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Author:

[Goodman, Alan L.](#)

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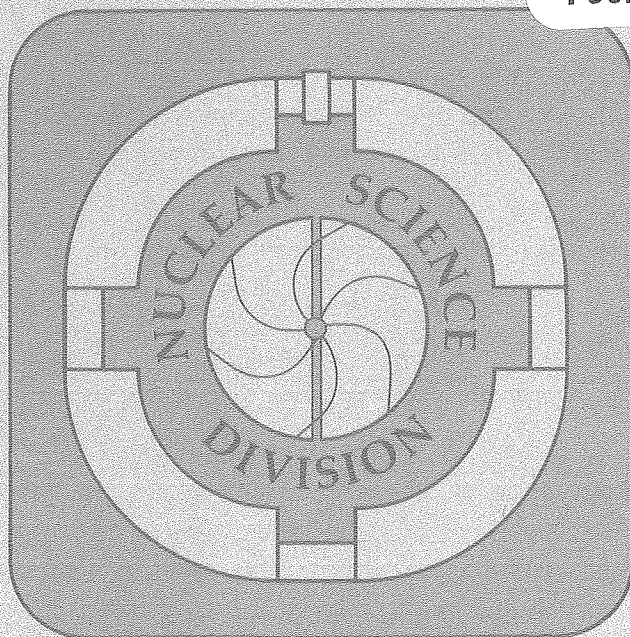
FINITE-TEMPERATURE HFB THEORY

Alan L. Goodman

July 1980

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FINITE-TEMPERATURE HFB THEORY

Alan L. Goodman^{*}

Physics Department and Quantum Theory Group
Tulane University
New Orleans, Louisiana 70118[†]

and

Nuclear Science Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

ABSTRACT

The finite-temperature Hartree-Fock-Bogoliubov (FTHFB) equations are derived. For the pairing Hamiltonian FTHFB simplifies to finite-temperature BCS (FTBCS). The solution of the FTBCS equations for the degenerate model displays a temperature-dependent pairing "phase transition."

[NUCLEAR STRUCTURE Finite-temperature,
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^{*}Supported in part by the National Science Foundation.

[†]Present address.

I. INTRODUCTION

The conventional HFB theory¹ is a zero-temperature theory in which the ground state is a quasiparticle vacuum. By including a cranking constraint, high-spin states along the yrast line can be described by HFB. This is because the excitation energy of yrast states is produced by collective rotations rather than statistical thermal excitations. Consequently the yrast band has a temperature $T=0$. Each yrast state is described by a quasiparticle vacuum which is re-defined for each spin.

Heavy-ion reactions produce nuclei which lie far above the yrast line. Since the time required to establish thermal equilibrium within a nucleus appears to be small compared to the de-excitation time of the nucleus, one can attempt to describe the region above the yrast line by temperature-dependent mean fields. It is therefore very desirable to derive a finite-temperature HFB (FTHFB) theory. Such a theory will be capable of describing temperature-dependent shape transitions and pairing "phase transitions." The FTHFB theory will include the interplay between single-particle, rotational, pairing and thermal degrees of freedom in a fully self-consistent fashion. For example, it will be possible to investigate the conjecture that the demarcation between the statistical decays which de-excite the nucleus down towards the yrast line and the collective rotational decays which de-excite the nucleus parallel to the yrast line is determined by a critical temperature above which the nucleus does not have a well-defined deformation.

It will be demonstrated that the FTHFB equations have exactly the same form as the conventional HFB equations. No additional terms are introduced into the definitions of the HF and pair potentials. That this

should occur is not obvious, since the FTHFB theory includes not only the quasiparticle vacuum energy, but also the quasiparticle excitation energies, and the interactions between the quasiparticles (see Appendix 1). The essential effect of introducing a finite-temperature is to produce a Fermi-Dirac distribution of quasiparticle excitations, so that the quasiparticles no longer have a zero occupation probability. This alters the equations for the particle densities.

The BCS limit of FTHFB is derived, and the FTBCS equations are solved for a simple model to illustrate the temperature-dependent pairing "phase transition."

II. REVIEW OF THERMODYNAMICS AND STATISTICAL MECHANICS

Those elements of thermodynamics and statistical mechanics which are essential for deriving FTHFB are now presented.

For a system which undergoes a transformation in which the chemical potential μ remains constant, the first law of thermodynamics is

$$\Delta E = \Delta Q - \Delta W + \mu \Delta N \quad , \quad (2.1)$$

where ΔE is the change in the internal energy E , ΔQ is the net amount of heat absorbed by the system, ΔW is the net amount of work done by the system, and ΔN is the change in the number of particles N . If the transformation occurs at a constant temperature T , then the second law of thermodynamics is

$$T \Delta S \geq \Delta Q \quad , \quad (2.2)$$

where ΔS is the change in the entropy S . Define the grand potential

$$\Omega = E - TS - \mu N \quad . \quad (2.3)$$

By combining the first and second laws, it follows that

$$\Delta\Omega \leq -\Delta W \quad . \quad (2.4)$$

For a mechanically isolated system, $\Delta W = 0$, so that

$$\Delta\Omega \leq 0 \quad . \quad (2.5)$$

Consequently, for a system which is mechanically isolated and maintained at constant temperature and constant chemical potential, the equilibrium state minimizes the grand potential. The equilibrium condition is

$$\delta\Omega = 0 \quad . \quad (2.6)$$

This variation may be used to define the density operator D , which has the property that

$$\text{Tr} D = 1 \quad . \quad (2.7)$$

The expectation value of any operator O is given by an ensemble average of O in the grand canonical ensemble

$$\langle O \rangle = \text{Tr}(DO) \quad . \quad (2.8)$$

The trace implies a sum over all states with any number of particles (or quasiparticles).

