

## Comparison between the temperature and the time-dependent Hartree-Fock-Bogoliubov descriptions of the pairing interaction

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The thermal and the time-dependent versions of the Hartree-Fock-Bogoliubov approximation are used to describe the effects of the pairing interaction in a simple model. Similarities and differences between the two approaches are discussed. In the one-shell case analytic results are obtained which clearly show that as the degeneracy increases the exact energies tend to the limits provided by the approximate methods. A relation between the quasiparticle occupation probability and the seniority is established. In the two-shell case the time-dependent approach approximates all the families of exact states labeled by the shell seniority and gives information on the two different phase transitions present in the model. The finite-temperature method, instead, only approximates the exact energy for the lowest state of each family.

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### I. INTRODUCTION

The Hartree-Fock-Bogoliubov (HFB) [1,2] description of fermion systems provides a single excitation image of the low energy part of the spectra of many-body systems. The thermal [3,4] and the time-dependent versions [5] give on the other hand descriptions that contain essentially all the information related with single-particle excitations for the whole spectrum of the Hamiltonian considered. Nevertheless the complexity of using one method or the other is completely different. In principle, the thermal version can be applied in a general case (in fact for a realistic situation the thermal calculations are not simple but they are feasible). On the other hand, except for very simple Hamiltonians it is quite complicated to perform the time-dependent version.

An interesting question that arises is if the two approximations provide the same information or which are the differences between them. Therefore the purpose of this work is to do a detailed comparison between the thermal and the time-dependent versions of HFB. With this aim we have decided to study the pairing interaction in a two-level model as in this case it is possible to perform the exact calculation as well as both approximate treatments and at the same time this problem contains the essential features of much more complex situations. We apply the temperature and time-dependent HFB approximations to study in particular the phase transitions this system presents, not only the one for the ground state, that appears as one changes the strength parameter, but also the one that resembles the disappearance

of superconductivity for higher temperatures that in our case correspond to higher excitation energies. These excitation energies can be thought of as related to the "critical temperature" at which the phase transition occurs. It is particularly helpful to use the scaling property discussed in the time-dependent results obtained previously [6].

We believe that the conclusions that can be drawn from this comparison will be more general than the particular case studied here.

In Sec. II we review the model studied and its exact treatment as well as the general features of the thermal and time-dependent HFB descriptions. In Sec. III we apply the two methods to the one-shell case, while the comparison between the results obtained for the two-shell case is discussed in Sec. IV. Finally, some conclusions are summarized in Sec. V.

### II. DISCUSSION OF THE MODEL AND DIFFERENT TREATMENTS

#### A. The model and its exact treatment

The model used consists of two nondegenerate shells of the same degeneracy  $\Omega$  ( $\Omega = j + \frac{1}{2}$ ), and energies  $\frac{\epsilon}{2}$  and  $\frac{\xi}{2}$ , where particles in both levels interact via a pairing residual Hamiltonian.

Defining

$$A_k^\dagger = \frac{1}{2\sqrt{\Omega}} \sum_{m_k} (-1)^{j_k - m_k} b_{j_k m_k}^\dagger b_{j_k - m_k}^\dagger, \quad (1)$$

$$N_k = \frac{1}{2} \sum_{m_k} b_{j_k m_k}^\dagger b_{j_k m_k}, \quad (2)$$

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the Hamiltonian used is

$$H = \epsilon(N_1 - N_2) - \frac{G\Omega}{2} [(A_1^\dagger + A_2^\dagger)(A_1 + A_2) + (A_1 + A_2)(A_1^\dagger + A_2^\dagger)], \quad (3)$$

where the two shells are denoted by 1 and 2.  $N_1(N_2)$  is the total number of pairs in level 1(2) and  $G$  is the interaction strength. The spectrum of this Hamiltonian can be obtained using the method described in Ref. [7]. For one shell the eigenstates are of the form

$$|k, \nu\rangle = \mathcal{N}_{k\nu} A^{\dagger k} B^\nu |0\rangle, \quad (4)$$

where  $\mathcal{N}_{k\nu}$  is a normalization constant,  $k$  is the number of paired particles,  $|0\rangle$  is the vacuum and the operator

$B^\nu$ , that satisfies the relations

$$AB^\nu |0\rangle = 0, \quad NB^\nu |0\rangle = \nu B^\nu |0\rangle, \quad (5)$$

creates  $\nu$  nonpaired particles. Consequently, the energy can be expressed in terms of the number of paired particles  $k$  and the "seniority"  $\nu$  as

$$E(k, \nu) = -Gk(\Omega - k - \nu + 1). \quad (6)$$

For two shells it is convenient to use the basis

$$|k_1 k_2 \nu_1 \nu_2\rangle = \mathcal{N}_{k_1 k_2 \nu_1 \nu_2} A_1^{\dagger k_1} A_2^{\dagger k_2} B_1^{\nu_1} B_2^{\nu_2} |0\rangle. \quad (7)$$

