Nuclear shape transitions at finite temperature

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(Received 24 January 1979)

Using the grand partition function, the stability conditions for nuclear shapes at finite nuclear temperature are derived. Pairing correlations and effects of deformation inducing residual interactions are taken into account.

[NUCLEAR STRUCTURE Nuclear level density; finite temperature Hartree-Fock and Hartree-Fock-Bogoliubov; stability conditions; deformation.]

I. INTRODUCTION

Theoretical investigations of nuclear shapes are usually done in the framework of Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) theories. In many cases the spherical solution is a self-consistent solution although the corresponding energy need not be a minimum. In such a case the stability matrix for the nucleus is not positive definite and a diagonalization of the secular matrix for the excitation energies, in the random-phase approximation (RPA) or quasiparticle RPA, leads to one or more imaginary eigenvalues. This is known as the Thouless theorem.[1]

The question arises as to whether the self-consistent field, pairing field, etc., for excited states are different from those in the ground state. It is not possible to answer this question for each and every individual excited state. If, however, we are willing to investigate instead the average properties of many excited states centered about a mean excitation energy, then the problem becomes tractable. One can assume a statistical distribution of the excited states, in which case the mean excitation energy is expressed in terms of the nuclear temperature τ. In the ground state $\tau = 0$.

An interesting possibility is that a nucleus which is spherical at $\tau = 0$ may prefer a deformed shape at some finite temperature. Since a deformed nucleus generates a much higher level density, shape transitions at some $\tau > 0$ may explain why spherical model calculations underestimate level densities in some "spherical" nuclei[2-5] by large factors. Indeed, in Ref. 4 it was shown, through a variational calculation, that the Sn isotopes may become deformed at $\tau > 0$ although they are spherical at $\tau = 0$.

In this paper we seek an extension of the Thouless theorem to study, in complete generality, the shape stability of the nucleus at a given excitation energy or finite temperature. Basically we assume that above the gap the nucleus very quickly becomes amenable to a statistical description where the grand canonical partition function can be used. This implies that at any given finite temperature the nucleus is in equilibrium with the heat source, which one identifies as the experimental instrument, say a particle beam, used to excite the nucleus. This makes it very clear that the present study only applies to processes which depend on statistical averages of nuclear properties such as level densities and strength function; it does not apply to exclusive reactions where one's interest lies in a set of very specific nuclear states.

In Sec. II we review the variational principle at finite temperature using the grand partition function. In Sec. III we derive the stability condition for Hartree-Fock solutions at finite temperature. We compare our result with the Thouless theorem. The most important part of this paper is Sec. IV, where we derive the stability condition at finite temperature for the more general and useful Hartree-Fock-Bogoliubov solutions.

In the last section we complete the derivation of the formalism by performing the necessary angular momentum coupling and separating the stability equations into distinct spin-parity channels. Furthermore, by comparing with the stability equations at $\tau = 0$, we identify the extra terms at $\tau > 0$ which do not have counterparts in the $\tau = 0$ equations. These extra terms reflect the extra degree of freedom in the averaging procedure at $\tau > 0$, and the role they play in the shape stability of spherical nuclei is the subject of another study.

II. THE VARIATIONAL PRINCIPLE AT FINITE TEMPERATURE

The variational principle of a grand canonical ensemble is well known in the literature.[6] For completeness, we state the contents of the principle that is pertinent to the present work.

The grand partition function Z is defined as

$$Z = \mathrm{Tr}\exp[-(H-\mu N)/\tau], \tag{1}$$

where Tr is the trace, H is the Hamiltonian, N is the number operator, and μ is the chemical potential. The true density matrix is

$$\omega = \frac{e^{-(H-\mu N)/\tau}}{Z}. \tag{2}$$

It is a matrix with unit trace. For variational calculations, one chooses trial values of ω, i.e., replaces ω by W which is a simpler matrix with unit trace. Now for any two matrices with unit trace, the following inequality holds[7]:

$$\mathrm{Tr}W\ln\omega \leq \mathrm{Tr}W\ln W.$$

The trial value of entropy, however, is

$$\sigma = -\mathrm{Tr}W\ln W. \tag{3}$$

We therefore get

$$\begin{aligned}\sigma &\leq -\mathrm{Tr}W\ln\omega\\ &= -\mathrm{Tr}W[-(H-\mu N)/\tau - \ln Z].\end{aligned} \tag{4}$$

Thus,

$$\langle H\rangle - \mu\langle N\rangle - \tau\sigma \geq -\tau\ln Z, \tag{5}$$

where we have introduced the notation that for any operator

$$\langle\theta\rangle = \langle\theta\rangle_W \equiv \mathrm{Tr}W\theta.$$

If we now call $\mathfrak{F}$, the left-hand side of Eq. (5), then the minimization principle tells us that we must have

$$\delta\mathfrak{F} = 0 \quad \text{(stationary condition)}, \tag{6}$$

$$\delta^2\mathfrak{F} > 0 \quad \text{(stability condition)}. \tag{7}$$

A trial wave function or configuration is stable if both (6) and (7) are satisfied; it is unstable if (7) is not satisfied. In the following sections, we first choose a trial density W; we then derive the stability conditions by expressing the left-hand sides of (6) and (7) in terms of variations in W.

III. THE STABILITY CONDITION AT FINITE TEMPERATURE IN THE HARTREE-FOCK APPROXIMATION

The stability condition in the Hartree-Fock approximation was derived by Mermin,[8] who studied a lattice gas having attractive interactions. In this section we rederive and extend his results using somewhat different methods. This paves the way for the considerably more complex derivation, in the next section, of the stability conditions in the Hartree-Fock-Bogoliubov approximation.