The internal energy E , the entropy S , and the particle number N are defined by

$$E = \langle H \rangle = \text{Tr}(DH) \quad , \quad (2.9)$$

$$S = \langle -k \ln D \rangle = -k \text{Tr}(D \ln D) \quad , \quad (2.10)$$

$$N = \langle \hat{N} \rangle = \text{Tr}(D\hat{N}) \quad , \quad (2.11)$$

where H is the Hamiltonian, k is Boltzmann's constant, and

$$\hat{N} = \sum_i c_i^\dagger c_i \quad . \quad (2.12)$$

The variational principle (2.6) is realized by²

$$\frac{\delta \Omega}{\delta D} = 0 \quad , \quad (2.13)$$

where the constraint (2.7) must be satisfied. The solution to Eqs. (2.13) and (2.7) is

$$D = Z^{-1} e^{-\beta(H - \mu N)} \quad , \quad (2.14)$$

$$Z = \text{Tr} [e^{-\beta(H - \mu N)}] \quad , \quad (2.15)$$

where Z is the grand partition function and $\beta = 1/kT$.

III. INDEPENDENT QUASIPARTICLE MODEL

The HFB theory approximates the Hamiltonian H by an independent quasiparticle Hamiltonian

$$H \approx H_{\text{HFB}} = E_0 + \sum_i E_i a_i^\dagger a_i \quad , \quad (3.1)$$

where E_0 is the energy of the quasiparticle vacuum, E_i is a quasiparticle energy, and a_i^\dagger is a quasiparticle creation operator

$$a_i^\dagger = \sum_j (U_{ij} c_j^\dagger + V_{ij} c_j) \quad . \quad (3.2)$$

The HFB density operator is obtained by substituting Eq. (3.1) into Eqs. (2.14) and (2.15), so that

$$D_{\text{HFB}} = Z_{\text{HFB}}^{-1} \exp \left(-\beta \sum_i E_i \hat{n}_i \right) \quad , \quad (3.3)$$

$$Z_{\text{HFB}} = \text{Tr} \left[\exp \left(-\beta \sum_i E_i \hat{n}_i \right) \right] \quad , \quad (3.4)$$

where the number operator \hat{n}_i is

$$\hat{n}_i = a_i^\dagger a_i \quad . \quad (3.5)$$

(Notice that the E_0 term cancels.)

The grand partition function (3.4) is

$$Z_{\text{HFB}} = \sum_{\{n_\alpha\}} \langle \{n_\alpha\} | \exp \left(-\beta \sum_i E_i \hat{n}_i \right) | \{n_\alpha\} \rangle \quad , \quad (3.6)$$

where $\{n_\alpha\}$ denotes a complete set of quasiparticle occupation numbers $n_1 n_2 n_3 \dots$, and each n_α is either 0 or 1. There is no restriction on the number of quasiparticles, $\sum_\alpha n_\alpha$, so that the trace in Eq. (3.4) sums over the quasiparticle vacuum, one-quasiparticle states, two-quasiparticle states, etc. By expanding the exponential in Eq. (3.6) and noting that $\hat{n}_i^m = \hat{n}_i$, where m is any positive integer, it follows that

$$Z_{\text{HFB}} = \sum_{\{n_\alpha\}} \prod_i e^{-\beta E_i n_i} \quad . \quad (3.7)$$

Inspection verifies that the sum and product can be inter-changed

$$Z_{\text{HFB}} = \prod_i \sum_{n_i=0,1} e^{-\beta E_i n_i} \quad , \quad (3.8)$$

so that the independent quasiparticle grand partition function is

$$Z_{\text{HFB}} = \prod_i (1 + e^{-\beta E_i}) \quad . \quad (3.9)$$

The density operator is evaluated by expanding the exponential in Eq. (3.3)

$$D_{\text{HFB}} = Z_{\text{HFB}}^{-1} \prod_i [e^{-\beta E_i \hat{n}_i} + (1 - \hat{n}_i)] \quad , \quad (3.10)$$

and substituting Eq. (3.9),

$$D_{\text{HFB}} = \prod_i [f_i \hat{n}_i + (1 - f_i)(1 - \hat{n}_i)] \quad , \quad (3.11)$$

where f_i is defined as

$$f_i = \frac{1}{1 + e^{\beta E_i}} \quad . \quad (3.12)$$

Define the single-quasiparticle density matrix $\bar{\rho}$

$$\bar{\rho}_{ij} = \langle a_j^\dagger a_i \rangle = \text{Tr}(D a_j^\dagger a_i) \quad . \quad (3.13)$$

