Time-dependent mean field description of a two-level bosonic model

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A time-dependent mean field approximation is applied to a simple bosonic model that is related to the phase transition from spherical to deformed nuclei. It is shown that this approximation is very appropriate for the detection of this phase transition. A method for extracting matrix elements is developed and applied for the two-particle transfer operator in this model.

I. INTRODUCTION

Boson expansions and models have been largely used in the last years for the description of the bosonic branch of interacting fermion systems. They have been useful in explaining properties of vibrational, transitional, and rotational nuclei. A simple two-level bosonic model has been recently presented [1] for studying the competition between a condensate of pairs of like particles and a condensate of α-like clusters. The former has been traditionally related to a superconductive description of nuclei as pairs of nucleons coupled to $J=0$, $T=1$, have been used in nuclear superfluidity [2,3] as well as in pairing vibrations [4]. A condensate of α-like clusters, instead, may be associated with deformed states [5–8].

This simple two-level bosonic model [1] presents a phase transition between a condensate of pairs of bosons and a condensate of bosons that strongly depends on the relations between the number of bosons and degeneracies of the two levels. In Ref. [9] a similar problem was studied, and it was concluded that simple bosonic models that take into account pair condensation cannot be relevant in the thermodynamical limit as the bosonic interaction that is responsible for the saturation properties of the system (i.e., that guarantees that the binding energy is proportional to the number of particles) must contain a repulsive core that will turn unstable the condensate of pairs of bosons. In Ref. [1] it was shown that this result depends strongly on the degeneracy of the bosonic levels.

It has been shown [10,11] that in nuclei phase transitions are smoother than the predictions of mean field theories. The main reason [12] is that in the deformed regions the matrix elements of "relevant" operators turn out to be proportional to the degeneracies (that we will call R), while in the normal or nondeformed regions they are proportional to $\sqrt{R}$. In nuclei the difference between these factors is not as noticeable as in large systems. That is, because of the finiteness of the number of particles and degeneracies, even in the exact calculations, the phase transition is not very sharp, and it is therefore quite difficult to determine the critical value of the parameters.

One can therefore be sure that it is difficult to see the interesting phase transition that appears in the referred to model [1]. One may also say that the transition from a boson condensate to a boson-pair condensate is smoothed because there is no sudden onset of collectivity. Any order parameter does not show discontinuities for a finite number of bosons and finite degeneracy, but a simple way to see clearly phase transitions is through the use of mean field theories, as they yield results similar to the ones obtained for infinite number of particles and degeneracies.

On the other hand, a study of a similar Hamiltonian but for fermions [12] has shown that a time-dependent mean field approximation provides the main dynamical features of the problem. It can be applied for all values of the coupling strength and number of particles and provides a description valid on both sides of the superconducting phase transition. And the more important property is that the time-dependent variational approach clearly points out the phase transitions through changes in the phase-space trajectories. It is also possible to extract matrix elements for the relevant operators from the variational solution.

The purpose of the present paper is to apply a time-dependent mean field approximation to the above-mentioned bosonic model in order to study the phase transitions that occur in the system, not only for the ground state, but also for higher excitation energies. These excitation energies can be thought as a "critical temperature" at which the phase transition occurs. We also want to make a detailed comparison with the fermionic case. An interesting question is if there is a scaling property such that the time-dependent results become exact in a certain limit, as happened in the fermionic case [12].

In the bosonic case there are several parameters that are candidates to be used as scaling parameters as they may become large, such as the number of bosons and degeneracies of both shells. In the fermionic case this free-

dom does not exist because in order to have normal systems it is necessary that the particles fill exactly the lowest shell (if not, the system is always superconductive). In this paper we have studied this problem in detail.

A second problem that we want to study is how to extend to the bosonic case the procedure used in Ref. [12] for evaluating the two-particle transfer-matrix elements. In the bosonic case the time-dependent mean value of the transfer operator is not any longer a periodic function; therefore, it is not possible to use its Fourier series as in the fermionic case. Instead, we use the information contained in the peaks of the Fourier transform, being the area of these peaks proportional to the corresponding transfer matrix elements. This problem is discussed in detail in Sec. IV.

In Sec. II we review the model studied and the results obtained in Ref. [1]. In Sec. III we describe the time-dependent mean field approximation applied to the simple model. The results obtained are shown and discussed in Sec. IV.

