# Statistical fluctuations in the $i_{13/2}$ model

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The finite-temperature Hartree-Fock-Bogoliubov cranking equations are solved for the  $i_{13/2}$  model. For any temperature below  $kT_c = 0.2$  MeV, rotations induce a sharp first-order phase transition. When statistical fluctuations in the pair gap  $\Delta$  are included, the phase transition is smoothed out for  $\frac{1}{2}T_c < T < T_c$ . The rotation-aligned  $i_{13/2}$  pair is unaffected by temperatures up to 0.5 MeV. The finite-temperature violation of the zero-temperature Hartree-Fock-Bogoliubov relation  $R^2 = R$  is given by the quasiparticle number fluctuation.

### I. INTRODUCTION

The finite-temperature Hartree-Fock-Bogoliubov cranking (FTHFBC) formalism has been applied to nuclei which are heated as well as rotating.<sup>1-3</sup> Properties such as pair gaps and deformations have been determined as functions of spin and temperature.<sup>4,5</sup> A variety of firstand second-order phase transitions have been identified.<sup>6-8</sup>

The FTHFBC theory ignores fluctuation effects, of which there are two types. First, the Hartree-Fock-Bogoliubov (HFB) theory provides a mean field approximation to the exact density operator D. Consequently, the HFB density operator  $D_{\rm HFB}$  violates the symmetries of the Hamiltonian H. This creates number and spin fluctuations in  $D_{\rm HFB}$ . This type of fluctuation has been treated for zero- and finite-temperature systems.<sup>4</sup>

The second type of fluctuation is statistical. It would exist even if the exact density operator were known. For example, if a system has a specified temperature, then there will be fluctuations in its energy. In a perfect classical gas the fractional fluctuation in the energy is proportional to  $1/\sqrt{N}$ . In the thermodynamic limit of large N, the fractional fluctuation vanishes, so that specifying the temperature is equivalent to specifying the energy. However, for small systems these fluctuations may be important.

Another example is given by statistical fluctuations in the order parameter. For macroscopic systems, these fluctuations are significant at a critical point. For other states the fluctuations are not important, and the order parameter has a specific well-defined value for each state. However, for finite systems such as nuclei, statistical fluctuations in the order parameter can be large even for states which are far from any critical point. Then the system will not have a specific value of the order parameter.

For nuclei the order parameter can be chosen as the pair gap  $\Delta$ . In the FTHFBC theory,  $\Delta$  has a specific value for each spin *I* and temperature *T*. Then there are sharp first- and second-order phase transitions. However, since a nucleus is a finite system, there will be significant statistical fluctuations in  $\Delta$  for any finite-temperature state. For the uniform model, Moretto has shown that these fluctuations wash out the second-order phase transi-

tion.<sup>9</sup> In this paper we will consider the effect of statistical fluctuations on first-order phase transitions in rotating heated nuclei.

### II. THE $i_{13/2}$ MODEL

Our previous applications of the FTHFBC theory used the two-level model.<sup>4,6,10</sup> We now consider the  $i_{13/2}$ model, which is more realistic than the two-level model. For example, the  $i_{13/2}$  model will probe the relative effects of temperature on the pair gap and on the rotationalignment effect. In this section calculations with the FTHFBC theory are described. In Sec. III the effect of statistical fluctuations will be discussed.

Consider the  $i_{13/2}$  shell with the cranked pairing Hamiltonian,

$$H' = H - \mu \hat{N} - \omega J_x , \qquad (2.1)$$

$$H = \sum_{m} \epsilon_m C_m^{\dagger} C_m - G \sum_{mm'>0} C_m^{\dagger} C_{\overline{m}} C_{\overline{m}'} C_{m'} , \qquad (2.2)$$

where *m* is the projection of the spin on the *z* axis and *x* is the rotation axis. The single-nucleon energies  $\epsilon_m$  are the eigenvalues of an axially symmetric potential with quadrupole deformation

$$\epsilon_m = \kappa \frac{3m^2 - j(j+1)}{j(j+1)} . \tag{2.3}$$

For  $j = \frac{13}{2}$  and a quadrupole deformation  $\beta = +0.24$ , the constant  $\kappa$  is 2.0 MeV. The implicit assumption is that the deformation is constant at low temperatures (kT < 0.5 MeV). The pair constant G is chosen as 0.448 MeV. Then  $\Delta = 1.0$  MeV for six nucleons in the  $i_{13/2}$  shell at zero spin and zero temperature.