With the HFB approximation (3.1) it follows that

$$\bar{\rho}_{ij} = \delta_{ij} f_i \quad . \quad (3.14)$$

Consequently the quantity f_i defined in Eq. (3.12) is shown to be the quasiparticle occupation probability. At zero-temperature ($\beta = \infty$), all f_i equal zero, and the density $\bar{\rho} = 0$ represents the quasiparticle vacuum. At finite-temperature, $0 < f_i < 1$, and $\bar{\rho}$ represents a statistical mixture of quasiparticle excitations. The quasiparticle pairing tensor \bar{t} is defined as

$$\bar{t}_{ij} = \langle a_j a_i \rangle = \text{Tr}(D a_j a_i) \quad . \quad (3.15)$$

With the HFB approximation (3.1), it follows that

$$\bar{t} = 0 \quad . \quad (3.16)$$

The single-particle density matrix ρ and the particle pairing tensor t are defined by

$$\rho_{ij} = \langle C_j^\dagger C_i \rangle = \text{Tr}(D C_j^\dagger C_i) \quad , \quad (3.17)$$

$$t_{ij} = \langle C_j C_i \rangle = \text{Tr}(D C_j C_i) \quad . \quad (3.18)$$

The HFB approximation to these particle densities is obtained by inverting the quasiparticle transformation (3.2) and inserting the quasiparticle densities (3.14) and (3.16), with the result that

$$\rho = \tilde{U} f U^* + V^\dagger (1-f) V \quad , \quad (3.19)$$

$$t = \tilde{U} f V^* + V^\dagger (1-f) U \quad , \quad (3.20)$$

where the tilde signifies transpose and $f_{ij} = \delta_{ij} f_i$. At zero-temperature, $f=0$, and the particle densities reduce to their usual form.

The internal energy (2.9) is given by the expectation value of

$$H = \sum_{ij} T_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} v_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \quad . \quad (3.21)$$

At finite-temperature a statistical ensemble of quasiparticle excitations is obtained, and the quasiparticle vacuum can no longer serve as a reference state to define normal products. Consequently Wick's theorem no longer applies for operators. However, Wick's theorem remains valid for the ensemble average of operators,³⁻⁶ such as

$$\langle c_i^\dagger c_j^\dagger c_l c_k \rangle = \langle c_i^\dagger c_k \rangle \langle c_j^\dagger c_l \rangle - \langle c_i^\dagger c_l \rangle \langle c_j^\dagger c_k \rangle + \langle c_i^\dagger c_j^\dagger \rangle \langle c_l c_k \rangle \quad . \quad (3.22)$$

Consequently the internal energy is given by

$$E = \text{Tr} \left[(T + \frac{1}{2} \Gamma) \rho + \frac{1}{2} \Delta t^\dagger \right] \quad , \quad (3.23)$$

where Tr here denotes the normal trace. The HF Hamiltonian \mathcal{H} , the HF potential Γ , and the pair potential Δ are defined by

$$\mathcal{H} = T - \mu + \Gamma \quad , \quad (3.24)$$

$$\Gamma_{ij} = \sum_{kl} v_{ikjl} \rho_{lk} \quad , \quad (3.25)$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} v_{ijkl} t_{kl} \quad . \quad (3.26)$$

Observe that the energy (3.23) and the potentials (3.24 - 3.26) have the same form at finite-temperature as they do at zero-temperature. An alternative derivation of Eq. (3.23) is given in Appendix 1.

The entropy (2.10) and the particle number (2.11) are evaluated with the HFB approximation (3.1)

$$S = -k \sum_i [f_i \ln f_i + (1 - f_i) \ln (1 - f_i)] \quad , \quad (3.27)$$

$$N = \text{Tr } \rho \quad . \quad (3.28)$$

The grand potential (2.3) is obtained from Eqs. (3.23)-(3.28)

$$\begin{aligned} \Omega = & \sum_{ij} (T - \mu)_{ij} \rho_{ji} + \frac{1}{2} \sum_{ijkl} v_{ijkl} \rho_{lj} \rho_{ki} \\ & + \frac{1}{4} \sum_{ijkl} v_{ijkl} t_{ij}^* t_{kl} + kT \sum_i [f_i \ln f_i + (1 - f_i) \ln (1 - f_i)] \quad . \end{aligned} \quad (3.29)$$

IV. FTHFB EQUATIONS

The FTHFB equations are derived by minimizing the grand potential

$$\delta\Omega = 0 \quad . \quad (4.1)$$

This variation has been considered by Lee and Das Gupta.⁷ However, they did not obtain the FTHFB equations. The quantities to be varied are U , V and f . Consider the infinitesimal variations

$$U' = U + \delta U \quad , \quad (4.2)$$

$$V' = V + \delta V \quad , \quad (4.3)$$

$$f' = f + \delta f \quad . \quad (4.4)$$

Since the quasiparticle transformation

$$\begin{pmatrix} a^\dagger \\ a \end{pmatrix} = \begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix} \begin{pmatrix} c^\dagger \\ c \end{pmatrix}, \quad (4.5)$$

is required to be unitary, the variations δU and δV are not independent.