The trial density matrix in HF is of the form

$$W = \exp\Big(-\sum_i \gamma_i c_i^\dagger c_i\Big)\Big/\mathrm{Tr}\Big[\exp\Big(-\sum \gamma_i c_i^\dagger c_i\Big)\Big], \tag{8}$$

where $c_i^\dagger(c_i)$ is a particle creation (annihilation) operator and the γ_i's are real c numbers. The denominator in (8) ensures that W is unitary. With W given by (8) it is most convenient to express $H-\mu N$ in terms of the creation and annihilation operators

$$H_\mu \equiv H - \mu N = \sum_{ij} t_{ij} c_i^\dagger c_j + \tfrac{1}{4}\sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k, \tag{9}$$

where t is the one-body term including the term μN, and V is the antisymmetrized two-body interaction. It is then easy to verify that

$$\begin{aligned}\mathfrak{F} = &\sum_{ij} t_{ij}\rho_{ji} + \tfrac{1}{2}\sum_{ijkl} V_{ikjl}\rho_{ji}\rho_{lk}\\ &+ \sum_i [f_i\ln f_i + (1-f_i)\ln(1-f_i)],\end{aligned} \tag{10}$$

where, in the diagonal basis,

$$\begin{aligned}\rho_{ji} &\equiv \langle c_i^\dagger c_j\rangle = \mathrm{Tr}(W c_i^\dagger c_j)\\ &= \delta_{ij}\frac{1}{1+e^{\gamma_i}} \equiv \delta_{ij} f_i.\end{aligned} \tag{11}$$

To obtain the appropriate expression for $\delta\mathfrak{F}$ and $\delta^2\mathfrak{F}$, we now consider the infinitesimal transformations

$$f_i \to f_i' = f_i + \eta_i, \tag{12a}$$

$$c_i^\dagger \to c_i'^\dagger,$$

$$c_i^\dagger = \sum_k [\delta_{ik} + \epsilon_{ik} + N_{ik}(\epsilon^2)] c_k'^\dagger. \tag{12b}$$

To ensure that the transformation (12b) is unitary to order ϵ^2, we require that ϵ be anti-Hermitian ($\epsilon = -\epsilon^\dagger$) and $N = -\frac{1}{2}\epsilon\epsilon^\dagger$, which is Hermitian. We now write

$$\rho_{ji} \to \rho_{ji}' = \rho_{ji} + \rho_{ji}^{(1)} + \rho_{ji}^{(2)}, \tag{13}$$

where $\rho_{ji}' = \mathrm{Tr}W' c_i^\dagger c_j = \langle c_i^\dagger c_j\rangle'$. Since $\langle c_i^\dagger{}' c_j{}'\rangle' = \delta_{ij}$

$(f_i+\eta_i)$, expressing $c_j^\dagger$, c_i in terms of $c_j^{\dagger\prime}c_i'$ and using the notation that $\rho^{(n)}$ is n^{th} order in ϵ and η, we find

$$\rho_{ji}^{(1)}=\delta_{ij}\eta_i+\epsilon_{ji}(f_i-f_j)\,, \tag{14a}$$

$$\rho_{ji}^{(2)}=\epsilon_{ji}(\eta_i-\eta_j)+\sum_k \epsilon_{jk}\epsilon_{ik}^* f_k+N_{ji}(f_i+f_j)\,. \tag{14b}$$

We note that both $\rho^{(1)}$ and $\rho^{(2)}$ are Hermitian. The variation in $\mathfrak{F}$ can now be obtained. To first order in ϵ and η,

$$\delta\mathfrak{F}=\sum_{ij}\left(t_{ij}+\sum_k V_{ikjk}f_k\right)[\delta_{ij}\eta_i+\epsilon_{ji}(f_i-f_j)] +\tau\sum_i \eta_i \ln\frac{f_i}{1-f_i}\,. \tag{15}$$

For $\delta\mathfrak{F}$ to vanish, the coefficients of ϵ_{ji} and η_i must vanish separately; thus we obtain the HF stationary conditions at finite temperature

$$t_{ij}+\sum_k V_{ikjk}f_k=\delta_{ij}E_i\,, \tag{16a}$$

$$f_i=[1+\exp(E_i/\tau)]^{-1}\,. \tag{16b}$$

To second order in ϵ and η we find

$$\delta^2\mathfrak{F}=\tfrac{1}{2}\sum_{ijkl}V_{ikjl}\rho_{ji}^{(1)}\rho_{lk}^{(1)}+\sum_i E_i\rho_{ii}^{(2)} +\frac{\tau}{2}\sum_i\frac{\eta_i^2}{f_i(1-f_i)}\,, \tag{17}$$

where we have used (16a). Using (14) and the limit

$$\lim_{E_i\to E_j}\frac{E_i-E_j}{f_j-f_i}=\frac{\tau}{f_i(1-f_i)}\,,$$

the last two terms on the right-hand side of Eq. (17) can be expressed in terms of $\rho^{(1)}$. The HF stability condition can thus be written as

$$\delta^2\mathfrak{F}=\tfrac{1}{2}\rho_{ij}^{(1)*}S_{jilk}\rho_{kl}^{(1)}>0\,, \tag{18}$$

where

$$S_{jilk}=\delta_{ik}\delta_{jl}\frac{E_i-E_j}{f_j-f_i}+V_{iljk}\,. \tag{19}$$

We introduce here a matrix multiplication notation $\theta_1\phi\theta_2$, where θ_1 and θ_2 have two indices and ϕ has four:

$$\theta_1\phi\theta_2\equiv(\theta)_{ik}(\phi)_{kijl}(\theta_2)_{lj}\,. \tag{20}$$

We will also use

$$(\theta_1\phi)_{jl}=(\theta_1)_{ik}(\phi)_{kijl} \tag{21}$$

and

$$(\phi\theta_2)_{ki}=\phi_{kijl}(\theta_2)_{lj}\,. \tag{22}$$

With the notation of Eq. (20), Eq. (18) can be written as

$$\delta^2\mathfrak{F}=\tfrac{1}{2}\rho^{(1)*}S\rho^{(1)}>0\,. \tag{23}$$

Since $\rho_{ij}^*=\rho_{ji}$ we can rewrite (18) in terms of ρ_{ii}(real), ρ_{ij}^* $(i>j)$, and ρ_{ij} $(i>j)$. Let there be n orbitals $(\sum_i=n)$, then we find that (18) can be written as

$$(\rho_{ii}\rho_{ij,\,i>j}^*\rho_{ij,\,i>j})\begin{pmatrix}P & D & D^*\\ D^\dagger & A & B\\ D^T & B^* & A^*\end{pmatrix}\begin{pmatrix}\rho_{ii}\\ \rho_{ij,\,i>j}\\ \rho_{ij,\,i>j}^*\end{pmatrix}\geqslant 0\,, \tag{24}$$

where P is an $n\times n$ matrix, D is $n\times(n-1)/2$, and A and B are each $n(n-1)/2\times n(n-1)/2$. Let x stand for $i\geqslant j$ and y for $k\geqslant l$, then

$$\begin{aligned}P_{xy}&=\delta_{xy}\tau\frac{1}{f_i(1-f_i)}+V_{ikik}=P_{xy}^*\,,\\ D_{xy}&=V_{ilik}\,,\\ A_{xy}&=\delta_{xy}\frac{E_i-E_j}{f_j-f_i}+V_{iljk}=A_{yx}^*\,,\\ B_{xy}&=V_{ikjl}=B_{yx}\,.\end{aligned} \tag{25}$$

The matrix B is exactly the same as in the zero temperature case[9]; except for the modification of the diagonal terms, the matrix A is also the same. The matrices P and D are new. The matrix P is real; in the limit of zero temperature the diagonal terms of P go to infinity.