II. MODEL

The model used consists of two nondegenerate shells of degeneracies 2 and $2R$ and single-boson energies $-D/2$ and $D/2$. The two lower levels simulate the proton and neutron pairing "bosons" that are used in the usual description of pairing vibrations. A condensate of this type of boson can be described as a superconductive system. The $2R$ upper levels simulate two-particle excitations formed by a proton and a neutron. If these proton-neutron excitations interact via a pairinglike residual Hamiltonian, one obtains collective pairs of proton-neutron pairs that may have the same quantum numbers as α particles. It has been shown [7] that this type of residual Hamiltonian has some resemblance with the effective interaction for the ^{212}Po nucleus.

In this work we will study a generalized version of this model in which the level degeneracies are $2R_0$ and $2R_1$, respectively. The Hamiltonian is therefore

$$H=\frac{D}{2}\left[\sum_{m=1}^{R_1}(\gamma_m^\dagger\gamma_m+\gamma_{\bar{m}}^\dagger\gamma_{\bar{m}})-\sum_{m'=1}^{R_0}(\gamma_{m'}'^\dagger\gamma_{m'}'+\gamma_{\bar{m}'}'^\dagger\gamma_{\bar{m}'}')\right]-G\sum_{m,m'>0}\gamma_m^\dagger\gamma_{\bar{m}}^\dagger\gamma_{\bar{m}'}'\gamma_{m'}'+\text{H.c.}\ , \tag{2.1}$$

where $\gamma_m^\dagger$ ($\gamma_{m'}'^\dagger$) are boson creation operators in the level 1 (0) and G is the interaction strength.

The exact solution may be found by diagonalization [1]. An important point when studying a simple model like this is the selection of appropriate scaling parameters. In Ref. [1], where R_0 was equal to 1, it has been shown that it is convenient to scale the energies with the parameter $GM\sqrt{MR_1}$, where M is half the number of bosons, whereas the appropriate dimensionless interaction parameter is $\xi=D/(G\sqrt{MR_1})$.

When the interaction is negligible the ground state of the system will be approximately described by a condensate of single bosons in the lower shell. As the interaction strength increases, one expects a ground-state phase transition to a condensate of a coherent combination of pairs of conjugate bosons. This phase transition has been found [1], but only for negative values of the interaction parameter ξ, at $\xi=-1$, and in the limit $R_1\to\infty$, $M\to\infty$, $M/R_1\ll 1$. For positive values of ξ, the ground state is always a condensate of pairs of bosons, no matter how large ξ (i.e., how small the interaction) may be.

This result was obtained through a variational treatment of the Holstein-Primakoff image of the Hamiltonian.

The most striking result obtained in Ref. [1] is that the number of α-like clusters is very high. Even for values of ξ as large as 2, one obtains a few percentage of α-like clustering in the approximate wave function. As the model Hamiltonian has similarities with the effective one obtained for the ^{208}Pb region [7], this may help to understand the high values of the preformation factor for α particles in this region [13,14].

III. TIME-DEPENDENT HARTREE-BOSE-BOGOLIUBOV TREATMENT

For implementing the time-dependent variational approach, we first introduce the boson-pair creation operators

$$\Gamma_1^\dagger=\sum_{m>0}^{R_1}\gamma_m^\dagger\gamma_{\bar{m}}^\dagger\ ,\qquad \Gamma_0^\dagger=\sum_{m'>0}^{R_0}\gamma_{m'}'^\dagger\gamma_{\bar{m}'}'^\dagger\ , \tag{3.1}$$

and the number operators

$$N_1=\sum_{m=1}^{R_1}\gamma_m^\dagger\gamma_m+\gamma_{\bar{m}}^\dagger\gamma_{\bar{m}}\ ,\qquad N_0=\sum_{m'=1}^{R_0}\gamma_{m'}'^\dagger\gamma_{m'}'+\gamma_{\bar{m}'}'^\dagger\gamma_{\bar{m}'}'\ . \tag{3.2}$$

With these definitions the Hamiltonian (2.1) is written as

$$H=\frac{D}{2}(N_1-N_0)-G(\Gamma_1^\dagger\Gamma_0+\Gamma_0^\dagger\Gamma_1)\ , \tag{3.3}$$

and the total number of bosons is $N=N_0+N_1=2M$.