To find δU and δV , consider the infinitesimal unitary transformation

$$\begin{pmatrix} a'^\dagger \\ a' \end{pmatrix} = \left[1 + \begin{pmatrix} \epsilon_1 & \epsilon_2 \\ \epsilon_2^* & \epsilon_1^* \end{pmatrix} \right] \begin{pmatrix} a^\dagger \\ a \end{pmatrix} = \begin{pmatrix} U' & V' \\ V'^* & U'^* \end{pmatrix} \begin{pmatrix} c^\dagger \\ c \end{pmatrix}, \quad (4.6)$$

where

$$\epsilon_1^\dagger = -\epsilon_1, \quad \tilde{\epsilon}_2 = -\epsilon_2. \quad (4.7)$$

The variations δU and δV are determined by substituting Eq. (4.5) into Eq. (4.6),

$$\delta U = \epsilon_1 U + \epsilon_2 V^*, \quad (4.8)$$

$$\delta V = \epsilon_1 V + \epsilon_2 U^*. \quad (4.9)$$

The transformed particle densities are obtained by substituting U' , V' and f' into Eqs. (3.19) and (3.20),

$$\rho' = \rho + \delta\rho, \quad t' = t + \delta t, \quad (4.10)$$

$$\delta\rho = \tilde{U}(\delta\bar{\rho})U^* - V^\dagger(\delta\bar{\rho})^*V + \tilde{U}(\delta\bar{t})V - V^\dagger(\delta\bar{t})^*U^*, \quad (4.11)$$

$$\delta t = \tilde{U}(\delta\bar{\rho})V^* - V^\dagger(\delta\bar{\rho})^*U + \tilde{U}(\delta\bar{t})U - V^\dagger(\delta\bar{t})^*V^*, \quad (4.12)$$

where

$$\delta\bar{\rho} = \delta f + [f, \epsilon_1^*]_-, \quad (4.13)$$

$$\delta\bar{t} = -\epsilon_2^* + [f, \epsilon_2^*]_+. \quad (4.14)$$

The terms $\delta\bar{\rho}$ and $\delta\bar{t}$ equal the variations in the quasiparticle densities caused by the infinitesimal transformations (4.4) and (4.6). The variation in the grand potential is found by substituting ρ' , t' and f' into Eq. (3.29),

$$\Omega' = \Omega + \delta\Omega, \quad (4.15)$$

$$\begin{aligned} \delta\Omega &= \text{Tr} [\mathcal{H}(\delta\rho) + \frac{1}{2}\{\Delta(\delta t)^\dagger + \text{c.c.}\}] + kT \sum_i \ln\left(\frac{f_i}{1-f_i}\right) (\delta f_i) \\ &= \text{Tr} [(H_{11} - E)(\delta\bar{\rho}) + \frac{1}{2}\{(H_{20})^\dagger (\delta\bar{t}) + \text{h.c.}\}] , \end{aligned} \quad (4.16)$$

where

$$H_{11} = U^* \mathcal{H} \tilde{U} - V^* \mathcal{H}^* \tilde{V} + U^* \Delta \tilde{V} - V^* \Delta^* \tilde{U}, \quad (4.17)$$

$$H_{20} = U^* \mathcal{H} V^\dagger - V^* \mathcal{H}^* U^\dagger + U^* \Delta U^\dagger - V^* \Delta^* V^\dagger, \quad (4.18)$$

$$E_{ij} = \delta_{ij} E_i, \quad E_i = kT \ln\left(\frac{1-f_i}{f_i}\right). \quad (4.19)$$

Equation (4.19) can be inverted to give

$$f_i = \frac{1}{\frac{\beta E_i}{1+e}}. \quad (4.20)$$

It should be noted that H_{11} and H_{20} have the same definitions as in the $T=0$ case, except that \mathcal{H} and Δ are now temperature-dependent. Are $\delta\bar{\rho}$ and $\delta\bar{t}$ independent variations? From the definitions (4.13) and (4.14) it follows that

$$(\delta\bar{\rho})_{ii} = \delta f_i, \quad (4.21)$$

$$(\delta\bar{\rho})_{ij} = (f_i - f_j)(\epsilon_i^*)_{ij}, \quad (i \neq j) \quad (4.22)$$

$$(\delta\bar{t})_{ii} = 0, \quad (4.23)$$

$$(\delta\bar{t})_{ij} = (f_i + f_j - 1)(\epsilon_2^*)_{ij}, \quad (i \neq j) \quad (4.24)$$

Now ϵ_1 , ϵ_2 and δf are varied independently. Therefore, except for the accidental case where $f_i - f_j = 0$ or $f_i + f_j - 1 = 0$, it follows that $\delta\bar{\rho}$ and $\delta\bar{t}$ are independent variations. The variational principle $\delta\Omega = 0$ therefore requires that the coefficients of $\delta\bar{\rho}$ and $\delta\bar{t}$ vanish

$$H_{11} = E \quad , \quad (4.25)$$

$$H_{20} = 0 \quad . \quad (4.26)$$

The remainder of the derivation is the same as for $T=0$ and is given here for the sake of completeness.⁸ Define the matrices

$$\alpha = (\mathcal{H}\tilde{U} + \Delta\tilde{V})E^{-1} \quad , \quad (4.27)$$

$$\beta = (-\Delta^*\tilde{U} - \mathcal{H}^*\tilde{V})E^{-1} \quad . \quad (4.28)$$