We can now show that in order that Eq. (24) be satisfied, the big matrix of Eq. (24) must be positive definite. It is a Hermitian matrix, thus all its eigenvalues are real. Let

$$\begin{pmatrix}E\\ F\\ G\end{pmatrix}$$

be an eigenvector with eigenvalue λ. Taking the complex conjugate we verify that

$$\begin{pmatrix}E^*\\ G^*\\ F^*\end{pmatrix}$$

is also an eigenvector with the same eigenvalue. Therefore

$$\begin{pmatrix}E+E^*\\ F+G^*\\ G+F^*\end{pmatrix}$$

is also an eigenvector with the same eigenvalue. However, this last vector is of the same form as the vector of Eq. (24). Therefore, if there is a negative eigenvalue, Eq. (24) will not always be satisfied.

In most practical calculations the matrix elements V_{iljk} are all real. In such cases further simplifications are possible. We write

$$\rho^{(1)} = \rho^r + i\rho^i ;$$

then Eq. (23) can be written as

$$\rho^{(1)*}S\rho^{(1)} = \rho^r S\rho^r + \rho^i S\rho^i + i(\rho^r S\rho^i - \rho^i S\rho^r) . \qquad (26)$$

One can now show that the quantity within parentheses on the right-hand side of Eq. (26) is zero. Since ρ^r is symmetric and ρ^i is antisymmetric, not all elements of ρ^r and ρ^i are linearly independent. We remove this degeneracy by defining the vectors $\rho^{(\pm)}$ spanned by the ordered pairs x, y, etc.:

$$x = i,j \quad i \geq j \text{ for } \rho^{(+)} ,$$
$$= i,j \quad i > j \text{ for } \rho^{(-)} .$$

Then

$$\rho^{(1)*}S\rho^{(1)} = 2\rho^{(+)}S^{(+)}\rho^{(+)} + 2\rho^{(-)}S^{(-)}\rho^{(-)} , \qquad (27)$$

where

$$S^{(\pm)}_{xy} = \delta_{xy} n_x \frac{E_i - E_j}{f_j - f_i} + n_x n_y (V_{iljk} \pm V_{ikjl}) , \qquad (28)$$

where $n_x^{-1} = 1 + \delta_{ij}$. The $\rho^{(+)}$, $\rho^{(-)}$ are now completely arbitrary, thus for stability one needs both $S^{(+)}$ and $S^{(-)}$ to be positive definite. We adopt the notation

$$\delta^2\mathfrak{F} = \sum \rho^{\odot} S^{\odot} \rho^{\odot} , \qquad (29)$$

where $\odot = (+)$ and $(-)$. Since all elements of $\rho^{(\pm)}$ are now linearly independent, $\delta^2\mathfrak{F} > 0$ only if *both* $S^{(+)}$ and $S^{(-)}$ are positive definite, i.e., *all* eigenvalues of $S^{(\pm)}$ are positive. The HF stability condition at finite temperature can be stated as follows: *The* HF *stationary conditions* [(16a) and (16b)] *are stable only if both the stability matrices* $S^{(+)}$ *and* $S^{(-)}$ *are positive definite.* It is interesting to note that $S^{(\pm)}$ are temperature dependent only through the temperature dependence of E_i and f_i.

We now wish to establish a connection with that part of the Thouless theorem which links the possible appearance of imaginary phonon energies in the random-phase approximation[1] (RPA) to the appearance of negative eigenvalues for the stability matrix. This connection is important because it enriches the physical content of the stability condition; when a state is unstable, it is natural to expect the existence of at least one state that has a lower energy and is tunneling underneath it. A tunneling state has imaginary energy.

As stated earlier, at $\tau = 0$, $f_p = 0$, $f_h = 1$, and pairs with $i = j$ do not appear in the stability formalism. At finite temperature, all terms with indices $i = j$ are therefore "extra terms" partly associated with the entropy in the free energy. We must bear this point in mind as we proceed.

The matrices

$$\mathcal{A} = \tfrac{1}{2}(S^{(+)} + S^{(-)}), \quad \mathcal{B} = \tfrac{1}{2}(S^{(+)} - S^{(-)})$$

calculated from $S^{(+)}$ and $S^{(-)}$ for $\tau = 0$ are precisely those that appear in the secular matrix for phonon energies in RPA

$$\omega = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} .$$

At the same time, under a similarity transformation

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

the stability matrix becomes

$$S_U \equiv U^{-1} \begin{pmatrix} S^{(+)} & 0 \\ 0 & S^{(-)} \end{pmatrix} U = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B} & \mathcal{A} \end{pmatrix} ,$$

which is identical to the Thouless stability matrix.[1] We have thus shown that Eq. (29) has the correct $\tau = 0$ limit. The connection between the nonpositive definiteness of S_U and the appearance of imaginary eigenvalues in ω was shown by Thouless[1].

IV. THE STABILITY CONDITIONS AT FINITE TEMPERATURE IN THE HARTREE-FOCK BOGOLIUBOV APPROXIMATION

In the HF approximation any nucleus that does not have a doubly closed shell would be deformed (at $\tau = 0$). The fact that most spherical nuclei are not doubly closed shell nuclei and also not deformed is due to pairing correlations that are totally ignored in HF. In the HFB approximation the pairing interaction, which inhibits deformation, is taken into account in such a way that it is in direct competition with the deformation inducing interactions. The nucleus is spherical when the pairing interaction is predominant, but becomes deformed when the pairing interaction is overcome, by whatever mechanism, by the deformation inducing interaction. In fact the phenomenon of a "phase transition" in nuclear shape with the atomic mass being the varying parameter is well known. Here we study changes in nuclear shape within a nucleus, and with the nuclear temperature acting as the variation parameter; such changes are phase transitions in the normal sense of the word.