Let  $|k\rangle$  denote one of the seven single-nucleon states  $|i_{13/2}m\rangle$ , where  $m - \frac{1}{2}$  is an even integer. Let  $|\bar{k}\rangle$  signify the time reverse of  $|k\rangle$ , i.e.,  $|i_{13/2}-m\rangle$ . The  $\sigma_x$  representation is defined by the unitary transformation<sup>11</sup>

$$|K\rangle = 2^{-1/2} (|k\rangle + |\bar{k}\rangle), \qquad (2.4)$$

$$|\overline{K}\rangle = 2^{-1/2}(-|k\rangle + |\overline{k}\rangle), \qquad (2.5)$$

where  $|\bar{K}\rangle$  is the time reverse of  $|K\rangle$ . The quasiparticle operators are chosen as

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$$a_i^{\dagger} = \sum_K \left( U_{iK} C_K^{\dagger} + V_{iK} C_{\overline{K}} \right) , \qquad (2.6)$$

$$a_{\hat{i}}^{\dagger} = \sum_{K} (\hat{U}_{iK} C_{\overline{K}}^{\dagger} + \hat{V}_{iK} C_{K}) . \qquad (2.7)$$

The advantage of the  $\sigma_x$  representation is that it block diagonalizes the FTHFBC energy matrix. The block which determines the quasiparticles  $a_i^{\dagger}$  and the quasiparticle energies  $E_i$  is

$$\begin{pmatrix} (\mathscr{H}_1 - \omega j_x) & \Delta_1 \\ \Delta_1^{\dagger} & -(\mathscr{H}_2 + \omega j_x)^* \end{pmatrix} \begin{bmatrix} U_i \\ V_i \end{bmatrix} = E_i \begin{bmatrix} U_i \\ V_i \end{bmatrix}. \quad (2.8)$$

The block which determines the quasiparticles  $a_{\hat{i}}^{\dagger}$  need not be solved, since

$$\hat{U}_i = V_i^*, \quad \hat{V}_i = U_i^*, \quad \hat{E}_i = -E_i$$
 (2.9)

The terms  $\mathscr{H}_1$  and  $\mathscr{H}_2$  are the Hartree-Fock (HF) Hamiltonians in the  $|K\rangle$  and  $|\overline{K}\rangle$  spaces, respectively. For the  $i_{13/2}$  model, the HF potential vanishes, so that  $\mathscr{H}_1$  and  $\mathscr{H}_2$  are equal and diagonal,

$$\mathscr{H}_1 = \mathscr{H}_2 = \epsilon - \mu . \tag{2.10}$$

The tridiagonal matrix  $j_x$  is

$$(j_x)_{KK'} = \langle K \mid J_x \mid K' \rangle = -\langle \overline{K} \mid J_x \mid \overline{K}' \rangle .$$
(2.11)

The pair potential  $\Delta_1$  is a multiple of the unit matrix. The diagonal elements of  $\Delta_1$  equal  $-\Delta$ , where

$$\Delta = G \sum_{K>0} t_{K\overline{K}} . \qquad (2.12)$$

The pair density is

$$t_{K\overline{K}'} = [\widetilde{U}fV^* + \widehat{V}^{\dagger}(1-\widehat{f})\widehat{U}]_{KK'}, \qquad (2.13)$$

and the HF density is

$$\rho_{KK'} = [\tilde{U}fU^* + \hat{V}^{\dagger}(1 - \hat{f})\hat{V}]_{KK'}, \qquad (2.14)$$

$$\rho_{\bar{K}\bar{K}'} = [\hat{U}\hat{f}\hat{U}^* + V^{\dagger}(1-f)V]_{KK'}. \qquad (2.15)$$

The probabilities for thermally exciting quasiparticles are given by the diagonal matrices f and  $\hat{f}$ , whose elements are

$$f_i = \frac{1}{1 + e^{\beta E_i}} , \qquad (2.16)$$

$$\hat{f}_i = \frac{1}{1 + e^{\beta \hat{E}_i}}$$
, (2.17)

where  $\beta = 1/kT$ , k is Boltzmann's constant, and T is the temperature. The chemical potential  $\mu$  and the rotational frequency  $\omega$  are adjusted to satisfy the number and spin constraints

$$N = \langle \hat{N} \rangle = \sum_{K} (\rho_{KK} + \rho_{\overline{K}\overline{K}}) , \qquad (2.18)$$

$$I = \langle J_x \rangle = \sum_{KK'} (\rho_{KK'} - \rho_{\overline{K}\,\overline{K}\,'})(j_x)_{K'K} \ . \tag{2.19}$$