Then the complex conjugates of Eqs. (4.25) and (4.26) are

$$(U\alpha^* + V\beta^*)E = E \quad , \quad (4.29)$$

$$(U\beta + V\alpha)E = 0 \quad . \quad (4.30)$$

The unitarity constraints on the quasiparticle transformations are

$$UU^\dagger + VV^\dagger = 1 \quad , \quad (4.31)$$

$$U\tilde{V} + V\tilde{U} = 0 \quad . \quad (4.32)$$

By comparing Eqs. (4.29) and (4.30) to Eqs. (4.31) and (4.32), it is obvious that a solution to Eqs. (4.29) and (4.30) is

$$\alpha = \tilde{U} \quad , \quad \beta = \tilde{V} \quad . \quad (4.33)$$

Substitute Eq. (4.33) into Eqs. (4.27) and (4.28)

$$\mathcal{H}\tilde{U} + \Delta\tilde{V} = \tilde{U}E \quad , \quad (4.34)$$

$$-\Delta^*\tilde{U} - \mathcal{H}^*\tilde{V} = \tilde{V}E \quad , \quad (4.35)$$

or

$$\begin{pmatrix} \mathcal{H} & \Delta \\ -\Delta^* & -\mathcal{H}^* \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix} \quad , \quad (4.36)$$

where U_i denotes the vector (U_{i1}, U_{i2}, \dots) , and similarly for V_i . Equation (4.36) is the finite-temperature HFB equation. Observe that the E_i which appears in f_i of Eq. (4.20) is indeed the quasiparticle energy.

The FTHFB equations have the same form as the $T=0$ HFB equations. Also the HF Hamiltonian (3.24), the HF potential (3.25), the pair potential (3.26), and the internal energy (3.23) have the same definitions as for zero-temperature. The only difference between the $T=0$ and the $T \neq 0$ cases is that the quasiparticle occupations f_i of Eq. (4.20) differ from zero at finite-temperature. Consequently the particle densities ρ and t , which are given by Eqs. (3.19) and (3.20), have different values at finite-temperature than for zero-temperature.

The FTHFB self-consistency conditions are that, (i) the U and V produced in successive iterations be the same, and (ii) the f produced in successive iterations be the same. The second condition is new and arises because the quasiparticle occupation f_i depends upon the quasiparticle energy E_i through Eq. (4.20), while E_i depends upon f_i through Eqs. (3.19) and (3.20). Otherwise the solution of the FTHFB equations proceeds in the same fashion as the $T=0$ HFB equations. As usual the chemical potential μ is adjusted so that the number constraint (3.28) is satisfied.

High-spin states at finite-temperature are easily obtained by including a cranking constraint. One should minimize

$$\Omega' = \Omega - \omega J_x, \quad (4.37)$$

with the constraint

$$\langle J_x \rangle = [I(I+1)]^{1/2}. \quad (4.38)$$

The resulting FTHFB-cranking equations are obtained from Eq. (4.36) by replacing the HF Hamiltonian \mathcal{H} with

$$\mathcal{H}' = \mathcal{H} - \omega J_x. \quad (4.39)$$

It is interesting to note that the zero-temperature variation produces Eq. (4.26), but not Eq. (4.25). The $T=0$ convention is to *arbitrarily* choose the quasiparticle transformations so that H_{11} is diagonal. However, for the finite-temperature case, the variational Eq. (4.25) *requires* that H_{11} equal the diagonal matrix E . The reason for this difference is easily seen by considering the generalized particle density matrix R and the generalized quasiparticle density matrix Q

$$R_{ij} = \langle d_j^\dagger d_i \rangle, \quad (4.40)$$

$$Q_{ij} = \langle b_j^\dagger b_i \rangle, \quad (4.41)$$

where

$$d^\dagger = \begin{pmatrix} c^\dagger \\ c \end{pmatrix}, \quad b^\dagger = \begin{pmatrix} a^\dagger \\ a \end{pmatrix}. \quad (4.42)$$

These densities are related by the quasiparticle transformation Z

$$R = Z^\dagger Q Z, \quad Z = \begin{pmatrix} U^* & V^* \\ V & U \end{pmatrix}, \quad Z Z^\dagger = 1. \quad (4.43)$$

The quasiparticle operators are given by the eigenvectors of R.

At zero-temperature

$$Q = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4.44)$$

and consequently,

$$R^2 = R \quad (T=0) \quad (4.45)$$

So at $T=0$, Q and R are highly degenerate with eigenvalues of 0 and 1.

This degeneracy is the cause of the arbitrariness in defining the quasiparticle transformations at $T=0$. For $T \neq 0$,

$$Q = \begin{pmatrix} f & 0 \\ 0 & 1-f \end{pmatrix}, \quad (4.46)$$

so that

$$R^2 \neq R \quad (T \neq 0) \quad (4.47)$$

At finite-temperature the degeneracy is broken. The eigenvalues of Q and R equal f_i and $1-f_i$. Except for accidental degeneracies in f_i , the quasiparticle transformations are therefore uniquely determined when $T \neq 0$.