In this case the matrix elements of the Hamiltonian are simply given by

$$\begin{aligned} H|k_1 k_2 \nu_1 \nu_2\rangle = & \left\{ \frac{\epsilon}{2} [2(k_1 - k_2) + \nu_1 - \nu_2] - G[k_1(\Omega - k_1 - \nu_1 + 1) + k_2(\Omega - k_2 - \nu_2 + 1)] \right\} |k_1 k_2 \nu_1 \nu_2\rangle \\ & - G\sqrt{k_1(\Omega + 1 - k_1 - \nu_1)(k_2 + 1)(\Omega - k_2 - \nu_2)} |k_1 - 1 k_2 + 1 \nu_1 \nu_2\rangle \\ & - G\sqrt{k_2(\Omega + 1 - k_2 - \nu_2)(k_1 + 1)(\Omega - k_1 - \nu_1)} |k_1 + 1 k_2 - 1 \nu_1 \nu_2\rangle. \end{aligned} \quad (8)$$

As the Hamiltonian does not change the seniority, it does not connect states of different seniority and therefore it is possible to diagonalize each seniority independently.

For one shell the number of states having seniority  $\nu$  is

$$D(\nu) = \binom{2\Omega}{\nu} - \binom{2\Omega}{\nu - 2} \quad (9)$$

and for two shells the degeneracy of the states with seniorities  $\{\nu_1, \nu_2\}$  is directly  $D(\nu_1) \times D(\nu_2)$ . In the latter case the exact energies can be obtained by diagonalizing a matrix of order  $\Omega - \nu + 1$  with elements implied by (8).

### B. Time-dependent Hartree-Fock-Bogoliubov treatment

For implementing the time-dependent variational approach we first introduce the operators

$$K_+^{(i)} = \sum_{m_i > 0} b_{j_i m_i}^\dagger b_{j_i \bar{m}_i}^\dagger, \quad (10)$$

$$K_-^{(i)} = \left(K_+^{(i)}\right)^\dagger, \quad (11)$$

$$K_0^{(i)} = \frac{1}{2} \sum_{m_i} \left( b_{j_i m_i}^\dagger b_{j_i m_i} - \frac{1}{2} \right). \quad (12)$$

With these definitions the Hamiltonian (3) is written as

$$\begin{aligned} H = \epsilon(K_0^{(1)} - K_0^{(2)}) - \frac{G}{2} \{ & (K_+^{(1)} + K_+^{(2)})(K_-^{(1)} + K_-^{(2)}) \\ & + (K_-^{(1)} + K_-^{(2)})(K_+^{(1)} + K_+^{(2)}) \}. \end{aligned} \quad (13)$$

Studying the commutator algebra for the operators defined in Eqs. (10), (11), and (12) one immediately sees that the group that is relevant for the two-level model described in the previous section is  $SU(2)*SU(2)$ , as the operators defined before have the commutation relations of  $SU(2)$

$$[K_+^{(i)}, K_-^{(i)}] = 2K_0^{(i)}, \quad (14)$$

$$[K_0^{(i)}, K_+^{(i)}] = K_+^{(i)}, \quad (15)$$

$$[K_0^{(i)}, K_-^{(i)}] = -K_-^{(i)}. \quad (16)$$

When the seniorities  $\nu_i$  are zero the vacuum state  $|0\rangle$  is characterized by

$$K_-^{(i)} |0\rangle = 0, \quad (17)$$

$$K_0^{(i)} |0\rangle = -\frac{\Omega_i}{2} |0\rangle, \quad (18)$$

which identify  $|0\rangle$  as the minimum weight state of the representation of  $SU(2)*SU(2)$  with weights  $\frac{\Omega_i}{2}$ . The coherent state in this representation is

$$|Z_1 Z_2\rangle = e^{\sum_i Z_i K_+^{(i)}} |0\rangle \quad (19)$$

and it is a BCS-like state (not normalized). The equations of motion obtained through the time-dependent variational principle with this state are equivalent to the TDHFB equations. To obtain them one has to use the variational principle appropriate for non-normalized states [5] with an action defined as

$$S = \int_{t_1}^{t_2} \frac{\langle Z_1 Z_2 | \{ i\hbar \frac{\partial}{\partial t} - H \} | Z_1 Z_2 \rangle}{\langle Z_1 Z_2 | Z_1 Z_2 \rangle} dt. \quad (20)$$