Studying the commutator algebra for the operators (3.1) and (3.2), one immediately sees that the group that is relevant for the two-level model described in the previous section is SU(1,1)×SU(1,1). In Ref. [15] the phase transitions that occur in a simple SU(1,1) model were extensively studied, but the sort of phase transitions displayed in that model does not correspond to the physical situation that we are studying in the present paper. The corresponding SU(1,1) generators for each level are

$$K_0^{(i)}=\frac{N_i+R_i}{2}\ ,\qquad K_+^{(i)}=\Gamma_i^\dagger\ ,\qquad K_-^{(i)}=\Gamma_i\ . \tag{3.4}$$

They have the commutation relations, of SU(1,1),

$$[K_+^{(i)},K_-^{(i)}]=-2K_0^{(i)} ,$$
$$[K_0^{(i)},K_+^{(i)}]=K_+^{(i)} , \tag{3.5}$$
$$[K_0^{(i)},K_-^{(i)}]=-K_-^{(i)} .$$

The vacuum state $|0\rangle$ is characterized by

$$K_-^{(i)}|0\rangle=0 ,$$
$$K_0^{(i)}|0\rangle=\frac{R_i}{2}|0\rangle , \tag{3.6}$$

which identifies $|0\rangle$ as the minimum weight state of the representation of SU(1,1)×SU(1,1) with weights $R_i/2$. The coherent state in this representation is

$$|Z_0Z_1\rangle=e^{\bar{Z}_0\Gamma_0^\dagger+\bar{Z}_1\Gamma_1^\dagger}|0\rangle , \tag{3.7}$$

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 so-called time-dependent Hartree-Bose-Bogoliubov (TDHBB) equations. To obtain them one has to use the variational principle appropriate for non-normalized states [16] with an action defined as

$$S=\int dt\left[\frac{1}{2}i\frac{\langle\psi|\dot{\psi}\rangle-\langle\dot{\psi}|\psi\rangle}{\langle\psi|\psi\rangle}-\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right] , \tag{3.8}$$

and use $|\psi\rangle=|Z_0Z_1\rangle$.

The calculation of the overlap and mean value of the Hamiltonian is a well-known calculation using group theory [16]. The overlap is given by

$$\langle Z_0Z_1|Z_0Z_1\rangle=(1-Z_0\bar{Z}_0)^{-R_0}(1-Z_1\bar{Z}_1)^{-R_1} , \tag{3.9}$$

and the mean values of the operators defined in (3.1) and (3.2) are

$$\langle\Gamma_i^\dagger\rangle=\frac{R_iZ_i}{1-Z_i\bar{Z}_i} ,$$
$$\langle\Gamma_i\rangle=\frac{R_i\bar{Z}_i}{1-Z_i\bar{Z}_i} , \tag{3.10}$$
$$\langle N_i\rangle=2R_i\frac{Z_i\bar{Z}_i}{1-Z_i\bar{Z}_i} .$$

Consequently, the mean value of the Hamiltonian (3.3) is

$$\mathcal{H}=D\left[R_1\frac{Z_1\bar{Z}_1}{1-Z_1\bar{Z}_1}-R_0\frac{Z_0\bar{Z}_0}{1-Z_0\bar{Z}_0}\right]$$
$$-GR_0R_1\frac{Z_0\bar{Z}_1+\bar{Z}_0Z_1}{(1-Z_0\bar{Z}_0)(1-Z_1\bar{Z}_1)} . \tag{3.11}$$

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 [12,17]. This is done with the transformation

$$\omega_i=\left[\frac{R_i}{1-Z_i\bar{Z}_i}\right]^{1/2}Z_i . \tag{3.12}$$

The new variables ω_i are canonical in the sense that the generalized Poisson brackets [16] have the standard form and that the variational equations look like the ordinary Hamilton equations

$$i\dot{\bar{\omega}}_i=\frac{\partial\mathcal{H}}{\partial\omega_i} , \tag{3.13}$$

and its Hermitian conjugate.