The only, but crucial, difference between HF and HFB is the replacement of (8) for HF by the new density matrix

$$W=\exp(-\sum_i \gamma_i a_i^\dagger a_i)/\mathrm{Tr}[\exp(-\sum_i \gamma_i a_i^\dagger a_i)] \tag{30}$$

for HFB. In (30) $a_i^\dagger$ and a_i are quasiparticle (qp) operators related to $c_\alpha^\dagger, c_\beta$ by a unitary transformation. Following the notation of Baranger,[9]

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix}_\alpha = (U_c)_{\alpha i} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}_i \equiv \begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix}_{\alpha i} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}_i , \tag{31}$$

where from now on repeated indices are to be summed over. The transformations A and B in (31) are not to be confused with those defined in (24). The unitarity of U_c demands that

$$AA^\dagger + B^*B^\dagger = 1, \quad AB^\dagger + B^*A^\dagger = 0 .$$

With W given by (30),

$$\rho_{ji} = \rho_{ij}^* \equiv \langle a_i^\dagger a_j \rangle = \delta_{ij} f_i, \quad f_i = \frac{1}{1+e^{\gamma_i}} , \tag{32a}$$

$$\kappa_{ji} = \kappa_{ij} \equiv \langle a_i a_j \rangle = 0 , \tag{32b}$$

in the diagonal basis. Therefore, if we write the Hamiltonian as

$$\begin{aligned} H_\mu &= H - \mu N \equiv t_{\alpha\beta} c_\alpha^\dagger c_\beta + \tfrac{1}{4} V_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma \\ &= H_0 + \tilde{t}_{ij} a_i^\dagger a_j + \tfrac{1}{4} \tilde{V}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \\ &\quad + \{aa \text{ terms} + a^\dagger aaa \text{ terms} + aaaa \text{ terms} + \text{H.c.}\} , \end{aligned} \tag{33}$$

the terms in the brackets do not contribute to $\mathrm{Tr}(WH_\mu)$. Anticipating the subsequent variational calculation we write

$$\begin{aligned} \mathrm{Tr}(WH_\mu) &= H_0 + \tilde{t}_{ii} + \tfrac{1}{4}(\tilde{V}_{ijij} - \tilde{V}_{ijji}) f_i f_j \\ &= t_{\alpha\beta} \tilde{\rho}_{\beta\alpha} + \tfrac{1}{2} V_{\alpha\beta\gamma\delta} \tilde{\rho}_{\delta\beta} \tilde{\rho}_{\gamma\alpha} + \tfrac{1}{4} \tilde{\kappa}_{\beta\alpha} G_{\alpha\beta\gamma\delta} \tilde{\kappa}_{\delta\gamma} \\ &= t\tilde{\rho} + \tfrac{1}{2}\tilde{\rho}^* F^* \tilde{\rho} + \tfrac{1}{4}\tilde{\kappa}^* G \kappa , \end{aligned} \tag{34}$$

where

$$F_{\alpha\gamma\delta\beta} = V_{\alpha\beta\gamma\delta} = V_{\beta\alpha\delta\gamma} = F_{\beta\delta\gamma\alpha} \tag{35a}$$

is the F matrix or particle-hole interaction and

$$G_{\alpha\beta\gamma\delta} = V_{\alpha\beta\gamma\delta} \tag{35b}$$

is the G matrix or the particle-particle interaction:

$$\begin{aligned} \tilde{\rho}_{\beta\alpha} = (\tilde{\rho}^\dagger)_{\beta\alpha} &= \langle c_\alpha^\dagger c_\beta \rangle \\ &= [A\rho A^\dagger + B^*(1-\rho^*)B^T + A\kappa B^T - B^*\kappa^* A^\dagger]_{\beta\alpha} , \end{aligned} \tag{36a}$$

$$\begin{aligned} \tilde{\kappa}_{\beta\alpha} = -\tilde{\kappa}_{\alpha\beta} &= \langle c_\alpha c_\beta \rangle \\ &= [A\rho B^\dagger + B^*(1-\rho^*)A^T + A\kappa A^T - B^*\kappa^* B^\dagger]_{\beta\alpha} . \end{aligned} \tag{36b}$$

The free energy is now

$$\begin{aligned} &= \mathrm{Tr}(WH_\mu) - \tau\sigma \\ &= t\tilde{\rho} + \tfrac{1}{2}\tilde{\rho}^* F^* \rho + \tfrac{1}{4}\tilde{\kappa}^* G \tilde{\kappa} \\ &\quad + \tau \sum_i [f_i \ln f_i + (1-f_i)\ln(1-f_i)] . \end{aligned} \tag{37}$$

For $\tilde{\rho}$, $\tilde{\kappa}$ given by (36) and (32), we have

$$\tilde{\rho} = AfA^\dagger + B^*(1-f)B^T ,$$

$$\tilde{\kappa} = AfB^\dagger + B^*(1-f)A^T .$$

To obtain variations in $\mathfrak{F}$, we consider the infinitesimal transformations

$$f \to f' = f + \eta , \tag{38a}$$

$$\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = U_a \begin{pmatrix} a' \\ a'^\dagger \end{pmatrix} , \tag{38b}$$

with

$$U_a = 1 + \begin{pmatrix} \epsilon & \phi \\ \phi^* & \epsilon^* \end{pmatrix} + \begin{pmatrix} N_1 & N_2 \\ N_2^* & N_1 \end{pmatrix} ,$$

$$\epsilon = -\epsilon^\dagger ; \quad \phi = -\phi ; \quad N_1 = N_1^\dagger = -\tfrac{1}{2}(\epsilon\epsilon^\dagger + \phi\phi^\dagger) ;$$

$$N_2 = N_2^T = -\tfrac{1}{2}(\epsilon\phi^T + \phi\epsilon^T) .$$

The N_1, N_2 terms are there to ensure that U_a is unitary to second order in ϵ and ϕ. Equation (38) implies

$$W \to W' = e^{-\gamma_i a_i'^\dagger a_i'}/\mathrm{Tr}(e^{-\gamma_i a_i'^\dagger a_i'}) , \tag{39}$$

resulting in

$$\rho \to \rho' = \langle a^\dagger a \rangle_{W'} \equiv \rho + \rho^{(1)} + \rho^{(2)} , \tag{40a}$$