The calculation of the overlap and the mean value of the Hamiltonian is a well-known group theoretical calculation [5]. The overlap is given by

$$\langle Z_1 Z_2 | Z_1 Z_2 \rangle = (1 + Z_1 \bar{Z}_1)^{\Omega_1} (1 + Z_2 \bar{Z}_2)^{\Omega_2} \quad (21)$$

and the mean values of the operators defined in (10), (11), and (12) are

$$\langle K_+^{(i)} \rangle = \frac{\Omega_i Z_i}{1 + Z_i \bar{Z}_i}, \quad (22)$$

$$\langle K_-^{(i)} \rangle = \frac{\Omega_i \bar{Z}_i}{1 + Z_i \bar{Z}_i}, \quad (23)$$

$$\langle K_0^{(i)} \rangle = -\frac{\Omega_i (1 - Z_i \bar{Z}_i)}{2 (1 + Z_i \bar{Z}_i)}. \quad (24)$$

Consequently, the mean value of the Hamiltonian (13) is

$$\begin{aligned} \mathcal{H} = & \frac{\epsilon}{2} \left( -\Omega_1 \frac{1 - Z_1 \bar{Z}_1}{1 + Z_1 \bar{Z}_1} + \Omega_2 \frac{1 - Z_2 \bar{Z}_2}{1 + Z_2 \bar{Z}_2} \right) - G \Omega_1 \Omega_2 \frac{Z_1 \bar{Z}_2 + \bar{Z}_1 Z_2}{(1 + Z_1 \bar{Z}_1)(1 + Z_2 \bar{Z}_2)} \\ & - G \left( \frac{\Omega_1 (\Omega_1 - 1) Z_1 \bar{Z}_1}{(1 + Z_1 \bar{Z}_1)^2} + \frac{\Omega_2 (\Omega_2 - 1) Z_2 \bar{Z}_2}{(1 + Z_2 \bar{Z}_2)^2} \right) - \frac{G}{2} (\Omega_1 + \Omega_2). \end{aligned} \quad (25)$$

Although all calculations could be performed in terms of the variables  $Z_i, \bar{Z}_i$ , it is more convenient to introduce new variables which are canonical [6,8]. This is done with the transformation

$$\omega_i = \sqrt{\frac{\Omega_i}{1 + Z_i \bar{Z}_i}} Z_i. \quad (26)$$

The new variables  $\omega_i$  are canonical in the sense that the generalized Poisson brackets [5] have the standard form and that the variational equations look like the ordinary Hamilton equations

$$i\dot{\omega}_i = \frac{\partial \mathcal{H}}{\partial \omega_i} \quad (27)$$

and its H.c. The dynamical problem has 2 degrees of freedom, the complex variables  $\omega_1$  and  $\omega_2$ . Therefore the existence of two constants of motion, the energy and

the number of particles, makes the system integrable. The most convenient variables for the integration are (for  $\Omega_1 = \Omega_2 = \Omega$ )

$$m = \frac{\omega_1 \bar{\omega}_1 + \omega_2 \bar{\omega}_2}{\Omega} - 1, \quad (28)$$

$$\varphi = \frac{1}{2}(\varphi_1 + \varphi_2), \quad (29)$$

$$\eta = \frac{\omega_2 \bar{\omega}_2 - \omega_1 \bar{\omega}_1}{\Omega}, \quad (30)$$

$$\alpha = \frac{1}{2}(\varphi_2 - \varphi_1), \quad (31)$$

where  $\varphi_i = \arg(\omega_i)$ . Noting that  $\omega_i \bar{\omega}_i$  is the mean number of pairs in the level  $i$  one gets that  $m$  is conserved and that the range of  $\eta$  is  $-1 \leq \eta \leq 1$ .

The energy can then be written as

$$\mathcal{E} = \frac{\mathcal{H}}{\epsilon \Omega} = -\eta + \frac{\xi}{4} \{ \eta^2 + m^2 - 1 - \cos(2\alpha) \sqrt{[(m+1)^2 - \eta^2][(m-1)^2 - \eta^2]} \}. \quad (32)$$

We have chosen  $\epsilon \Omega$  as the energy unit because in this case the equations of motion become independent of both parameters. We have also used a natural strength parameter  $\xi = \frac{2G\Omega}{\epsilon}$ .