The free energy in a rotating frame is



FIG. 1. The pair gap  $\Delta$  versus the temperature T for the nonrotating system. The quantities kT,  $\hbar\omega$ ,  $\kappa$ , and G have units of MeV.

$$F' = E - TS - \omega I , \qquad (2.20)$$

where the energy and the entropy are

$$E = \sum_{K} \epsilon_{K} (\rho_{KK} + \rho_{\overline{K}\overline{K}}) - \Delta^{2}/G , \qquad (2.21)$$

$$S = -k \sum_{i} [f_i \ln f_i + (1 - f_i) \ln(1 - f_i)] . \qquad (2.22)$$

The sum in Eq. (2.22) includes *i* and  $\hat{i}$ .

Since the HF and pair fields each have a dimension of 7, the HFB energy matrix (2.8) has a dimension of 14. Equation (2.8) is solved by iteration. The final self-consistent energy matrix is completely defined by specifying four numbers T,  $\omega$ ,  $\mu$ , and  $\Delta$ . All quantities are chosen to be real.

For a nonrotating system where  $\omega = 0$ , the FTHFBC equation (2.8) reduces to the much simpler finite-temperature Bardeen-Cooper-Schrieffer (BCS) (FTBCS) equation<sup>1</sup>



FIG. 2. The pair gap  $\Delta$  versus the rotational frequency  $\omega$  for various temperatures.



FIG. 3. The angular momentum I versus the rotational frequency  $\omega$  for various temperatures.

$$1 = \frac{G}{2} \sum_{m>0} \frac{\tanh(\frac{1}{2}\beta E_m)}{E_m} , \qquad (2.23)$$

where the quasiparticle energies are

$$E_m = E_{\bar{m}} = [(\epsilon_m - \mu)^2 + \Delta^2]^{1/2} . \qquad (2.24)$$

The FTBCS equation (2.23) is solved for the pair gap  $\Delta(T)$  at  $\omega = 0$ , which is shown in Fig. 1. Heating creates a second-order phase transition from the superfluid to the



FIG. 4. Critical frequency curve and phase diagram: critical rotational frequency  $\omega_c$  versus temperature *T*. The solid line follows the Maxwell or Ehrenfest convention and the dashed lines follow the delay convention for first-order phase transitions.



FIG. 5. Matrix element of  $J_x$  for one rotation-aligned nucleon.

normal state at the critical temperature  $kT'_c = 0.545$  MeV.

The FTHFBC equation (2.8) is solved for the pair gap  $\Delta(\omega)$  at various temperatures, as depicted in Fig. 2. There is a critical point at  $kT_c = 0.2$  MeV. For  $T < T_c$  the function  $\Delta(\omega)$  exhibits backbending. This indicates that rotation induces a first-order phase transition from superfluid to normal. For  $T_c < T < T'_c$  the function  $\Delta(\omega)$  does not backbend, and rotation induces a second-order phase transition.

For each temperature below  $T_c$ , the critical frequency  $\omega_c$  is defined by<sup>6</sup> the crossing point in the isothermal function  $F'(\omega)$  where F' is the free energy in the rotating frame (2.20). Alternatively,  $\omega_c$  can be found by applying the Maxwell construction to the isothermal equation of state  $\omega(I)$  given in Fig. 3. For  $T > T_c$ ,  $\omega_c$  is defined as the frequency at which  $\Delta$  vanishes. The critical frequency curve  $\omega_c(T)$  is given by the solid line in Fig. 4. This is the phase diagram for the rotating heated system.

How does temperature affect the rotation-aligned pair? The single-nucleon matrix element  $\langle \alpha | J_x | \alpha \rangle$  is calculated, where  $|\alpha\rangle$  diagonalizes the HF density  $\rho$ . Figures 5 and 6 show the matrix element for the two orbitals which become aligned along the rotation axis at high spin. For small  $\omega$  raising the temperature increases the orbital alignment. This is reasonable, since increasing T decreases  $\Delta$ , which permits a more rapid particle alignment. However, the alignment is completed at the same  $\omega$ , regardless of the temperature. Once the nucleon is rotation aligned at





FIG. 7. The orbital occupation probability  $\rho$ , the quasiparticle transformation coefficient  $v^2$ , and the quasiparticle occupation probability f, versus the temperature T. The orbital has  $m = \frac{5}{2}$ .

T=0, raising the temperature to 0.5 MeV has no effect on the alignment.