$$\kappa \to \kappa' = \langle aa \rangle_{W'} \equiv \kappa + \kappa^{(1)} + \kappa^{(2)} , \tag{40b}$$

where $\langle\ \rangle_{W'}$ denotes evaluation with the new density matrix and the superscript indicates the order of variation. From (38) we obtain

$$\rho^{(1)} = \rho^{(1)\dagger} = \{\epsilon, f\}_- + \eta , \tag{41a}$$

$$\kappa^{(1)} = -\kappa^{(1)T} = \tfrac{1}{2}\{\phi, (1-2f)\}_+ , \tag{41b}$$

$$\rho^{(2)} = \rho^{(2)\dagger} = \{\epsilon, \eta\}_- + \phi(1-f)\phi^\dagger + \epsilon f \epsilon^\dagger + \{N_1, f\}_+ , \tag{41c}$$

$$\kappa^{(2)} = -\kappa^{(2)T} = -\{\phi, \eta\}_+ + \tfrac{1}{2}\phi(1-2f)\epsilon^T - \tfrac{1}{2}\epsilon(1-2f)\phi^T . \tag{41d}$$

The notation of (41) is, e.g.,

$$[\phi(1-2f)\epsilon^\dagger]_{ij} = \phi_{ik}(1-2f_k)\epsilon^*_{jk},$$

and $\{a,b\}_\pm = ab \pm ba$. Substituting (41) into (36), we have

$$\tilde{\rho} \to \tilde{\rho}' = \tilde{\rho} + \tilde{\rho}^{(1)} + \tilde{\rho}^{(2)}, \tag{42a}$$

$$\tilde{\kappa} \to \tilde{\kappa}' = \tilde{\kappa} + \tilde{\kappa}^{(1)} + \tilde{\kappa}^{(2)}, \tag{42b}$$

where from (36)

$$\tilde{\rho}^{(n)} = \tilde{\rho}^{(n)\dagger} = A\rho^{(n)}A^\dagger - B^*\rho^{(n)*}B^{\mathcal{T}} + A\kappa^{(n)}B^{\mathcal{T}} - B^*\kappa^{(n)*}A^\dagger, \tag{42c}$$

$$\tilde{\kappa}^{(n)} = -\tilde{\kappa}^{(n)\dagger} = A\rho^{(n)}B^\dagger - B^*\rho^{(n)*}A^{\mathcal{T}} + A\kappa^{(n)}A^{\mathcal{T}} - B^*\kappa^{(n)*}B^\dagger, \tag{42d}$$

$n=1,\ 2$. It follows that

$$\begin{aligned}\delta\mathfrak{F} &= (t+\tilde{\rho}^*F^*)\tilde{\rho}^{(1)} + \tfrac{1}{4}\tilde{\kappa}^*G\tilde{\kappa}^{(1)} + \tfrac{1}{4}\tilde{\kappa}^{(1)*}G\tilde{\kappa} + \tau\sum_i \eta_i \ln\frac{f_i}{1-f_i} \\ &= \left(U_{ij} + \delta_{ij}\tau\ln\frac{f_i}{1-f_i}\right)\rho^{(1)}_{ij} + (R_{ij}\kappa^{(1)}_{ij} + \mathrm{cc}).\end{aligned} \tag{43}$$

The stationary conditions $\delta\mathfrak{F}=0$ are thus

$$R_{ij} = R^*_{ij} = 0, \tag{44a}$$

$$U_{ij} = 0, \quad i \neq j \tag{44b}$$

and

$$U_{ii} + \tau\ln\frac{f_i}{1-f_i} = 0, \quad \text{or } f_i = 1/(1+e^{U_{ii}/\tau}). \tag{44c}$$

U_{ii} is identified as the quasiparticle energy

$$U_{ii} \equiv E_i = (t+\tilde{\rho}^*F^*)_{\alpha\beta}(A_{\beta i}A^*_{\alpha i} - B^*_{\beta i}B_{\alpha i}) + \tfrac{1}{4}[(\tilde{\kappa}^*G)_{\alpha\beta}(A_{\beta i}B^*_{\alpha i} - B^*_{\beta i}A_{\alpha i}) + \mathrm{cc}], \tag{45}$$

where i is *not* summed over. We do not need the explicit expression for R_{ij} except to note that (32a) is useful to identify certain terms in $\delta^2\mathfrak{F}$ as being zero. Because of (36), it is clear that $\delta^2\mathfrak{F}$ takes the form

$$\delta^2\mathfrak{F} = U_{ij}\rho^{(2)}_{ij} + \frac{\tau}{2}\sum_i \frac{\eta_i^2}{f_i(1-f_i)} + (R_{ij}\kappa^{(2)}_{ij} + \mathrm{cc}) + \tfrac{1}{2}\tilde{\rho}^{(1)\dagger}F^*\tilde{\rho}^{(1)} + \tfrac{1}{4}\tilde{\kappa}^{(1)\dagger}G\tilde{\kappa}^{(1)}. \tag{46}$$

From (44) all coefficients of $R^{(2)}_{ij}$ vanish; from (44b) all off-diagonal terms of U_{ij} vanish. After some manipulation, we find that

$$U_{ii}\rho^{(2)}_{ii} + \frac{\tau}{2}\sum_i \frac{\eta_i^2}{f_i(1-f_i)} = \tfrac{1}{2}(\rho^{(1)\dagger})_{ji}\frac{E_i - E_j}{f_j - f_i}\rho^{(1)}_{ij} + \tfrac{1}{2}(\kappa^{(1)\dagger})_{ji}\frac{E_i + E_j}{1-f_i-f_j}\kappa^{(1)}_{ij}. \tag{47}$$