The dynamical problem has two degrees of freedom, the complex variables ω_0 and ω_1. Therefore, the existence of two constants of motion, the energy and number of particles, makes the system integrable. The most adequate variables for the integration are

$$m=\frac{\omega_0\bar{\omega}_0+\omega_1\bar{\omega}_1}{M} ,$$
$$\varphi=\tfrac{1}{2}(\varphi_0+\varphi_1) ,$$
$$n=\frac{\omega_1\bar{\omega}_1-\omega_0\bar{\omega}_0}{M} , \tag{3.14}$$
$$\alpha=\tfrac{1}{2}(\varphi_1-\varphi_0) ,$$

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

The energy function (3.11) becomes

$$\mathcal{H}=DMn-GM\left[R_1+\frac{M}{2}(m+n)\right]^{1/2}$$
$$\times\left[R_0+\frac{M}{2}(m-n)\right]^{1/2}$$
$$\times(m^2-n^2)^{1/2}\cos(2\alpha) , \tag{3.15}$$

and the equations of motion are ($\mathcal{H}^*=\mathcal{H}/DM$)

$$\dot{m}=-\frac{\partial\mathcal{H}^*}{\partial\varphi}=0 ,$$
$$\dot{\varphi}=\frac{\partial\mathcal{H}^*}{\partial m} ,$$
$$\dot{n}=-\frac{\partial\mathcal{H}^*}{\partial\alpha} , \tag{3.16}$$
$$\dot{\alpha}=\frac{\partial\mathcal{H}^*}{\partial n} .$$

IV. RESULTS AND DISCUSSION

The TDHBB results are obtained solving Eqs. (3.16). However, the trajectories are best represented implicitly in the phase plane (n,α) as constant-energy curves $\mathcal{H}=$const. It is clear from expression (3.15) that the appropriate scaling to be used depends on the relation between the number of pairs of bosons M and the degeneracies R_0 and R_1. In the case considered in Ref. [1] ($R_0=1$, $M<R_1$), it is convenient, as already mentioned, to scale the energies with the parameter $GM\sqrt{MR_1}$, whereas the corresponding interaction parameter is $\xi=D/(G\sqrt{MR_1})$.

The energy function (3.15) becomes (fixing $m=1$)

$$\mathcal{E}=\frac{\mathcal{H}}{GM\sqrt{MR_1}}$$
$$=\xi n-\left[1+\frac{M}{2R_1}(1+n)\right]^{1/2}\times\left[\frac{1}{M}+\frac{1}{2}(1-n)\right]^{1/2}\times(1-n^2)^{1/2}\cos(2\alpha)\ . \quad (4.1)$$

It is also interesting to consider a symmetric model, as the fermionic one studied in Ref. [12], in which $R_0=R_1=R$. The appropriate energy scaling for $M<R$ is GMR with an interaction parameter defined as $\varepsilon=D/GR$. Equation (3.15) becomes

$$\mathcal{E}=\frac{\mathcal{H}}{GMR}=\varepsilon n-\left[\left[1+\frac{M}{2R}\right]^2-\left[\frac{Mn}{2R}\right]^2\right]^{1/2}\times(1-n^2)^{1/2}\cos(2\alpha)\ . \quad (4.2)$$

Since we are working with bosons, the number of pairs M may be greater than the degeneracies R_0 and R_1. For studying the limit $M\gg R_0$, $M\gg R_1$, the appropriate energy scaling is GM^2 with an interaction parameter $\zeta=D/GM$ and an energy function

$$\mathcal{E}=\frac{\mathcal{H}}{GM^2}=\zeta n-\left[\frac{R_0}{M}+\frac{1-n}{2}\right]^{1/2}\left[\frac{R_1}{M}+\frac{1+n}{2}\right]^{1/2}\times(1-n^2)^{1/2}\cos(2\alpha)\ . \quad (4.3)$$

Comparing the exact ground-state results obtained by diagonalizing the Hamiltonian (2.1) with the TDHBB energies, one concludes that the latter tend to the exact energies for large number of bosons and large degeneracies. In the fermionic case it has been shown [12] that there exists a scaling property such that the time-dependent results provide a universal (i.e., degeneracy-independent) curve to which the exact energies converge for large degeneracies. For the bosonic model studied in the present work, this is not the case, as the limits provided by TDHBB for different relations between the number of bosons and degeneracies of the levels correspond to different energy scalings. This is clearly seen from Eqs. (4.1)–(4.3).