V. FINITE-TEMPERATURE BCS

It is instructive to derive the BCS limit of the FTHFB equations.

Consider the pairing Hamiltonian

$$H = \sum_i \epsilon_i c_i^\dagger c_i - \sum_{ij>0} G_{ij} c_i^\dagger c_i^\dagger c_j^- c_j, \quad (5.1)$$

where $|\bar{i}\rangle$ is the time-reverse of $|i\rangle$, $\epsilon_{\bar{i}}$ is equal to ϵ_i , ϵ_i includes the chemical potential $-\mu$, and it is assumed that the only non-zero matrix elements v_{ijkl} are

$$v_{i\bar{i}j\bar{j}} = -G_{ij} \quad . \quad (5.2)$$

As usual, the contribution of G to the HF potential is neglected, so that $\Gamma=0$, and the HF Hamiltonian is

$$\mathcal{H}_{ij} = \epsilon_i \delta_{ij} \quad . \quad (5.3)$$

The pair potential (3.26) reduces to

$$\Delta_{ij} = \Delta_i \delta_{ij} \quad , \quad (5.4)$$

$$\Delta_i = -\sum_{k>0} G_{ik} t_{k\bar{k}} \quad . \quad (5.5)$$

Just as in the $T=0$ theory, the FTHFB energy matrix (4.36) separates into 2×2 subspaces with eigenvalues

$$E_i = E_{\bar{i}} = [\epsilon_i^2 + \Delta_i^2]^{\frac{1}{2}} \quad , \quad (5.6)$$

and eigenvectors

$$a_i^\dagger = u_i C_i^\dagger - v_i C_{\bar{i}} \quad , \quad (5.7)$$

$$a_{\bar{i}}^\dagger = u_i C_{\bar{i}}^\dagger + v_i C_i \quad , \quad (5.8)$$

where

$$u_i^2 = \frac{1}{2} (1 + \epsilon_i/E_i) \quad , \quad (5.9)$$

$$v_i^2 = \frac{1}{2} (1 - \epsilon_i/E_i) \quad . \quad (5.10)$$

So far this derivation is the same as for $T=0$. The only difference

between finite-temperature BCS and zero-temperature BCS is in evaluating the pairing tensor $t_{k\bar{k}}$, which is given by Eq. (3.20). The matrices U , V , and f are block diagonal in each two-dimensional subspace consisting of $|i\rangle$ and $|\bar{i}\rangle$. These matrices are

$$U = \begin{pmatrix} u_i & 0 \\ 0 & u_i \end{pmatrix}, \quad V = \begin{pmatrix} 0 & -v_i \\ v_i & 0 \end{pmatrix}, \quad f = \begin{pmatrix} f_i & 0 \\ 0 & f_i \end{pmatrix}. \quad (5.11)$$

Since $E_{\bar{i}} = E_i$, therefore $f_{\bar{i}} = f_i$. The pairing tensor is evaluated by substituting Eq. (5.11) into Eq. (3.20),

$$t_{i\bar{i}} = u_i v_i (1 - 2f_i), \quad (5.12)$$

where

$$u_i v_i = -\frac{\Delta_i}{2E_i}, \quad (5.13)$$

$$1 - 2f_i = \tanh(\frac{1}{2}\beta E_i). \quad (5.14)$$

The FTBCS equations are found by substituting Eqs. (5.12)-(5.14) into Eq. (5.5),

$$\Delta_i = \frac{1}{2} \sum_{j>0} G_{ij} \frac{\Delta_j}{E_j} \tanh(\frac{1}{2}\beta E_j). \quad (5.15)$$

When $T=0$, the factor $\tanh(\frac{1}{2}\beta E_j)$ equals 1, and Eq. (5.15) reduces to the zero-temperature BCS equation. When $T \rightarrow \infty$, $\tanh(\frac{1}{2}\beta E_j)$ equals 0, and the pair gap Δ_i vanishes. Pairing correlations are destroyed by increasing the temperature.

The number conservation constraint (3.28) is given by substituting Eq. (5.11) into Eq. (3.19),

$$N = 2 \sum_{i>0} [v_i^2 + (u_i^2 - v_i^2) f_i] \quad (5.16)$$

The FTBCS equations (5.15) simplify for the pairing force

$$G_{ij} = G \quad . \quad (5.17)$$

Then the pair potential has the same value for all states

$$\Delta_i = \Delta = -G \sum_{j>0} t_{jj} \quad , \quad (5.18)$$

and the gap equations are

$$1 = \frac{G}{2} \sum_{j>0} \frac{\tanh(\frac{1}{2} \beta E_j)}{E_j} \quad . \quad (5.19)$$

VI. THE DEGENERATE MODEL

The manner in which temperature destroys pairing correlations and the critical temperature at which the pair gap disappears will now be discussed. Consider the simple pairing Hamiltonian for one half-filled degenerate j -shell,

$$H = -G \sum_{mm'>0} c_m^\dagger c_m^\dagger c_{\bar{m}}, c_{m'} \quad . \quad (6.1)$$