The equations of motion can be written as

$$\dot{m} = -\frac{\partial \mathcal{E}}{\partial \varphi} = 0, \quad (33)$$

$$\dot{\varphi} = \frac{\partial \mathcal{E}}{\partial m}, \quad (34)$$

$$\dot{\eta} = \frac{\partial \mathcal{E}}{\partial \alpha}, \quad (35)$$

$$\dot{\alpha} = -\frac{\partial \mathcal{E}}{\partial \eta}. \quad (36)$$

When the seniorities  $\nu_i$  are not zero one gets the same equations but with  $\Omega_i$  replaced by  $\Omega_i - \nu_i$ . In particular, for Eqs. (28)–(32) we have also considered  $\nu_1 = \nu_2 = \nu$  and replaced  $\Omega$  by  $\Omega - \nu$ .

The TDHFB energy levels are determined by a Bohr-Sommerfeld-like quantization condition for the action.

### C. The thermal treatment

We will now discuss the thermal treatment following closely the description done in Ref. [4]. We start by considering a general two-body Hamiltonian:

$$H = \sum_{ij} T_{ij} b_i^\dagger b_j + \frac{1}{4} \sum_{ijkl} V_{ij,kl} b_i^\dagger b_j^\dagger b_l b_k, \quad (37)$$

which as usual, is approximated by a one-body Hamiltonian describing noninteracting quasiparticles, i.e.,

$$F = H - \mu N \simeq H_{\text{HFB}} = E_0 + \sum_i E_i \alpha_i^\dagger \alpha_i, \quad (38)$$

where the chemical potential  $\mu$  is fixed by imposing the condition that the mean number of particles is well defined.  $E_i$  are the quasiparticles energies while  $\alpha_i^\dagger$  creates one quasiparticle and is defined by the unitary transformation

$$\alpha_i^\dagger = \sum_j \{U_{ij} b_j^\dagger + V_{ij} b_j\}. \quad (39)$$

If we want to obtain a thermal HFB description we must remember that the density operator and the partition function that are defined as

$$\mathbf{D} = Z^{-1} e^{-\beta(H - \mu N)}, \quad (40)$$

$$Z = \text{Tr}\{e^{-\beta(H - \mu N)}\}, \quad (41)$$

when treated by the HFB approximation (38) become

$$Z_{\text{HFB}} = \prod_i (1 + e^{-\beta E_i}), \quad (42)$$

$$\mathbf{D}_{\text{HFB}} = \prod_i \{f_i \mathbf{n}_i + (1 - f_i)(1 - \mathbf{n}_i)\}, \quad (43)$$

where  $\mathbf{n}_i$  is the quasiparticle number operator corresponding to the state  $i$  while

$$f_i = \frac{1}{1 + e^{\beta E_i}} \quad \text{and} \quad \beta = \frac{1}{KT}. \quad (44)$$

The usual density and pairing matrices are

$$\begin{aligned} \rho_{ij} &= \langle b_j^\dagger b_i \rangle = \text{Tr}\{\mathbf{D}_{\text{HFB}} b_j^\dagger b_i\} \\ &= [\mathbf{U}^T f \mathbf{U}^* + \mathbf{V}^\dagger (1 - f) \mathbf{V}]_{ij}, \end{aligned} \quad (45)$$

$$\begin{aligned} t_{ij} &= \langle b_j b_i \rangle = \text{Tr}\{\mathbf{D}_{\text{HFB}} b_j b_i\} \\ &= [\mathbf{U}^T f \mathbf{V}^* + \mathbf{V}^\dagger (1 - f) \mathbf{U}]_{ij}. \end{aligned} \quad (46)$$

The energy is evaluated using Wick's theorem [2] for  $T \neq 0$ . One then obtains

$$E_{\text{FT}} = \text{Tr}\{\mathbf{D}_{\text{HFB}} H\} = \text{Tr}\{(T + \frac{1}{2}\Gamma)\rho + \frac{1}{2}\Delta t^\dagger\}, \quad (47)$$

where the HF Hamiltonian as well as the self-consistent and pairing potentials are defined as usual as

$$H_{\text{HF}} = T - \mu + \Gamma, \quad (48)$$

$$\Gamma_{ij} = \sum_{k,m} V_{ik,jm} \rho_{mk}, \quad (49)$$

$$\Delta_{ij} = \frac{1}{2} \sum_{k,m} V_{ij,km} t_{km}. \quad (50)$$

The coefficients  $\mathbf{U}$  and  $\mathbf{V}$  of Eq. (39) are obtained by

solving the eigenvalue equations

$$\begin{pmatrix} H_{\text{HF}} & \Delta \\ -\Delta^* & -H_{\text{HF}}^* \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = E_i \begin{pmatrix} U_i \\ V_i \end{pmatrix}. \quad (51)$$

These equations are the FTHFB equations and it is to be noted that for  $T = 0$  one gets the usual HFB description.