How does temperature affect the occupation probability of an orbital? There are two competing effects. First, raising the temperature reduces the pair gap. This depletes orbitals above the chemical potential. Second, increasing the temperature creates thermal excitations of quasiparticles. This populates orbitals above the chemical potential. For a nonrotating system FTHFBC simplifies to FTBCS. Then the occupation probability of the orbital  $|i_{13/2}m\rangle$  is

$$\rho_m = v_m^2 + (u_m^2 - v_m^2) f_m , \qquad (2.25)$$

where the quasiparticles are

$$a_m^{\dagger} = u_m C_m^{\dagger} - v_m C_{\overline{m}} \tag{2.26}$$

and  $u_m^2 + v_m^2 = 1$ . Figures 7 and 8 show how  $\rho_m$ ,  $v_m^2$ , and  $f_m$  vary with temperature for the  $m = \frac{5}{2}$  orbital, which is



FIG. 8. See Fig. 7. The orbital has  $m = \frac{7}{2}$ .

just below the chemical potential, and the  $m = \frac{7}{2}$  orbital, which is just above the chemical potential. Although  $v_m^2$ and  $f_m$  change rapidly with temperature, the occupation  $\rho_m$  is nearly independent of temperature. So the two competing effects mentioned above nearly cancel.

Whereas the yrast line is described by a quasiparticle vacuum, the region above the yrast line contains thermally excited quasiparticles. The average quasiparticle number is  $N = \langle \hat{N} \rangle$ , where

$$\widehat{N} = \sum_{i} \widehat{n}_{i} = \sum_{i} a_{i}^{\dagger} a_{i} . \qquad (2.27)$$

The temperature dependence of N is given in Fig. 9 for the nonrotating system.

## **III. STATISTICAL FLUCTUATIONS**

In Sec. II, statistical mechanics was applied with the assumption that the system was in a state of thermal equilibrium. This section considers statistical fluctuations around the equilibrium state.

### A. Energy fluctuations

A system at constant temperature has fluctuations in the energy. We must distinguish between statistical fluctuations and fluctuations due to the approximate nature of the mean field density operator. The energy fluctuation is defined by

$$(\delta E)^2 = \langle H^2 \rangle - \langle H \rangle^2 . \tag{3.1}$$

This fluctuation does not vanish at T=0 when it is evaluated with the Hartree-Fock-Bogoliubov cranking (HFBC) wave function. Then  $\delta E$  is a measure of the approximate nature of the wave function. However, statistical fluctuations must disappear at T=0. So Eq. (3.1) cannot be directly applied to determine statistical fluctuations around FTHFBC states. Using exact wave functions it may be shown that



FIG. 9. The quasiparticle number  $N_{qp}$  versus the temperature T for  $\omega = 0$ .

$$(\delta E)^2 = kT^2 C_I , \qquad (3.2)$$

where  $C_I$  is the specific heat at constant spin

$$C_I = \left\lfloor \frac{\partial E}{\partial T} \right\rfloor_I \,. \tag{3.3}$$

The third law of thermodynamics requires that  $C_I$  approach 0 as T approaches 0. Notice that with Eq. (3.2) the statistical energy fluctuation vanishes at T=0 even for approximate wave functions.

The specific heat and the energy fluctuation are shown in Figs. 10 and 11 for I = 0. The peak in these functions at  $kT'_c = 0.55$  MeV signals the second-order phase transition from superfluid to normal. The graphs for I = 2, 4, and 6 are similar to the I = 0 results. At the critical temperature  $\delta E = 1.76$  MeV. Is this fluctuation large or small? There are two interpretations. To address this question in a realistic fashion we will use numbers appropriate to real nuclei, and not simply the  $i_{13/2}$  model. Tanabe *et al.*<sup>5</sup> have solved the FTHFBC equations for  $^{164}$ Er. For  $I^{\pi} = 6^+$  and kT = 0.6 MeV, the thermal excitation energy is 5.3 MeV and  $C_I = 24k$ , so that  $\delta E = 2.9$ MeV. Now 2.9 MeV is certainly a large fluctuation when compared to an energy of 5.3 MeV. However, it is common to define the fractional fluctuation in the energy

$$\mathscr{F} = \left[\frac{(\delta E)^2}{E^2}\right]^{1/2},\tag{3.4}$$

where E is the average energy. For <sup>164</sup>Er the ground state value of |E| is approximately (8 MeV) (164)=1312 MeV. For  $I^{\pi}=6^+$  and kT=0.6 MeV,  $|E|\approx1306$ MeV. The fractional fluctuation is  $\mathcal{F}=2.9$  MeV/1306 MeV=0.002. This is extremely small, even compared to  $1/\sqrt{N}=0.08$ .