From Eqs. (46), (47), and (42), it is clear that $\delta^2\mathfrak{F}$ can be expressed in terms $\rho^{(1)}$ and $\kappa^{(1)}$ only. We now specialize to the case where all two-body matrix elements are real. In order to further reduce the expression such that only linearly independent elements of $\rho^{(1)}$ and $\kappa^{(1)}$ are involved, we separate them into real and imaginary parts

$$\rho^{(1)} \equiv \rho^{(+)} + i\rho^{(-)}, \quad \kappa^{(1)} = \kappa^{(+)} + i\kappa^{(-)}, \tag{48}$$

where $\rho^{(\pm)}$, $\kappa^{(\pm)}$ are real, $\rho^{(+)}$ is symmetric, and the three others are antisymmetric. We now write

$$\tilde{\rho}^{(1)} = P^{(+)}\rho^{(+)} + iP^{(-)}\rho^{(-)} + Q^{(+)}\kappa^{(+)} + iQ^{(-)}\kappa^{(-)}, \tag{49a}$$

$$\tilde{\kappa}^{(1)} = M^{(+)}\rho^{(+)} + iM^{(-)}\rho^{(-)} + N^{(+)}\kappa^{(+)} + iN^{(-)}\kappa^{(-)}, \tag{49b}$$

where the notation is

$$(P\rho)_{\alpha\beta} = \sum_{i\geq j} P^{ij}_{\alpha\beta}\rho_{ij},$$

and from now on only *ordered* pairs $(i \geq j)$ are summed over. Comparing (49) and (42), we have

$$P^{(\pm)ij}_{\alpha\beta} = (A_{\alpha i}A^*_{\beta j} \pm A_{\alpha j}A^*_{\beta i} - B^*_{\alpha j}B_{\beta i} \mp B^*_{\alpha i}B_{\beta j})\frac{1}{1+\delta_{ij}}, \tag{50a}$$

$$Q^{(\pm)ij}_{\alpha\beta} = (A_{\alpha i}B_{\beta j} \pm B^*_{\alpha j}A^*_{\beta i} - A_{\alpha j}B_{\beta i} \mp B^*_{\alpha i}A^*_{\beta j})\frac{1}{1+\delta_{ij}}, \tag{50b}$$

$$M^{(\pm)ij}_{\alpha\beta} = (A_{\alpha i}B^*_{\beta j} \pm A_{\alpha j}B^*_{\beta i} - B^*_{\alpha j}A_{\beta i} \mp B^*_{\alpha i}A_{\beta j})\frac{1}{1+\delta_{ij}}, \tag{50c}$$

$$N^{(\pm)ij}_{\alpha\beta} = (A_{\alpha i}A_{\beta j} \pm B^*_{\alpha j}B^*_{\beta i} - A_{\alpha j}A_{\beta i} \mp B^*_{\alpha i}B^*_{\beta j})\frac{1}{1+\delta_{ij}}. \tag{50d}$$

Owing to the Hermiticity of the Hamiltonian and W, $\mathfrak{F}$ must be real, therefore all (+) (−) cross terms, which are imaginary, cannot contribute to $\delta^2\mathfrak{F}$. We can therefore write, similar to (28),

$$\delta^2\mathfrak{F} = \sum_{\odot=(+),(-)} (\Gamma^\odot)^\dagger \cdot S^\odot \cdot \Gamma^\odot, \tag{51}$$

where for $\odot = (+)$ or $(-)$

$$\Gamma = \begin{pmatrix}\rho \\ \kappa\end{pmatrix}, \quad S = \begin{pmatrix} C & E \\ E^\dagger & D\end{pmatrix}, \tag{52}$$

the indices for the vectors ρ and κ and the matrices C, E, and D are the ordered pairs $x = (i \geq j)$. Thus

$$\Gamma^\dagger \cdot S \cdot \Gamma = \rho^*_x C_{xy}\rho_y + (\rho^*_x E_{xy}\kappa_y + \mathrm{cc}) + \kappa^*_x D_{xy}\kappa_y.$$

The submatrices of S are

$$C_{xy}=\delta_{xy}\frac{1}{1+\delta_{ij}}\frac{E_i-E_j}{f_j-f_i}+\tfrac{1}{2}(P^*FP)_{xy}+\tfrac{1}{4}(M^*GM)_{xy}, \tag{53a}$$

$$D_{xy}=\delta_{xy}\frac{1}{1+\delta_{ij}}\frac{E_i+E_j}{1-f_i-f_j}+\tfrac{1}{2}(Q^*FQ)_{xy}+\tfrac{1}{4}(N^*GN)_{xy}, \tag{53b}$$

$$E_{xy}=\tfrac{1}{2}(P^*FQ)_{xy}+\tfrac{1}{4}(M^*GN), \tag{53c}$$

$$(E^\dagger)_{xy}=\tfrac{1}{2}(Q^*FP)_{xy}+\tfrac{1}{4}(N^*GM)_{xy}, \tag{53d}$$

with the notation being, e.g.,

$$(P^*FQ)_{ij,kl}=P^{*ij}_{\beta\alpha}F_{\alpha\beta\gamma\delta}Q^{kl}_{\delta\gamma}.$$

Since all elements in $\Gamma^{(+)}$ and $\Gamma^{(-)}$ are linearly independent, the HFB stability condition is as follows: *The stationary conditions* (44) *are stable, or* $\delta^2\mathfrak{F}>0$, *only if both the stability matrices* $S^{(+)}$ *and* $S^{(-)}$ *are positive definite.*

V. ANGULAR MOMENTUM COUPLING FOR A SPHERICAL NUCLEUS

Equations (51)–(53) are the stability conditions for a general HFB configuration at finite temperature. To bring the development of the formalism one step further so that angular momentum becomes an apparently good quantum number, we restrict our consideration to spherical nuclei only. In this case Eq. (31) can be reduced to a Bogoliubov-Valatin[10] transformation

$$A_{\alpha i}=\delta_{\alpha i}u_a,\quad B_{\alpha i}=\delta_{\bar\alpha i}s_\alpha v_a, \tag{54}$$

where the u, v factors are τ dependent; a stands for all quantum numbers of an orbit except its magnetic quantum number m_a, $\alpha\equiv(a,m_a)$, $\bar\alpha\equiv(a,-m_a)$, $s_\alpha\equiv(-)^{j_a-m_a}$. By a judicious choice of phase, u and v can be made real, resulting in all quantities in Eqs. (51)–(53) being real.