We will now consider the pairing Hamiltonian in the case of two shells with the same degeneracy  $\Omega$  and energies  $\epsilon_1 = \frac{\epsilon}{2}, \epsilon_2 = -\frac{\epsilon}{2}$ . The pairing potential reduces in this case to a constant  $\Delta$  that is state independent. One also obtains for the relevant variables, such as the quasiparticle energies and occupation probabilities ( $E_i, V_i^2, U_i^2$ ), very simple expressions, namely,

$$E_i = \sqrt{(\epsilon_i - \mu)^2 + \Delta^2}, \quad (52)$$

$$U_i^2 = \frac{1}{2} \left\{ 1 + \frac{(\epsilon_i - \mu)}{E_i} \right\}, \quad (53)$$

$$V_i^2 = \frac{1}{2} \left\{ 1 - \frac{(\epsilon_i - \mu)}{E_i} \right\}. \quad (54)$$

The ground-state energy is

$$\begin{aligned} E_{\text{FT}} &= \epsilon\Omega \{V_1^2 - V_2^2 + (U_1^2 - V_1^2)f_1 - (U_2^2 - V_2^2)f_2\} \\ &\quad - \frac{\Delta^2}{G} \end{aligned} \quad (55)$$

while the gap and number equations are written as

$$\frac{2}{G\Omega} = \frac{\tanh\{\frac{\beta E_1}{2}\}}{E_1} + \frac{\tanh\{\frac{\beta E_2}{2}\}}{E_2} = \frac{1 - 2f_1}{E_1} + \frac{1 - 2f_2}{E_2}, \quad (56)$$

$$N = 2\Omega \{V_1^2 + V_2^2 + (U_1^2 - V_1^2)f_1 + (U_2^2 - V_2^2)f_2\}. \quad (57)$$

### III. ONE-SHELL CASE

In this section we apply the results obtained in the previous section to the one-shell case. This not only implies the consideration of the limit  $\epsilon$  going to zero but also amounts to a rescaling of the energies. Even if it is a very simple case in which the system is always superconductive it is worthwhile to study it because one gets analytic results and clear-cut conclusions may be arrived at.

#### A. Time-dependent description

To perform the TDHFB treatment in one shell it is worthwhile to note that the expression of the mean energy obtained for the two-shell case can be applied to the one-shell situation by considering in a simple way the limit when  $\epsilon$  tends to zero. In this case the energy

must be scaled in terms of  $G\Omega^2$  and one must take into account that the degeneracy of the level obtained when  $\epsilon = 0$  is twice the degeneracy of each one of the original levels, i.e., [cf. Eq. (32)]

$$\frac{\mathcal{H}}{G\Omega^2} = -\frac{1}{8}\{1 - \eta^2 - m^2 + \cos(2\alpha)\sqrt{[(m+1)^2 - \eta^2][(m-1)^2 - \eta^2]}\}. \quad (58)$$

In the  $m = 0$  case it is possible to obtain an analytic relation between the action  $S_\alpha$  and the mean energy, namely,

$$S_\alpha = \Omega \int \eta d\alpha = 2\pi\Omega \left\{ 1 - \sqrt{-4\frac{\mathcal{H}}{G\Omega^2}} \right\}. \quad (59)$$

Then

$$\frac{\mathcal{H}}{G\Omega^2} = -\frac{1}{4} \left( 1 - \frac{S_\alpha}{2\pi\Omega} \right)^2. \quad (60)$$

This expression corresponds to the case of seniority zero. When the seniority is not zero one replaces  $\Omega$  by  $\Omega - \nu$  and gets

$$E_{\text{TD}} = \mathcal{H} = -\frac{1}{4}G \left( \Omega - \nu - \frac{S_\alpha}{2\pi} \right)^2. \quad (61)$$

The exact energy is given by Eq. (6). The number of pairs  $k$  may be related to the variable  $m$  using the definition (28) and the fact that  $\omega_i \bar{\omega}_i$  is the number of pairs in level  $i$ ,

$$k = \frac{1}{2}(m+1)(\Omega - \nu). \quad (62)$$

Therefore, the exact energy for very large  $\Omega$  is

$$E_{\text{exact}} \simeq -\frac{1}{4}G(\Omega - \nu)^2(1 - m^2). \quad (63)$$

As was already discussed in Ref. [6] the TDHFB result is the limit to which the exact energy tends for  $\Omega$  going to infinity. Consequently, one has to compare Eq. (61) with Eq. (63) for  $m = 0$ . Two different interpretations are possible. If one performs the TDHFB treatment for  $\nu = 0$ , which is the seniority in the ground state, then the approximate energy levels are obtained through a Bohr-Sommerfeld-like quantization rule [6,9,10], i.e., by imposing

$$S_\alpha = 2\pi n, \quad (64)$$

where  $n$  is an integer number. In this case the TDHFB and the exact (for very large  $\Omega$ ) energies coincide, as expected.