FIG. 10. The specific heat C versus the temperature T for  $\omega = 0$ . The quantity C has units of Boltzmann's constant.



FIG. 11. The energy fluctuation  $\delta E$  versus the temperature T for  $\omega = 0$ .

#### **B.** Quasiparticle number fluctuations

The fluctuation in the quasiparticle number is

$$(\delta N)^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 , \qquad (3.5)$$

where  $\hat{N}$  is the quasiparticle number operator of Eq. (2.27). Since  $\hat{n}_i^2 = \hat{n}_i$ , it follows that

$$\hat{N}^2 = \sum_i \hat{n}_i + \sum_{i \neq j} \hat{n}_i \hat{n}_j , \qquad (3.6)$$

so that

$$\langle \hat{N}^2 \rangle = \sum_i f_i + \sum_{i \neq j} f_i f_j . \qquad (3.7)$$

From Eq. (2.27) it follows that

$$\langle \hat{N} \rangle^2 = \sum_i f_i^2 + \sum_{i \neq j} f_i f_j .$$
(3.8)

Combining Eqs. (3.7) and (3.8), the fluctuation is

$$(\delta N)^2 = \sum_i f_i (1 - f_i) .$$
 (3.9)

At T = 0, all  $f_i = 0$ , so that  $\delta N = 0$  as expected. Figure 12 shows how this fluctuation increases with temperature. Observe that  $\delta N$  and N are similar in magnitude.

At zero temperature the HFBC quasiparticle vacuum satisfies the unitarity relation



$$R^2 = R, (T = 0)$$
 (3.10)

where R is the generalized particle density matrix

$$R = \begin{bmatrix} \rho & t \\ -t^* & 1 - \rho^* \end{bmatrix} . \tag{3.11}$$

However, at finite-temperature Eq. (3.10) is violated. It will now be demonstrated that  $\delta N$  provides a measure of  $(R^2 - R)$ . The generalized quasiparticle density matrix is

$$Q = \begin{bmatrix} f & 0\\ 0 & 1-f \end{bmatrix}.$$
 (3.12)

The densities Q and R are related by a similarity transformation

$$R = Z^{\dagger} Q Z , \qquad (3.13)$$

where Z is the quasiparticle transformation

$$\boldsymbol{Z} = \begin{bmatrix} \boldsymbol{U}^* & \boldsymbol{V}^* \\ \boldsymbol{V} & \boldsymbol{U} \end{bmatrix}, \quad \boldsymbol{Z}\boldsymbol{Z}^{\dagger} = 1 \;. \tag{3.14}$$

It follows that

$$R^2 = Z^{\dagger} Q^2 Z \tag{3.15}$$

and

and

$$R - R^2 = Z^{\dagger}(Q - Q^2)Z$$
. (3.16)

Since  $(R - R^2)$  and  $(Q - Q^2)$  are related by this similarity transformation, they have equal traces. From Eq. (3.12) it follows that

$$Q - Q^{2} = \begin{bmatrix} f(1-f) & 0\\ 0 & f(1-f) \end{bmatrix}, \qquad (3.17)$$

$$\Gamma r(Q - Q^2) = 2 \sum_i f_i (1 - f_i) = 2(\delta N)^2 , \qquad (3.18)$$

$$\Gamma r(R - R^2) = 2(\delta N)^2$$
. (3.19)

The finite-temperature violation of the relation  $R^2 = R$  is trivially obtained from the quasiparticle number fluctuation.

A related question is the reduction of the HFB densities  $\rho$  and t to canonical form. At zero temperature, Eq. (3.10) implies that there exist pairs of nucleon orbits  $|\alpha\rangle$  and  $|\hat{\alpha}\rangle$  such that

$$\rho_{\hat{a}\hat{a}} = \rho_{aa} , \qquad (3.20)$$

$$|t_{\alpha\hat{\alpha}}| = [\rho_{\alpha\alpha}(1-\rho_{\alpha\alpha})]^{1/2}, \qquad (3.21)$$

where all other elements of  $\rho$  and t equal zero. Since  $R^2 \neq R$  if T > 0, the canonical form of Eqs. (3.20) and (3.21) does not exist at finite temperatures. For the special case of nonrotating systems, Eq. (3.20) will be satisfied when T > 0 because of the time-reversal symmetry, but the pair density will not have the canonical form. However, for a rotating system, even Eq. (3.20) is violated when T > 0. One cannot define two orbitals  $|\alpha\rangle$  and  $|\hat{\alpha}\rangle$  which have equal occupation. In this case the identification of paired orbitals is somewhat arbitrary. The labeling of paired orbitals can be accomplished by continuation from the T=0 identification. Because Eq. (3.10) is violated at finite temperature and the canonical form is lost, the Bloch-Messiah theorem, which plays such an important role in analyzing zero-temperature HFBC wave functions, is not very useful for interpreting finitetemperature HFB density operators.