The interactions of Eq. (35) can be multipole expanded,

$$v_{\alpha\beta\gamma\delta}\equiv\sum_{\lambda\mu}G_{abcd\lambda}C^{\lambda\mu}_{\alpha\beta}C^{\lambda\mu}_{\gamma\delta}$$
$$\equiv\sum_{\lambda'\mu'}F_{acdb\lambda'}C^{\lambda'\mu'}_{\alpha\bar\gamma}s_\gamma C^{\lambda'\mu'}_{\delta\bar\beta}s_\beta, \tag{55}$$

where $C^{\lambda\mu}_{\alpha\beta}$ is the Clebsch-Gordan coefficient

$$C^{\lambda\mu}_{\alpha\beta}\equiv\langle j_am_aj_bm_b|j_aj_b;\lambda\mu=m_a+m_b\rangle.$$

We now want to find the angular momentum-coupled expression for (46) and (47),

$$2\delta^2\mathfrak{F}=\rho^\dagger E_\rho\rho+\kappa^\dagger E_\kappa\kappa+\tilde\rho^\dagger F^*\tilde\rho+\tfrac{1}{2}\tilde\kappa^\dagger G\tilde\kappa,$$

where the superscript (1) for the density matrices has been suppressed and

$$(E_\rho)_{ab}=\frac{E_a-E_b}{f_b-f_a},\quad (E_\kappa)_{ab}=\frac{E_a+E_b}{1-f_a-f_b}. \tag{56}$$

For the spherical case, from (42) and (55),

$$\tilde\rho_{\beta\alpha}=u_au_b\rho_{\beta\alpha}-v_av_bs_\alpha s_\beta\rho^*_{\bar\beta\bar\alpha}-u_bv_as_\alpha\kappa_{\beta\bar\alpha}-v_bu_as_\beta\kappa^*_{\bar\beta\alpha}, \tag{57a}$$

$$\tilde\kappa_{\beta\alpha}=u_bv_as_\alpha\rho_{\beta\bar\alpha}-v_bu_as_\beta\rho^*_{\bar\beta\alpha}+u_au_b\kappa_{\beta\alpha}-v_bv_as_\alpha s_\beta\kappa^*_{\bar\beta\bar\alpha}. \tag{57b}$$

We multipole decompose ρ and κ by defining

$$\rho_{ab\lambda\mu}\equiv n_{ab}\sum_{m's}C^{\lambda\mu}_{\alpha\bar\beta}s_\beta\rho_{\beta\alpha},\quad \kappa_{ab\lambda\mu}\equiv n_{ab}\sum_{m's}C^{\lambda\mu}_{\alpha\beta}\kappa_{\beta\alpha}, \tag{58}$$

where the normalization $n_{ab}=(1+\delta_{ab})^{-1/2}$ is inserted for convenience. We then find, from (55), (57), and (58)

$$\tilde\rho^\dagger F\tilde\rho=\sum_{abcd\lambda\mu}\tilde\rho^*_{ab\lambda\mu}F^*_{abcd\lambda}\tilde\rho_{cd\lambda\mu}, \tag{59a}$$

$$\tilde\kappa^\dagger G\tilde\kappa=\sum_{abcd\lambda\mu}\tilde\kappa^*_{ab\lambda\mu}G_{abcd\lambda}\tilde\kappa_{cd\lambda\mu}, \tag{59b}$$

where

$$\tilde\rho_{ab\lambda\mu}=\frac{1+\delta_{ab}}{2}[U^{(+)}_{ab}\rho^{(+)}_{ab\lambda\mu}+U^{(-)}_{ab}\rho^{(-)}_{ab\lambda\mu}-V^{(+)}_{ab}\kappa^{(-)}_{ab\lambda\mu}-V^{(-)}_{ab}\kappa^{(+)}_{ab\lambda\mu}] \tag{60a}$$
$$\equiv\frac{1+\delta_{ab}}{2}[U^{(+)}\rho^{(+)}+U^{(-)}\rho^{(-)}-V^{(+)}\kappa^{(-)}-V^{(-)}\kappa^{(+)}]_{ab\lambda\mu},$$

$$\tilde\kappa_{ab\lambda\mu}=\frac{1+\delta_{ab}}{2}[V^{(-)}\rho^{(+)*}+V^{(+)}\rho^{(-)*}+U^{(+)}\kappa^{(+)*}+U^{(-)}\kappa^{(-)*}]_{ab\lambda\mu}, \tag{60b}$$

$$\rho^{(\pm)}_{ab\lambda\mu}=\rho_{ab\lambda\mu}\mp s_\lambda\rho^*_{ab\lambda-\mu},\quad s_\lambda=(-)^{\lambda-\mu}, \tag{61a}$$

$$\kappa^{(\pm)}_{ab\lambda\mu}=\kappa^*_{ab\lambda\mu}\mp s_\lambda\kappa_{ab\lambda-\mu}, \tag{61b}$$

$$U^{(\pm)}_{ab}=n_{ab}(u_au_b\pm v_av_b), \tag{61c}$$

$$V^{(\pm)}_{ab}=n_{ab}(u_av_b\pm v_au_b). \tag{61d}$$

The reason we use quantities with superscripts ($\pm$) is to show their definite symmetry properties under the permutation of a and b. Exploiting these properties and further taking note of the symmetry relations between $\rho^{(\pm)}_{ab\lambda\mu}$ and $\rho^{(\pm)}_{ab\lambda-\mu}$, and between $\kappa^{(\pm)}_{ab\lambda\mu}$ and $\kappa^{(\pm)}_{ab\lambda-\mu}$, we find that

$$\tilde\rho^\dagger F\tilde\rho=\sum_{a\ge b}\sum_{c\ge d}\sum_{\lambda,\mu\ge0}\frac{1}{1+\delta_{\mu0}}\times\sum_{\phi=\pm}(U^{(\phi)}\rho^{(\phi)}-V^{(-\phi)}\kappa^{(\phi)})^*_{ab\lambda\mu}\times F^{(\phi)}_{abcd\lambda}(U^{(\phi)}\rho^{(\phi)}-V^{(-\phi)}\kappa^{(\phi)})_{cd\lambda\mu}, \tag{62a}$$

$$\tfrac{1}{2}\tilde{\kappa}^\dagger G\tilde{\kappa}=\sum_{a\geq b}\sum_{c\geq d}\sum_{\lambda,\mu\geq 0}\frac{1}{1+\delta_{\mu 0}}\times\sum_{\phi=\pm}(V^{(-\phi)}\rho^{(\phi)}+U^{(\phi)}\kappa^{(\phi)})^*_{ab\lambda\mu}\times G_{abcd\lambda}(V^{(-\phi)}\rho^{(\phi)}+U^{(\phi)}\kappa^{(\phi)})_{cd\lambda\mu}, \tag{62b}$$

where

$$F^{(\pm)}_{abcd\lambda}=F^*_{abcd\lambda}\pm(-)^{j_a+j_b+\lambda}F^*_{bacd\lambda}. \tag{61e}$$

The diagonal terms are straightforwardly found to be

$$\rho^\dagger E_\rho\rho=\sum_{a\geq b}\sum_{\lambda,\mu\geq 0}\frac{1}{1+\delta_{\mu 0}}\sum_{\phi=\pm}\rho^{(\phi)*}_{ab\lambda\mu}(E_\rho)_{ab}\rho^{(\phi)}_{ab\lambda\mu} \tag{63}$$

with a similar expression for $\kappa^\dagger E_\kappa\kappa$ obtainable from (63) by replacing ρ by κ everywhere. The factor $(1+\delta_{\mu 0})^{-1}$ in (62) and (63) can be absorbed into $\rho^{(\phi)}$ and $\kappa^{(\phi)}$ by a redefinition of these quantities and shall be suppressed from now on.