Analyzing the minimum value of the scaled energy $\mathcal{E}$ as a function of the interaction parameter (ξ, ε, or ζ, depending on the case considered), one may determine if there exists a ground-state phase transition from a condensate of single bosons in the lower level (normal state) to a condensate of a coherent combination of pairs of conjugate bosons (superconductive state). The normal-state energy is $\mathcal{E}_n=-|\xi|$ (or $\mathcal{E}_n=-|\varepsilon|$ or $\mathcal{E}_n=-|\zeta|$). If the minimum value of $\mathcal{E}$ is smaller than $\mathcal{E}_n$ only for interaction parameters up to a certain value ξ_c, one says that a ground-state phase transition occurs for that critical interaction parameter ξ_c. For a fixed value of the interaction parameter, the energies below $\mathcal{E}_n$ correspond to superconductive systems. Similarly, energies above $-\mathcal{E}_n$ also correspond to superconductive systems. Consequently, normal systems are only found in the energy region $\mathcal{E}_n<\mathcal{E}<-\mathcal{E}_n$.

In the case considered in Ref. [1], when the energy function is given by (4.1), a ground-state phase transition is found at $\xi_c=-\sqrt{1+M/R_1}$ for $M\to\infty$, $R_1\to\infty$, $M<R_1$. For positive values of the interaction parameter, no ground-state phase transition occurs. These results coincide with the ones obtained in Ref. [1]. In the symmetric case in which $R_0=R_1=R$, no ground-state phase transition is found for $M<R$. On the other hand, when the number of bosons is greater than the degeneracies of the levels, analyzing Eq. (4.3), one finds two ground-state phase transitions, one for positive values of the interaction parameter ζ and the other for negative values. The positive critical strength is $\zeta_c=\sqrt{1+R_0/M}$, and it is obtained in the limit $R_1/M\to 0$, whereas for negative values one gets $\zeta_c=-\sqrt{1+R_1/M}$ in the limit $R_0/M\to 0$. Therefore, in the symmetric model $R_0=R_1=R$, the ground-state phase transition only occurs if $M\gg R$. Performing a similar analysis in the symmetric fermionic model (cf. Ref. [12]), the result obtained is quite different. In this case the ground-state phase transition only occurs in the middle of the shell, i.e., for $M=R$.

The phase-space trajectories $n(\alpha)$ obtained for fixed values of the energy $\mathcal{E}$ given by (4.1) are shown in Fig. 1 for $R_0=1$, $R_1=500$, $M=50$, and interaction parameter $\xi=0.3$. Two different kinds of trajectories are observed. The closed ones correspond to superconductive systems [12], and they may be interpreted as vibrations around a well-deformed minimum. The open trajectories, instead, may be associated with normal systems. As in the fermionic case [12], the superconductive system becomes normal when the excitation energy increases. This phase transition and also the ground-state one are clearly pointed out in the TDHBB description by a change in the trajectories behavior. Similar results are obtained for other

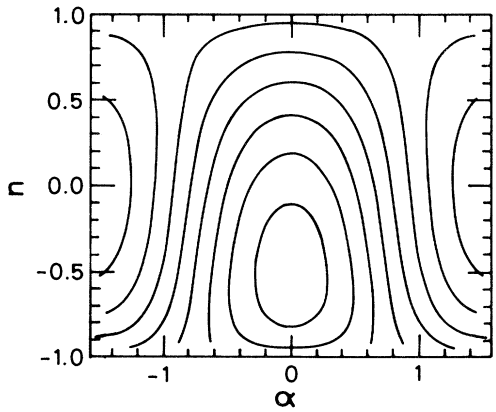

FIG. 1. Phase-space trajectories for $M=50$, $R_0=1$, and $R_1=500$ for equally spaced energies with $\xi=0.3$.