# C. Pairing fluctuations

The FTHFBC theory predicts first- and second-order phase transitions in rotating heated nuclei. Do statistical fluctuations wash out these phase transitions?

For a nucleus with a given temperature, rotational frequency and particle number, the free energy in a rotating frame, F' of Eq. (2.20), is minimized. The equilibrium state has a sharp value of  $\Delta$ , as in the FTHFBC theory. However, statistical fluctuations create values of  $\Delta$  which deviate from the equilibrium value.

In the Landau theory of phase transitions, F' is treated as a function of  $\Delta$ , where  $\Delta$  is an independent variable not constrained by T,  $\omega$ , and N.<sup>12,13</sup> The extrema of  $F'(\Delta)$ define the equilibrium or FTHFBC states. In the Landau theory the entire surface  $F'(\Delta, T, \omega)$  is constructed, and not simply the equilibrium states.

The probability that the nucleus has any given value of  $\Delta is^{12}$ 

$$P(\Delta) \propto e^{-F'(\Delta)/kT} . \tag{3.22}$$

According to Eq. (3.22), there are no fluctuations at T=0. This equation determines the thermodynamic fluctuations. However, if the temperature is too small or if nonequilibrium states vary too rapidly with time, then the quantum fluctuations dominate and Eq. (3.22) is no longer meaningful.<sup>12</sup>





FIG. 13. The free energy F versus the pair gap  $\Delta$  for various temperatures and  $\omega = 0$ . The quantity F has units of MeV.

To evaluate  $P(\Delta)$ , first choose T,  $\omega$ , and N. Second, diagonalize the HFB energy matrix (2.8),

$$\begin{bmatrix} (\epsilon - \mu - \omega j_x) & -\delta \\ -\delta & -(\epsilon - \mu + \omega j_x) \end{bmatrix}, \qquad (3.23)$$

where  $\delta$  is an arbitrary multiple of the unit matrix. Use the eigenvectors (*U*, *V*) and eigenvalues *E* of Eq. (3.23) to calculate the HFB densities  $\rho$  and *t*, which are defined in



FIG. 14. The probability P versus the pair gap  $\Delta$  for various temperatures and  $\omega = 0$ .

Eqs. (2.13)–(2.17). Next calculate  $\Delta$  with Eq. (2.12) and F' with Eqs. (2.19)–(2.22). For one value of  $\delta$  this procedure determines one point in the  $F'(\Delta)$  plane. By varying  $\delta$  from zero to infinity, the function  $F'(\Delta)$  is mapped out. The extrema of  $F'(\Delta)$  are the FTHFBC equilibrium solutions, where  $\delta = \Delta$ . At all other states  $\delta \neq \Delta$ . Finally, calculate  $P(\Delta)$  from  $F'(\Delta)$  using Eq. (3.22).

Consider the second-order phase transition produced by heating a nonrotating nucleus. Figure 13 shows  $F'(\Delta)$  for various temperatures with  $\omega = 0$ . As T increases from 0 to  $T'_c = 0.55$  MeV/k, the minimum in  $F'(\Delta)$  shifts continuously from  $\Delta = 1.0$  MeV to  $\Delta = 0$ . Also, the barrier separating the superfluid and normal states decreases as the nucleus is heated. From Fig. 13 and Eq. (3.22) the probability distribution  $P(\Delta)$  is calculated, as shown in Fig. 14. Since the FTHFBC theory minimizes  $F'(\Delta)$ , it finds the  $\Delta$  which maximizes  $P(\Delta)$ , i.e., the most probable  $\Delta$ . For kT = 0.1 MeV,  $P(\Delta)$  has a narrow peak, so the fluctuations in  $\Delta$  are small. Also  $P(\Delta)$  is almost symmetric. For kT = 0.3 MeV,  $P(\Delta)$  is less symmetric and broader, so the fluctuations are large. At  $kT'_c = 0.55$ MeV the equilibrium  $\Delta$  is zero. However, there are large fluctuations in  $\Delta$  extending to  $\Delta \approx 1.4$  MeV. Even at kT = 2.0 MeV, which is four times the critical temperature, the fluctuations in  $\Delta$  are still large.