On the other hand, one may perform the TDHFB calculation for each value of  $\nu$  independently. As there is only one energy level for each  $\nu$ , these are obtained looking for the minimum TDHFB energy in each calculation. Obviously, the minimum corresponds to  $S_\alpha = 0$  [cf. Eq. (64)] and then the approximate and the exact values

also coincide in this case.

One may also obtain the minimum TDHFB energy minimizing Eq. (58). The result is

$$E_{\text{TD}} = -\frac{1}{4}G(\Omega - \nu)^2(1 - m^2) \quad (65)$$

which coincides with the exact energy in the limit of  $\Omega$  going to infinity that is given by Eq. (63).

In Fig. 1 we show, for  $m = 0$ , the exact energy as a function of the seniority  $\nu$  for different values of  $\Omega$ , as well as the approximate energy obtained with TDHFB (that is shown in full line). It is seen that as  $\Omega$  increases the exact values tend to the TDHFB ones, as already mentioned.

## B. Thermal description

To obtain the thermal results for one shell we must consider the limit  $\epsilon$  tending to zero in Eqs. (52) to (57) obtaining therefore

$$E_{\text{FT}} = -\frac{G\Omega^2}{4} \left\{ -\left(\frac{N}{\Omega}\right)^2 + 2\left(\frac{N}{\Omega}\right) + 4f^2 - 4f \right\}. \quad (66)$$

The exact energy for very large  $\Omega$  expressed in terms of the total number of particles  $N = 2k + \nu$  and the seniority is [cf. Eq. (6)]

$$E_{\text{exact}} \simeq -\frac{G\Omega^2}{4} \left\{ -\left(\frac{N}{\Omega}\right)^2 + 2\left(\frac{N}{\Omega}\right) + \left(\frac{\nu}{\Omega}\right)^2 - 2\left(\frac{\nu}{\Omega}\right) \right\}. \quad (67)$$

Comparing the two expressions it is seen that if the quasiparticle occupation probability  $f$  is related to the seniority through  $f = \frac{\nu}{2\Omega}$  then the FTHFB energy is the limit to which the exact energy tends for  $\Omega$  going to infinity.

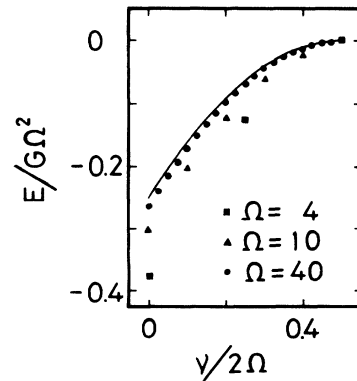


FIG. 1. Exact energies (in units of  $G\Omega^2$ ) are shown by dots as function of  $\frac{\nu}{2\Omega}$  for the values of  $\Omega$  shown in the inset. The values (that coincide) obtained using FTHFB and TDHFB are shown in full line, as functions of  $f$  and  $\frac{S_\alpha}{2\pi\Omega}$ , respectively.

ity, as is the case in the TDHFB approach. Consequently, with this recipe the thermal and the time-dependent expressions for the energy coincide. This recipe is in principle rather arbitrary as in the thermal description one has only one parameter, the temperature, that is in fact defined through the density of states. However, it seems reasonable because for  $T = 0$  one has  $f = 0$  [see Eq. (44)] and as this temperature corresponds to the ground state,  $\nu$  is also zero. For increasing temperature  $f$  increases and as increasing temperature means increasing excitation energy also  $\nu$  increases. The maximum value for  $f$ , and also for  $\frac{\nu}{2\Omega}$ , is one half.

#### IV. COMPARISON IN THE TWO-SHELL CASE

##### A. Time-dependent description

It has been shown in Ref. [6] that the TDHFB description is particularly good for this model when considering shell seniority zero states. In particular the approximation turned out to be exact for an infinite  $\Omega$ . In this work we have studied in TDHFB not only the shell seniority zero states but also states having shell seniorities  $(\nu, \nu)$ . We can then label the family of states by their shell seniority.