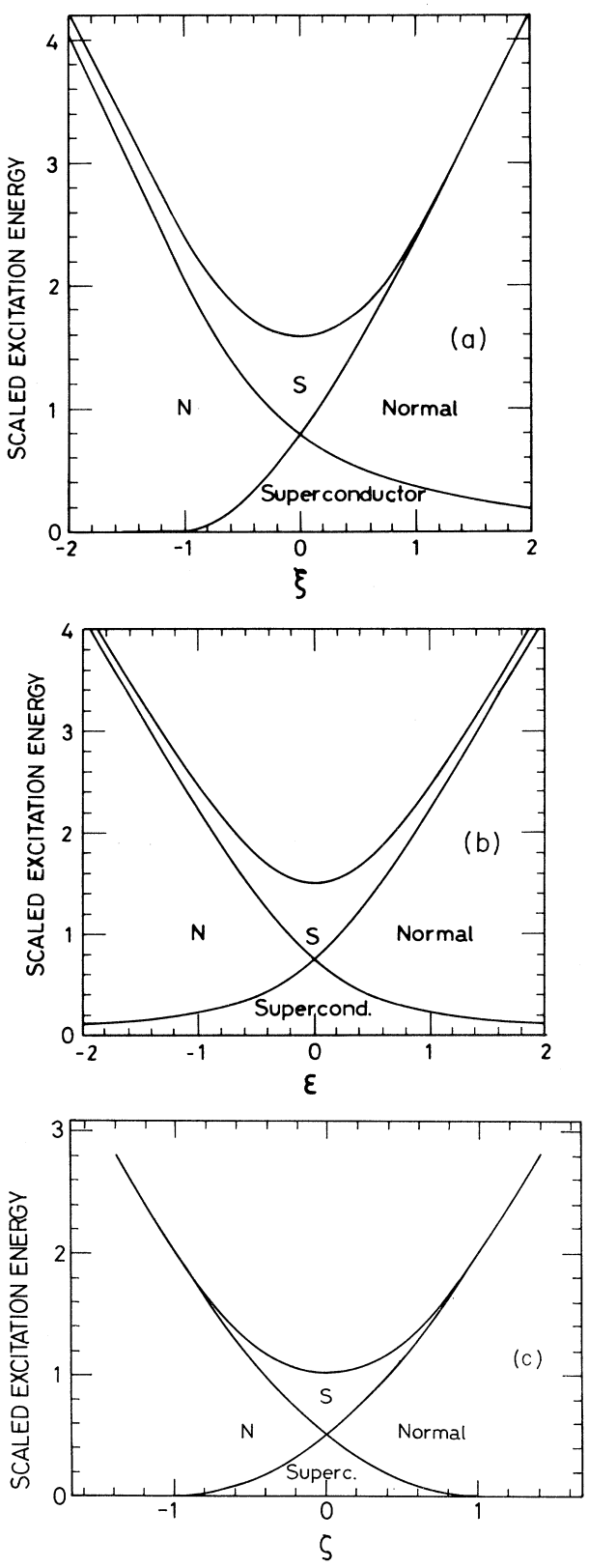

FIG. 2. "Phase diagrams" for the different cases studied. In (a) $M=50$, $R_0=1$, and $R_1=500$; (b) $M=R_0=R_1=50$; and (c) $M=5000$, $R_0=R_1=50$. In each case the appropriate scaled interaction parameter is displayed.

values of the parameters and also in the other cases considered in the present work in which the energies are given by (4.2) and (4.3).

The excitation energies in which the phase transition between both types of orbits occurs are shown in Fig. 2 as functions of the interaction parameter. Figure 2(a) corresponds to the same case shown in Fig. 1, whereas Figs. 2(b) and 2(c) correspond to the cases in which the energies are given by (4.2) and (4.3), respectively. It is to be noted that the appearance of a second phase transition in a higher excitation energy in which the system turns to be superconductive once again is due to the fact that the residual Hamiltonian considered has only off-diagonal terms. The upper curve corresponds to the maximum excitation energy in the system. These results agree with the above discussion in which we concluded that the normal systems are only found in the energy region $-|\xi|<\mathcal{E}<|\xi|$.

The ground-state phase transitions analyzed before are clearly observed. In Fig. 2(a) only one ground-state phase transition appears at $\xi=-1$, in Fig. 2(b) there is none, and in Fig. 2(c) there are two. One may summarize the results obtained relating the existence or not of a superconductive ground state with the ratio M/R_i. When this ratio is small, the system has always a superconductive ground state, while when it is large, the system has a normal ground state for small interaction.