Define the average  $\Delta$  by

$$\langle \Delta \rangle = \frac{\int_0^\infty \Delta P(\Delta) d\Delta}{\int_0^\infty P(\Delta) d\Delta} .$$
 (3.24)

Figure 15 compares the average  $\Delta$  with the BCS  $\Delta$ , which is the equilibrium or most probable  $\Delta$ . Whereas the BCS  $\Delta$  exhibits a sharp second-order phase transition from superfluid to normal, the average  $\Delta$  remains large even at very high temperatures. The conclusion is that statistical fluctuations in  $\Delta$  wash out the second-order phase transition.<sup>9</sup>

Next consider the first-order phase transition induced by rotating the nucleus. Figure 16 shows  $F'(\Delta)$  for various  $\omega$  at T=0. For  $\omega=0$  there is a large barrier between the superfluid minimum at  $\Delta=1.0$  MeV and the normal maximum at  $\Delta=0$ . At  $\hbar\omega'_c=0.126$  MeV the normal state



FIG. 15. The pair gap  $\Delta$  versus the temperature T for  $\omega = 0$ . The dashed curve is the BCS or most probable  $\Delta$ , and the solid curve is the average  $\Delta$ .

F'

- 9.4

-9.6

- 9.8

- 10.0

- 10.2

- 10.4

- 10.6





becomes an inflection point. For  $\hbar\omega_c = 0.157$  MeV there are two degenerate minima, one superfluid and one normal, as well as a relative maximum. These three extrema are self-consistent solutions of the FTHFBC equations. For  $\hbar\omega_c''=0.181$  MeV the superfluid minimum becomes an inflection point.

How were  $\omega_c$ ,  $\omega'_c$ , and  $\omega''_c$  determined? The crossing point of the loop in  $F'(\omega)$  defines  $\omega_c$  (Ref. 6). The point where  $\Delta \rightarrow 0$  in Fig. 2 defines  $\omega'_c$ . The maximum  $\omega$  for which  $\Delta > 0$  in Fig. 2 defines  $\omega''_c$ . This explains the peculiar backbending feature of  $\Delta(\omega)$ . Why is it that FTHFBC solutions exist with large  $\Delta$  for frequencies up to  $\omega''_c$ , but no paired solutions exist for  $\omega > \omega''_c$ ? Because at  $\omega''_c$  the superfluid minimum in  $F'(\Delta)$  disappears.

There are two definitions for the critical frequency of a first-order phase transition. In previous papers the author used the Maxwell or Ehrenfest convention, which is  $\omega_c$ , the frequency for which there are two degenerate minima. The essential idea is that the system is always in the absolute minimum. As  $\omega$  is varied past  $\omega_c$  the absolute minimum suddenly jumps from one minimum to the other producing a sudden discontinuity in the order parameter  $\Delta$ . This is the signature of a first-order phase transition.

An alternative definition of the critical frequency is given by the delay convention. Imagine that the curves  $F'(\Delta)$  are physical surfaces and place a small sphere at the minimum of the  $\omega=0$  surface. As  $\omega$  increases past  $\hbar\omega_c=0.157$  MeV the sphere remains in the same potential well, which then becomes a relative minimum. It is not until  $\omega$  reaches  $\hbar\omega_c''=0.181$  MeV where the relative minimum disappears that the sphere rolls down to the absolute minimum at  $\Delta=0$ . Similarly, start with a rapidly rotating system and place the sphere at  $\Delta=0$ . As  $\omega$  decreases below  $\omega_c$ , the normal state becomes a relative minimum, but the sphere remains there until  $\omega$  decreases



FIG. 17. See Fig. 16. The temperature is 0.1 MeV/k.

to  $\hbar\omega'_c = 0.126$  MeV. Then the normal minimum disappears and the sphere rolls down to the superfluid minimum. So at each temperature there are three critical frequencies  $\omega_c$ ,  $\omega'_c$ , and  $\omega''_c$ .

The free energy for kT = 0.1 MeV is shown in Fig. 17. The differences from T = 0 are that all minima shift to smaller  $\Delta$ , all barrier heights decrease, and the three critical frequencies come closer together.

There is a critical point at  $kT_c = 0.2$  MeV and  $\hbar\omega_c = 0.1505$  MeV. Figure 18 shows that  $F'(\Delta)$  is horizontal from  $\Delta = 0$  to  $\Delta \approx 0.7$  MeV. At the critical point all minima and maxima disappear, and the three critical



FIG. 18. See Fig. 16. The temperature is 0.2 MeV/k.