Then $\epsilon_m = 0$ and $\mu = 0$, so that all quasiparticle energies equal Δ . The gap equations (5.19) then simplify to

$$\Delta = \Delta_0 \tanh(\frac{1}{2} \beta \Delta) \quad , \quad (6.2)$$

where

$$\Delta_0 = (2j+1) \frac{G}{4} \quad , \quad (6.3)$$

is the $T=0$ gap. The critical temperature T_c at which the gap Δ vanishes is determined by Eq. (6.2),

$$kT_c = \frac{1}{\beta_c} = \frac{\Delta_0}{2} \lim_{\Delta \rightarrow 0} \frac{\tanh(\frac{1}{2} \beta_c \Delta)}{\frac{1}{2} \beta_c \Delta} = \frac{\Delta_0}{2} . \quad (6.4)$$

The gap equation (6.2) provides the function $\Delta(T)$, which is given in Fig. 1. Increasing the temperature produces a "phase transition" from a paired state to a normal state.

VII. CONCLUSION

The finite-temperature HFB equations have been derived by minimizing the grand potential. The HFB equations as well as the HF and pair potentials have the same form for finite-temperature as for zero-temperature. The only difference between the $T \neq 0$ and $T = 0$ cases is the presence of non-zero quasiparticle occupations when $T \neq 0$. This results in different expressions for the particle densities. The BCS limit of FTHFB was obtained. The FTBCS equations were solved for the degenerate model, demonstrating that a "phase transition" from a superfluid state to a normal state is caused by raising the temperature.

In a separate article the FTHFB-cranking equations are solved for the two-level R(5) model, and various nuclear properties, such as the pair gap and the moment-of-inertia, are presented as a function of spin and temperature.

APPENDIX 1

The internal energy E of Eq. (3.23) was obtained by using the finite-temperature Wick's theorem. Alternatively, the particle Hamiltonian (3.21) can be expressed in terms of the quasiparticle operators (3.2)

$$H = H_0 + H_{11} + H_{20} + H_{22} + H_{31} + H_{40} \quad , \quad (A.1)$$

where

$$H_0 = \text{Tr}[(T + \frac{1}{2}\Gamma_0)\rho_0 + \frac{1}{2}\Delta_0 t_0^\dagger] \quad , \quad (A.2)$$

$$H_{11} = \sum_{ij} (H_{11})_{ij} a_i^\dagger a_j \quad , \quad (A.3)$$

$$H_{20} = \sum_{i>j} [(H_{20})_{ij} a_i^\dagger a_j^\dagger + (H_{20}^*)_{ij} a_j a_i] \quad , \quad (A.4)$$

$$H_{22} = \sum_{ijkl} (H_{22})_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \quad , \quad (A.5)$$

and

$$(H_{11})_{ij} = (U^* \mathcal{K}_0 \tilde{U} - V^* \mathcal{K}_0^* \tilde{V} + U^* \Delta_0 \tilde{V} - V^* \Delta_0^* \tilde{U})_{ij} \quad , \quad (A.6)$$

$$(H_{20})_{ij} = (U^* \mathcal{K}_0 V^\dagger - V^* \mathcal{K}_0^* U^\dagger + U^* \Delta_0 U^\dagger - V^* \Delta_0^* V^\dagger)_{ij} \quad , \quad (A.7)$$

$$\begin{aligned} (H_{22})_{ijkl} = & \frac{1}{4} \sum_{mnrs} v_{mnrs} [U_{im}^* U_{jn}^* U_{kr} U_{ls} \\ & + (U_{im}^* v_{ln} - U_{in}^* v_{lm})(U_{ks} v_{jr}^* - U_{kr} v_{js}^*) \\ & + v_{is}^* v_{jr}^* v_{kn} v_{lm}] \quad , \end{aligned} \quad (A.8)$$

$$\mathcal{K}_0 = T + \Gamma_0 \quad , \quad (A.9)$$

$$(\Gamma_0)_{ij} = \sum_{kl} v_{ikjl} (\rho_0)_{lk} \quad , \quad (A.10)$$

$$(\Delta_0)_{ij} = \frac{1}{2} \sum_{kl} v_{ijkl} (t_0)_{kl} \quad , \quad (\text{A.11})$$

$$\rho_0 = V^\dagger V \quad , \quad (\text{A.12})$$

$$t_0 = V^\dagger U \quad . \quad (\text{A.13})$$

Since

$$\langle H_{20} \rangle = \langle H_{31} \rangle = \langle H_{40} \rangle = 0 \quad , \quad (\text{A.14})$$

it follows that

$$\langle H \rangle = \langle H_0 \rangle + \langle H_{11} \rangle + \langle H_{22} \rangle \quad . \quad (\text{A.15})$$