Finally, we have calculated the two-particle transfer-matrix elements, both exactly and within the TDHBB approach. Assuming that both levels have a similar radial dependence, the two-particle transfer operator may be defined by $\Gamma_0^+ + \Gamma_1^+$ [see Eq. (3.1)]. Its exact matrix elements are evaluated using

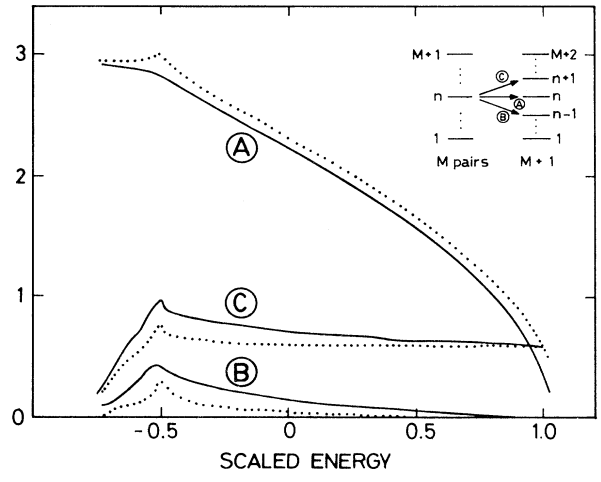

FIG. 3. Matrix elements of the two-particle transfer operator for $M=50$, $R_0=1$, $R_1=500$, and $\xi=-0.5$ as functions of the scaled energy $\mathcal{E}$. The dots represent the exact results, and the values obtained with the Fourier analysis are shown as solid lines. The labels to the lines are explained in the inset.

$$\langle N_i+2|\Gamma_i^+|N_i\rangle=\left[\left(\frac{R_i+N_i}{2}\right)\left(\frac{R_i+N_i}{2}+1\right)-\frac{R_i}{2}\left(\frac{R_i}{2}-1\right)\right]^{1/2}, \tag{4.4}$$

and the eigenfunctions obtained from the exact diagonalization of the Hamiltonian.

The TDHBB matrix elements are evaluated, as proposed in Ref. [12], from the time-dependent mean value in the state which is a solution of the variational equations at a certain energy $\mathcal{E}$. Using (3.10), (3.12), and (3.14), this mean value is written as

$$\frac{f(t)}{M}=\frac{1}{2}e^{i\varphi}\left\{e^{-i\alpha}\left[(m-n)\left(\frac{2R_0}{M}+m-n\right)\right]^{1/2}+e^{i\alpha}\left[(m+n)\left(\frac{2R_1}{M}+m+n\right)\right]^{1/2}\right\}. \tag{4.5}$$

The time dependence of n, α, and φ is obtained integrating the equations of motion (3.16) for a given energy $\mathcal{E}$. If $f(t)$ is periodic, of period $T(\mathcal{E})$, its Fourier components

$$\tilde{f}_k(\mathcal{E})=\frac{1}{T}\int_0^T e^{ik(2\pi/T)t}f(t)dt \tag{4.6}$$

may be compared with the exact two-particle transfer-matrix elements. This procedure is the one that was used in the fermionic case.

Unfortunately, in the present case, the period of φ is not equal to the one corresponding to the trajectory $n(\alpha)$. As the function $f(t)$ is not any longer periodic, we propose, as a procedure for obtaining the approximate matrix elements in this case, to perform the Fourier transform of $f(t)$ that has been evaluated at the energy $\mathcal{E}$ corresponding to the TDHBB solution. This Fourier transform has only few peaks (in general, we find at most three peaks that are noticeable over the background), and those peaks appear at energies that are related to the excitation energies at energy $\mathcal{E}$. The matrix elements can be obtained from the areas of the peaks. We have checked that in the fermionic case, where the function $f(t)$ is periodic, this procedure yields the same results as the ones obtained in Ref. [12].

In Fig. 3 we display the matrix elements of the two-particle transfer operator for $M=50$, $R_0=1$, $R_1=500$, and $\xi=-0.5$ as functions of the scaled energy $\mathcal{E}$. The dots represent the exact results, and the values obtained with the Fourier analysis are shown as solid lines. The labels of the lines are explained in the inset.

The nice agreement between the exact and approximate results supports the recipe that we have developed for the evaluation of matrix elements when using time-dependent variational solutions. It must be noted that this recipe can be used for any time-dependent variational problem and provides therefore a solution to a long-standing problem [18].

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