In Figs. 2 and 3 we show the exact results presented as families of states labeled by their shell seniority, for  $\Omega = 40$ ,  $N = 80$  (i.e.,  $m = 0$ ) and  $\xi = 0.5$  and 3, respectively. As it is already known [6] this model presents two phase transitions. One is a ground-state phase transition that appears at the critical interaction strength  $\xi_c = 1$ . This means that for small coupling constants the ground state is normal and for  $\xi > \xi_c$  the ground state is superconductive. In this second case another phase transition appears for higher excitation energy such that the energies below the critical value correspond to superconductive states and the energies above it to normal ones. For  $\nu = 0$  this critical energy is  $\mathcal{E} = -1$  and in the exact results it is pointed out by a maximum in the density of states. In Figs. 2 and 3 it can be seen that all the families present the same behavior and that for  $\xi > \xi_c$  there also exists a critical shell seniority  $\nu_c$  such that for  $\nu > \nu_c$  all the states are normal.

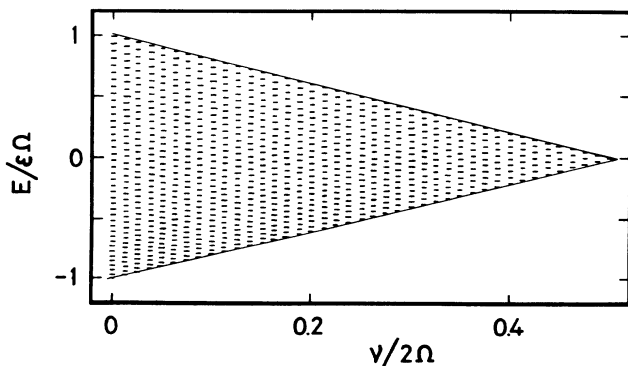


FIG. 2. Exact energies (in units of  $\epsilon\Omega$ ) for the  $(\nu, \nu)$  families as function of  $\frac{\nu}{2\Omega}$  for  $N = 2\Omega = 80$  and  $\xi = 0.5$ .

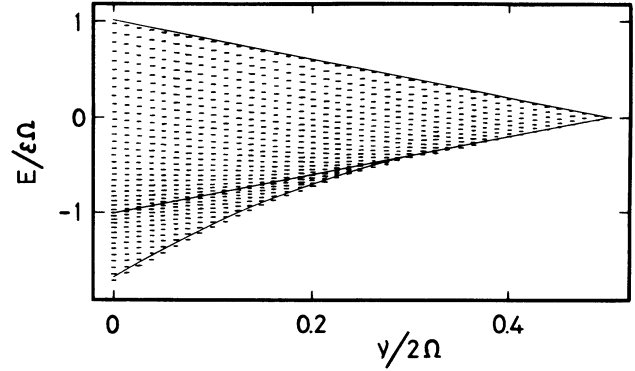


FIG. 3. Exact energies (in units of  $\epsilon\Omega$ ) for the  $(\nu, \nu)$  families as function of  $\frac{\nu}{2\Omega}$  for  $N = 2\Omega = 80$  and  $\xi = 3$ .

Within the TDHFB approach one calculates the action  $S_\alpha$  as function of the energy. As for  $\nu = 0$  (see Fig. 2 of Ref. [6]) one gets continuous functions labeled by the shell seniority that are the limits to which the exact results for each family tend when  $\Omega$  goes to infinity.

In particular, it is very easy to study the extrema of the energy functional. For example, for  $m = 0$  one has [cf. Eq. (32)]

$$\frac{\mathcal{H}}{\epsilon(\Omega - \nu)} = -\eta - \frac{\kappa}{2}(1 - \eta^2)\cos^2\alpha, \quad (68)$$

where

$$\kappa = \xi \left(1 - \frac{\nu}{\Omega}\right). \quad (69)$$

For  $\xi < 1$  the minimum and maximum energies are

$$\left(\frac{\mathcal{H}}{\epsilon\Omega}\right)_{\min} = -1 + \frac{\nu}{\Omega}; \quad \left(\frac{\mathcal{H}}{\epsilon\Omega}\right)_{\max} = 1 - \frac{\nu}{\Omega} \quad (70)$$

which agree quite well with the exact results as can be seen in Fig. 2 where they are represented as full lines.

