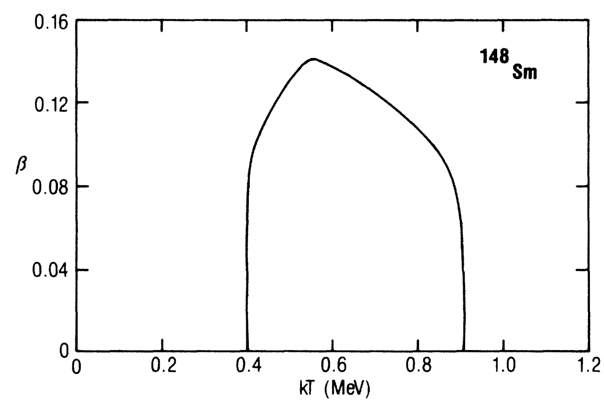


FIG. 2. The quadrupole deformation vs the temperature for $^{148}$Sm.

The nature of the phase transition at $kT = 0.40$ MeV is illuminated by considering the deformation free energy

$$F_{\rm def}(\beta,T) = F(\beta,T) - F(0,T) \ , \tag{3}$$

which is depicted in Fig. 3. At $T = 0$ the static shape is given by the minimum at $\beta = 0$. For $kT = 0.40$ MeV, $F_{\rm def}$ is nearly flat for $-0.05 < \beta < +0.10$. This is characteristic of a critical point, and large thermal shape fluctuations should be expected. At $kT = 0.6$ MeV, the minimum describes a prolate shape with $\beta = 0.14$. The inflection point at $\beta = 0$ is a metastable spherical state. Since there is only one minimum at each temperature, the spherical to deformed phase transition is second order.

What is the cause of the spherical to deformed transition at $kT = 0.40$ MeV? The pairing-plus-quadrupole Hamiltonian contains the two primary components of the nucleon-nucleon effective interaction. First there is the quadrupole-quadrupole ($QQ$) interaction, which attempts to create deformed nuclear shapes. Second is the monopole pairing interaction, which favors spherical shapes. The competition between these two interactions determines the nuclear shape. For the open shell nucleus $^{170}$Er, the $QQ$ interaction dominates, and the ground state is prolate. For the transitional nucleus $^{148}$Sm, which is closer to a closed shell configuration, the pair interaction is dominant, and the ground state is spherical. The nucleus $^{148}$Sm is selected because it is on the border between transitional and deformed nuclei. Simply adding two neutrons ($^{150}$Sm) creates a prolate HFB ground state, with $\beta = 0.20$. If the pair interaction is "turned off," then the HFB ground state of $^{148}$Sm becomes prolate with $\beta = 0.21$. Therefore, $^{148}$Sm would be deformed at zero temperature if the pair correlations did not exist.

Figure 4 gives the FTHFB pair gaps $\Delta_p$ and $\Delta_n$ versus the temperature for $^{148}$Sm. The pair gaps are starting to decrease at $kT < 0.4$ MeV. The pairing energy of the spherical shape is reduced by 1.9 MeV when the temperature is raised from 0 to 0.4 MeV. It then becomes energetically favorable to acquire a deformation and the attendant deformation energy. When the shape becomes prolate at $kT = 0.4$ MeV, the pair gaps quickly adjust to new values of $\Delta$ appropriate to the new intrinsic wave function. This causes the near vertical part of $\Delta(T)$ at $kT = 0.4$ MeV. As the temperature is increased further, the pair correlations decrease rapidly, disappearing at $kT_c = 0.56$ MeV for the neutrons and $kT_c = 0.90$ MeV for the protons. This illustrates how thermal excitations destroy the *BCS* variety of pair correlations, producing a second-order phase transition from the superfluid (or superconducting) state to the normal state. When the neutron pair correlations diminish, the quadrupole interaction is able to create a deformed shape.

When $\Delta_n$ vanishes at $kT_c = 0.56$ MeV, the quadrupole deformation in Fig. 2 attains its maximum value, $\beta = 0.14$. Although the pair correlation energy is 8.1 MeV smaller for the prolate shape than for the spherical shape at $kT_c = 0.56$ MeV, this loss is more than compensated for by the deformation energy of 9.4 MeV. Also, the entropy of the deformed state is larger than the entropy of the spherical state at $kT_c = 0.56$ MeV, resulting in a $TS$ differential of 0.8 MeV in favor of the prolate state. (Recall that the minimized quantity is the free energy $E - TS$.)

The argument may be summarized as follows: The nucleus $^{148}$Sm has a spherical ground state because the pairing interaction (which favors spherical shapes) dominates over the quadrupole interaction (which favors deformed shapes). Raising the temperature quenches both the pair gap $\Delta$ and the quadrupole deformation $\beta$. However, the critical temperature for the elimination of $\Delta_n$ is 0.56 MeV, whereas the critical temperature for the vanishing of $\beta$ is 0.91 MeV. Since the neutron pair correlations disappear at the lower temperature, the quadrupole interaction can create a deformation for temperatures between 0.56 and 0.91 MeV. The nucleus $^{148}$Sm exhibits a delicate balance between two competing tendencies, and the balance is shifted simply by changing the temperature. This effect was found by Smith *et al.*[5] in $^{116}$Sn. However, the dramatic "window of deformation" shown in our Fig. 2 does not appear in Ref. 5.

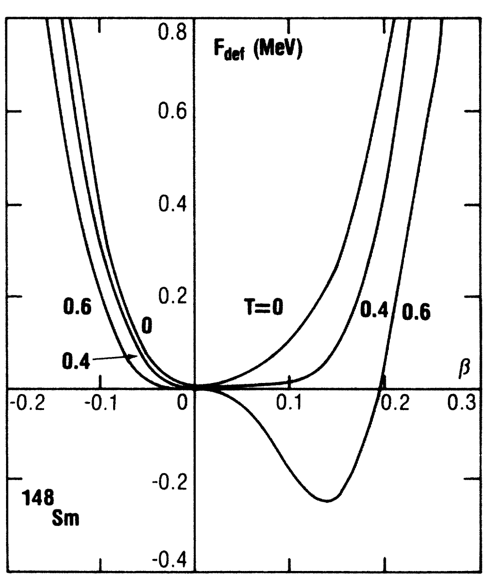


FIG. 3. The deformation free energy vs the quadrupole deformation for $^{148}$Sm. Each curve corresponds to a different temperature.

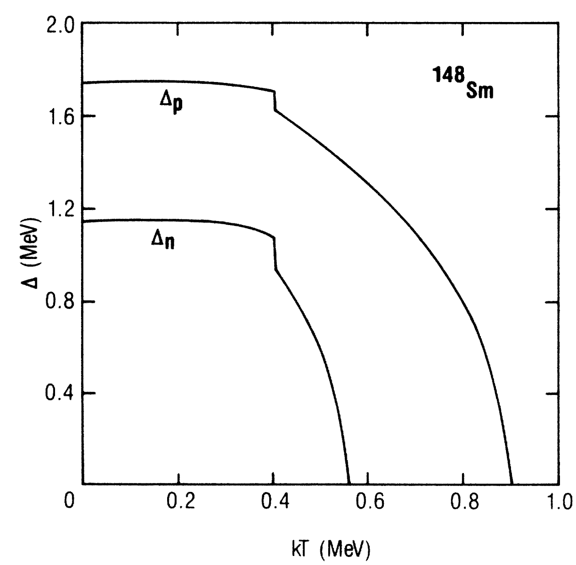


FIG. 4. The proton pair gap and neutron pair gap vs the temperature for $^{148}$Sm.

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