FIG. 19. The probability P versus the pair gap  $\Delta$  for various temperatures and critical rotational frequencies.

frequencies converge to a single value. This is shown in the phase diagram of Fig. 4. The dashed lines are  $\omega'_c(T)$ and  $\omega''_c(T)$ , which define the first-order phase transition in the delay convention.

The statistical fluctuations in  $\Delta$  are calculated with  $F'(\Delta)$  and Eq. (3.22). The probability P that the system has a given value of  $\Delta$  is shown in Fig. 19 for several choices of T and  $\omega_c$ . For kT = 0.02 MeV,  $P(\Delta)$  has two well-defined peaks which correspond to the two degenerate minima in  $F'(\Delta)$ . The probability P falls to a relative minimum of 0.05. Consequently, statistical fluctuations do not wash out the barrier in  $F'(\Delta)$ , which separates the two degenerate phases.

For kT = 0.05 MeV, the relative minimum in  $P(\Delta)$ rises to 0.35. For kT = 0.10 MeV the two peaks in  $P(\Delta)$ are disappearing and the relative minimum in  $P(\Delta)$  is 0.78. Then the probability that the system occupies the relative maximum in  $F'(\Delta)$  is 78% of the probability that it occupies one of the degenerate minima. The statistical



FIG. 20. See Fig. 16. The temperature is 0.3 MeV/k.



fluctuations in the pairing gap have almost eliminated the effect of the barrier in  $F'(\Delta)$ . Consequently when kT = 0.10 MeV, which is  $kT_c/2$ , the first-order phase transition is smoothed out by statistical fluctuations.

At the critical point, curve D in Fig. 19 shows that there is equal probability for  $\Delta$  to have any value between 0 and 0.7 MeV. Fluctuations in the order parameter are unusually large at a critical point.

Finally, we consider second-order phase transitions induced by rotating a system with  $T_c < T < T'_c$ , where  $kT_c = 0.2$  MeV and  $kT'_c = 0.545$  MeV. The phase transition is second order in this temperature range because for any rotational frequency  $F'(\Delta)$  contains only one minimum rather than two. This is shown in Fig. 20 for kT = 0.3 MeV. At the critical frequency of 0.143 MeV,  $F'(\Delta)$  rises very slowly. Figure 21 shows the corresponding  $P(\Delta)$ . Although the most probable value of  $\Delta$  is zero, the probability distribution has a long tail. The average value of  $\Delta$  is marked by the dot at  $\Delta = 0.54$  MeV. Consequently, the second-order phase transition induced by rotations is also smoothed out by statistical fluctuations.

#### **IV. CONCLUSIONS**

For the  $i_{13/2}$  model, equilibrium statistical mechanics predicts that (a) heating the nonrotating system induces a second-order phase transition from superfluid to normal at  $kT'_c = 0.55$  MeV; (b) rotating the system at constant temperature produces a first-order phase transition from superfluid to normal if  $0 < T < T_c$ , where  $kT_c = 0.2$  MeV; and (c) rotating the system at constant temperature creates a second-order phase transition from superfluid to normal if  $T_c < T < T'_c$ . These transitions are all accompanied by the alignment of two  $i_{13/2}$  nucleons along the rotation axis. This rotation-aligned pair is unaffected by temperatures up to 0.5 MeV.

When statistical fluctuations in the pair gap  $\Delta$  are included, then (a) the first-order phase transition is washed out for temperatures in the range  $\frac{1}{2}T_c < T < T_c$ , and (b) the second-order phase transitions are also smoothed out. For infinite systems statistical fluctuations are important only at critical points. However, for finite systems, statistical fluctuations around equilibrium states are important even for states far from critical points. Descriptions

of finite systems which ignore these fluctuations are not adequate.

These conclusions are obtained for calculations restricted to a single *j* shell. Would the inclusion of many *j* shells alter these conclusions? Fluctuations in the pair gap  $\Delta$  occur in the vicinity of the chemical potential. Including *j* shells which lie below or above the chemical potential would not affect the fluctuations. Only those few shells which are near the chemical potential will change the results. Therefore it is unlikely that extending the model space from one *j* shell to many *j* shells would appreciably alter the conclusions. The effect of statistical fluctuations on second-order phase transitions has been studied by Moretto<sup>9</sup> using the uniform model, which contains a large number of particles, and the results are similar to the  $i_{13/2}$  model.

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