For  $\xi > 1$  the maximum energy is the same as before but the minimum is

$$\left(\frac{\mathcal{H}}{\epsilon\Omega}\right)_{\min} = -\frac{1}{2} \left[ \xi + \frac{1}{\xi} - 2\xi \frac{\nu}{\Omega} + \xi \left(\frac{\nu}{\Omega}\right)^2 \right], \quad (71)$$

whereas  $-1 + \frac{\nu}{\Omega}$  is now the critical energy corresponding to the phase transition described above. These three energies are represented as full lines in Fig. 3 and agree quite well with the exact results. On the other hand, the critical seniority is determined by the point in which the minimum and the critical energies join themselves and is

$$\nu_c = \Omega \left(1 - \frac{1}{\xi}\right). \quad (72)$$

##### B. Thermal description

In the two-shell case when there are enough particles so as to fill completely the lower shell the Fermi energy  $\mu$  is equal to zero for all temperatures, making all the FTHFB results very simple, as in this case one has  $f_1 = f_2 = f$ ,

$E_1 = E_2 = E$ ,  $U_1 = V_2$ , and consequently  $V_1 = U_2$ . Using these relations one obtains  $E = (1 - 2f)G\Omega$ ,

$$\Delta = \sqrt{[G\Omega(1 - 2f)]^2 - \frac{\epsilon^2}{4}} \quad (73)$$

and therefore the scaled ground-state energy can be written as

$$\frac{E_{\text{FT}}}{\epsilon\Omega} = -\frac{1}{2\xi} - \frac{\xi}{2}(1 - 2f)^2. \quad (74)$$

The expression (73) allows us to define a critical  $f$ , or temperature, when the gap vanishes,

$$f_c = \frac{1}{2} \left( 1 - \frac{1}{\xi} \right). \quad (75)$$

If one relates the thermal occupation factor  $f$  to the seniority through  $f = \frac{\nu}{2\Omega}$ , as in the one-shell case, then the FTHFB ground-state energy (74) coincides with the minimum TDHFB energy (71) and is represented by the lowest full line in Fig. 3. Consequently, the FTHFB energy agrees quite well with the exact energy for the lowest  $(\nu, \nu)$  states when  $\Omega$  is large. This can be understood if one realizes that in the thermal approach it is possible to obtain in principle just two numbers for each temperature: the ground-state energy and the energy of the simple excitations (or quasiparticles). The thermal excitation energies are essentially determined by the highest seniority states (as at a given excitation energy there are much more states with the higher possible seniority than with smaller seniorities), and therefore these states dominate completely the thermal picture.

Finally, using the above-mentioned relation between  $f$  and  $\nu$  it can be seen that the expressions for the critical seniority obtained in TDHFB [Eq. (72)] and in FTHFB [Eq. (75)] also coincide and reproduce the exact result (see Fig. 3).

## V. CONCLUSIONS

With the aim of establishing similarities and differences between the time-dependent and the finite-temperature Hartree-Fock-Bogoliubov approaches we have applied them in a simple model with a pairing interaction.

In the one-shell case the results obtained are analytic. In the thermal description we have established a relation

between the quasiparticle occupation probability  $f$  and the seniority  $\nu$ . Using it it is clearly shown that in this case the two approaches provide the same results. Moreover, one gets the limit to which the exact energies tend as the degeneracy increases.

In the two-shell case and within the TDHFB approximation we have performed a more complete analysis than the one in Ref. [6] using as trial states not only the shell seniority zero states but also states having shell seniorities  $(\nu, \nu)$ . We conclude that the method provides the limits to which the exact results for each family of states labeled by the shell seniority tend when  $\Omega$  goes to infinity. Moreover, it can be applied for all values of the coupling strength and the number of particles and displays all the relevant physical information contained in the model. In particular, one gets the correct dependence on the seniority of the phase transition that appears at higher excitation energy where superconductivity disappears.

On the other hand, the energy provided by the FTHFB method agrees quite well with the exact energy for the lowest  $(\nu, \nu)$  states in the superconductive region when  $\Omega$  is large. It also gives the correct value for the critical seniority where superconductivity disappears. These two conclusions are based on the above-mentioned relation between the thermal occupation probability  $f$  and the seniority  $\nu$ .

Comparing the two methods one concludes that the TDHFB one is more powerful because in the two-shell case it is capable of approximating all the families of exact states for any value of the coupling constant and it gives information on the two different phase transitions present in the model. Nevertheless, it must be mentioned that the FTHFB method is simpler to apply in realistic situations. On the other hand, the results obtained in the FTHFB approach are also got with the TDHFB treatment. In this respect an interesting conclusion is that in those cases in which the two methods provide results, these coincide. Once again, this coincidence is based on the relation established between  $f$  and  $\nu$ .

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