In order to express (62) and (63) in a more compact form, we consider $\rho^{(\phi)}_{\lambda\mu}$, $\kappa^{(\phi)}_{\lambda\mu}$, $U^{(\phi)}$, and $V^{(\phi)}$ to be vectors in the Hilbert space spanned by the indices x representing the *ordered pair* of orbits $a_x\geq b_x$, and E_ρ, E_κ, $F^{(\phi)}_\lambda$, and G_λ to be matrices in this Hilbert space, the former two matrices being diagonal. In this notation we find

$$2\delta^2\mathfrak{F}=\sum_{\lambda,\mu\geq 0,\phi=\pm}\Gamma^{(\phi)\dagger}_{\lambda\mu}\mathcal{S}^{(\phi)}_\lambda\Gamma^{(\phi)}_{\lambda\mu}, \tag{64}$$

where

$$\Gamma^{(\phi)}_{\lambda\mu}=\begin{pmatrix}\rho^{(\phi)}_{\lambda\mu}\\ \kappa^{(\phi)}_{\lambda\mu}\end{pmatrix}=\begin{pmatrix}\rho^{(\phi)}\\ \kappa^{(\phi)}\end{pmatrix}_{\lambda\mu}, \tag{65a}$$

$$\mathcal{S}^{(\phi)}_\lambda=\begin{pmatrix}\mathfrak{C}^{(\phi)}_\lambda & \mathcal{E}^{(\phi)}_\lambda\\ \mathcal{E}^{(\phi)}_\lambda & \mathfrak{D}^{(\phi)}_\lambda\end{pmatrix}, \tag{65b}$$

$$\mathfrak{C}^{(\phi)}_\lambda=E_\rho+[U^{(\phi)}]^T F^{(\phi)}U^{(\phi)}+[V^{(-\phi)}]^T G_\lambda V^{(-\phi)}, \tag{65c}$$

$$\mathcal{E}^{(\phi)}_\lambda=-[U^{(\phi)}]^T F^{(\phi)}_\lambda V^{(-\phi)}+[V^{(-\phi)}]^T G_\lambda U^{(\phi)}, \tag{65d}$$

$$\mathfrak{D}^{(\phi)}_\lambda=E_\kappa+[V^{(-\phi)}]^T F^{(\phi)}_\lambda V^{(-\phi)}+[U^{(\phi)}]^T G_\lambda U^{(\phi)}. \tag{65e}$$

Equations (64) and (65) are our final expressions for $\delta^2\mathfrak{F}$. Since all elements of $\rho^{(\pm)}_{\lambda\mu}$ and $\kappa^{(\pm)}_{\lambda\mu}$ are linearly independent, $\delta^2\mathfrak{F}>0$ only if $S^{(\pm)}_\lambda$ for each and every spin-parity channel λ are positive definite. Notice that the stability matrices $S^{(\pm)}_\lambda$ are independent of the magnetic quantum number μ, as expected for a system with spherical symmetry.

We can now establish contact with the stability condition for ground state ($\tau=0$) HFB configurations. In the limit $\tau\to 0$, the diagonal terms in $C^{(\pm)}_\lambda\to\infty$, and for practical purposes $S^{(\pm)}_\lambda\to D^{(\pm)}_\lambda$ since the submatrices C and D become decoupled. In a situation which is completely analogous to that of the HF approximation discussed at the end of Sec. III, the matrices

$$P_\lambda\equiv\tfrac{1}{2}(D^{(+)}_\lambda+D^{(-)}_\lambda),\quad R_\lambda\equiv\tfrac{1}{2}(D^{(+)}_\lambda-D^{(-)}_\lambda)$$

are precisely those that appear in the secular equation for phonon energies in the quasiparticle RPA (QRPA) theory[11]

$$\omega_\lambda=\begin{pmatrix}P_\lambda & R_\lambda\\ -R_\lambda & -P_\lambda\end{pmatrix}.$$

Similarly the stability condition in QRPA is

$$S^{\mathrm{QRPA}}_\lambda=\begin{pmatrix}P_\lambda & R_\lambda\\ R_\lambda & P_\lambda\end{pmatrix},$$

which again like Eq. (23) can be obtained by a similarity transformation from

$$\begin{pmatrix}D^{(+)}_\lambda & 0\\ 0 & D^{(-)}\end{pmatrix}.$$

This shows that our stability condition (64) has the correct zero temperature limit. The more important lesson we learn from this comparison, however, is that the stability matrix at $\tau>0$ is more than giving the $\tau=0$ stability condition the appropriate τ dependence. The terms in $C^{(\pm)}_\lambda$ and $E^{(\pm)}_\lambda$ do not have counterparts in the $\tau=0$ stability condition. These terms are associated with the extra degree of freedom in the finite temperature theory which allows f to vary from zero (or from unity, for hole orbits in the HF approximation). This is a direct result of the averaging process, using the density matrix W, over the grand canonical ensemble. In this case one is not seeking for one best configuration which is then defined as a quasiparticle vacuum, or $\langle a^\dagger a\rangle\equiv f=0$.

ACKNOWLEDGMENTS

This work started when one of the authors (S.D.G.) began his visit to Chalk River Nuclear Laboratories in the summer of 1977. He wishes to thank CRNL for its hospitality. He also wishes to thank L. Zamick and A. Mekjian of Rutgers University for useful discussions. The other author (H.C.L.) spent part of the summer at Brookhaven National Laboratory during which time part of this work was done. He wishes to thank BNL for its hospitality.

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