At finite-temperature the independent quasiparticle term H_{11} and the quasiparticle interaction H_{22} both contribute to the energy, whereas at zero-temperature their averages vanish. These contributions are

$$\langle H_{11} \rangle = \sum_i (H_{11})_{ii} f_i = \text{Tr} [\mathcal{H}_0(\rho - \rho_0) + \Delta_0(t - t_0)^\dagger] \quad , \quad (\text{A.16})$$

$$\begin{aligned} \langle H_{22} \rangle &= \sum_{ij} \left[(H_{22})_{ijij} - (H_{22})_{ijji} \right] f_i f_j \\ &= \sum_{ijkl} v_{ijkl} \left[\frac{1}{2} (\rho - \rho_0)_{lj} (\rho - \rho_0)_{ki} + \frac{1}{4} (t - t_0)_{ij}^* (t - t_0)_{kl} \right] , \end{aligned} \quad (\text{A.17})$$

where ρ and t are defined by Eqs. (3.19) and (3.20). The internal energy (A.15) is

$$\langle H \rangle = \text{Tr} \left[(T + \frac{1}{2} \Gamma) \rho + \frac{1}{2} \Delta t^\dagger \right] \quad , \quad (\text{A.18})$$

where Γ and Δ are defined by Eqs. (3.25) and (3.26). Observe that Eq. (A.18) agrees with Eq. (3.23).

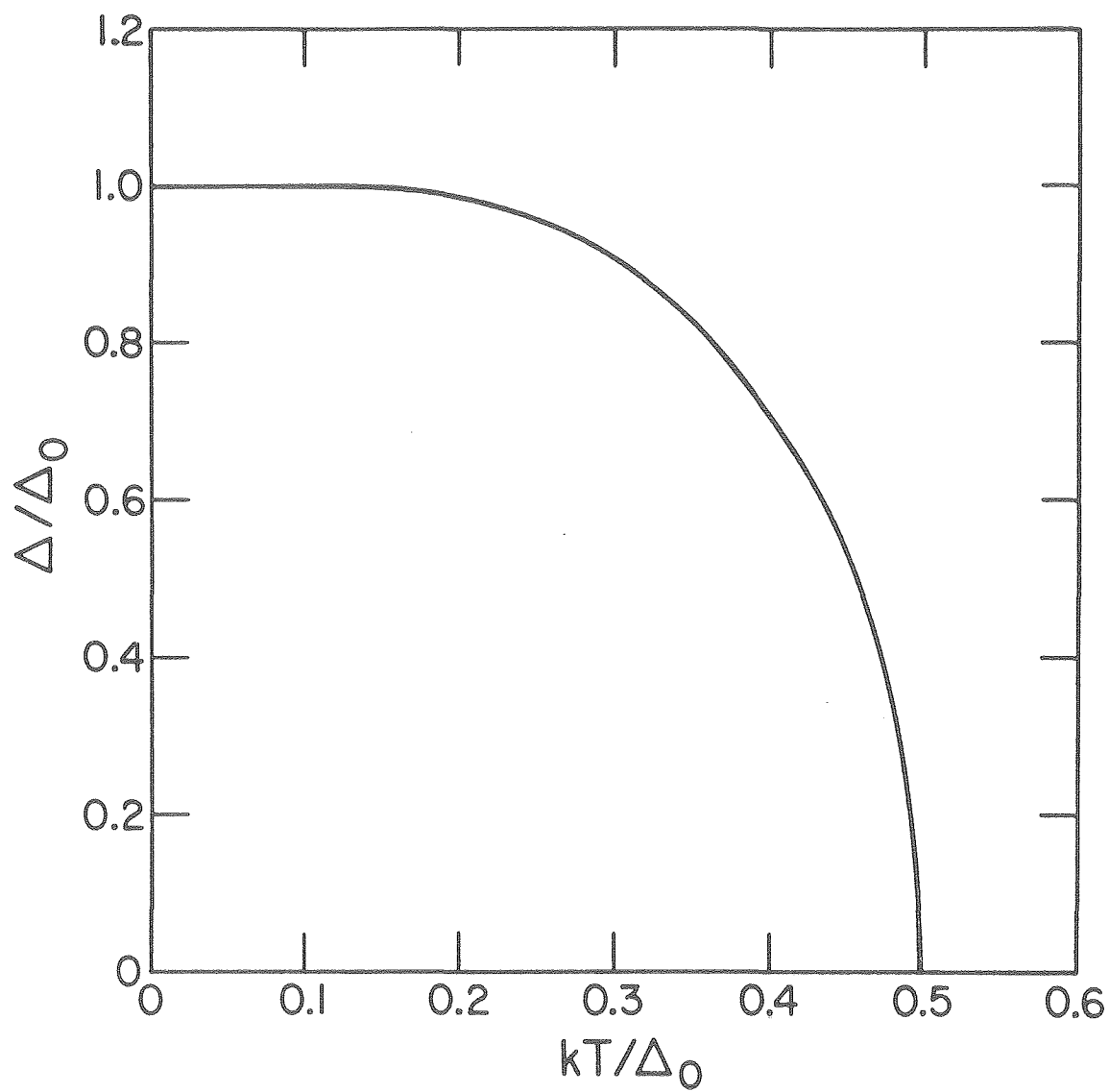
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Fig. 1. Pairing gap versus temperature in the degenerate model.

The quantity Δ_0 is the gap at $T=0$.