Self-consistent random phase approximation in the Schütte–Da Providencia fermion-boson model

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(Received 27 May 2003; published 30 January 2004)

The self-consistent random phase approximation (SCRPA) is applied to the exactly solvable model with fermion-boson coupling proposed by Schütte and Da Providencia. Very encouraging results in comparison with the exact solution of the model for various observables are obtained. The transition from the normal phase to the phase with a spontaneously broken symmetry is carefully investigated. The strong reduction of the variance in SCRPA vs Hartree-Fock is pointed out.

DOI: 10.1103/PhysRevC.69.017306 PACS number(s): 21.60.Jz, 24.10.Cn

During the last decade the so-called self-consistent version of the random phase approximation (SCRPA) has seen very encouraging successes in a number of nontrivial model cases (see, for example, Ref. [1] for a detailed description of the method and Ref. [2] for the application of SCRPA to the many-level pairing model). In spite of these performances of the theory, there are remaining problems. In first place this concerns situations with spontaneously broken symmetries. Such situations were treated in Refs. [1,3,4]. Whereas in the Lipkin model [3] the symmetry broken ("deformed") phase caused no problem because the broken symmetry is discrete (parity), in the other two cases [1,4], with a continuous broken symmetry, problems appeared with the low-lying mode known to be exactly at zero energy in the standard HF-RPA approach (the spurious or Goldstone mode), where HF stands for Hartree-Fock. In the two cases cited [1,4] the low-lying mode does not appear at zero energy in SCRPA because the RPA operator does not contain the symmetry operator as a limit case. Indeed, e.g., the number operator in quasiparticle (BCS) representation contains a purely Hermitian piece $\alpha_k^\dagger \alpha_k$ which cannot be incorporated in the RPA operator which by definition is non-Hermitian. The same situation is present in the Schütte-Da-Providenica boson-fermion model [5] where the symmetry operator contains the boson and fermion number operators. The violation of the Goldstone theorem signifies that the Ward identities and conservation laws are not respected. Though this violation seems relatively mild and to go away in macroscopic systems (the Hermitian pieces becoming of zero weight), the situation remains annoying for finite systems.

In this paper which can be considered as a sequel of Ref. [4] we want again to investigate the Schütte–Da Providenica model:

$$H = \bar{n} + \alpha b^\dagger b + G(\tau^+ b^\dagger + \tau^- b) \tag{1}$$

with $b^\dagger$, b ideal boson operators and

$$n = \sum_{i=1}^N a_{0i}^\dagger a_{0i}, \quad \bar{n} = \sum_{i=1}^N a_{1i}^\dagger a_{1i}, \quad \tau^+ = \sum_{i=1}^N a_{1i}^\dagger a_{0i},$$
$$\tau^- = \sum_{i=1}^N a_{0i}^\dagger a_{1i}, \quad \tau^0 = \tfrac{1}{2}(\bar{n} - n),$$

where the $a^\dagger$, a are fermion operators. In analogy to the work in Ref. [4] we will introduce the more general RPA operator

$$Q_\nu^\dagger = X_\nu t^+ - Y_\nu t^- + \lambda_\nu B^\dagger - \mu_\nu B + U_\nu \beta^\dagger \beta^\dagger - V_\nu \beta\beta,$$
$$\nu = 1, 2, 3, \tag{2}$$

where

$$t^\pm = \frac{T^\pm}{\sqrt{-2\langle T^0\rangle}} \quad \text{and} \quad \beta^\dagger\beta^\dagger = \frac{B^\dagger B^\dagger}{\sqrt{2(1+2\langle B^\dagger B\rangle)}}. \tag{3}$$

The operators $T^\pm$, T^0 are obtained from $\tau^\pm$, τ^0, by writing the latter ones in the deformed basis

$$\begin{pmatrix} \alpha_{1k}^\dagger \\ \alpha_{0k} \end{pmatrix} = \begin{pmatrix} u & -v \\ v & u \end{pmatrix} \begin{pmatrix} \alpha_{1k}^\dagger \\ a_{0k}^\dagger \end{pmatrix}, \quad u^2 + v^2 = 1. \tag{4}$$

The bosons operators $B^\dagger$ and B are obtained from the original ones by a shift transformation $B \to b - \sigma$, where σ is a c number characterizing the appearance of the Bose condensate. The introduction of the boson pair operators $\beta^\dagger\beta^\dagger$ is motivated by the fact that otherwise there exists a certain dissymmetry between fermions and bosons, the fermions being in any case bilinear whereas the bosons are otherwise only contained to linear order in Eq. (2). Also the symmetry operator $P = b^\dagger b - \bar{n}$ contains the bosons quadratically and the extended ansatz (2) may therefore show improved behavior with respect to the Goldstone mode. The formalism goes exactly in the same way as in Refs. [1,2,4] using the equation of motion method

$$\langle [\delta Q, [H', Q_\nu^\dagger]]\rangle = \Omega_\nu \langle [\delta Q, Q_\nu^\dagger]\rangle \tag{5}$$

to determine the amplitudes in Eq. (2). As in Ref. [4], in order to fix the value $L = \langle P\rangle$, we use in Eq. (5) the cranked Hamiltonian $H' = H - \mu P$ in the symmetry broken phase, otherwise $H' = H$. The mean-field amplitudes u, v, and σ are readily obtained from a minimization of the ground-state energy, leading to $\langle [H', t^+]\rangle = \langle [H', B^\dagger]\rangle = 0$. The amplitudes in Eq. (2) form a complete orthonormal set when calculated from Eq. (5). Then Eq. (2) can be inverted and with the usual condition for the RPA ground state

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TABLE I. Chemical potential: exact, SCRPA(6), SCRPA(4), and standard RPA; L values, in the deformed region for different values of the interaction strength x.

x	L	μ(exact)	$\mu(6)$	$\mu(4)$	μ(RPA)
1.1	−1	−0.0131	−0.0485	−0.0485	0.1160
1.4	−3	0.0325	0.0348	0.0405	0.1303
1.8	−3	−0.0341	−0.0315	−0.0329	0.0060
2.2	0	0.0320	0.0300	0.0240	0.0345
2.6	4	0.0305	0.0285	0.0221	0.0207
3.0	9	0.0204	0.0195	0.0135	0.0071

$$Q_\nu|\mathrm{RPA}\rangle = 0, \quad \nu = 1, 2, 3. \tag{6}$$

All expectation values appearing in Eq. (5), for example, $\langle t^+B^\dagger\rangle$, $\langle t^+B\rangle$, and $\langle B^\dagger B\rangle$ can directly be expressed in terms of the RPA amplitudes. The only unknown quantity at this point preventing a fully self-consistent solution of the SCRPA equations, Eq. (5), is the expectation value $\langle T^0\rangle$. However, in analogy to our previous study for the two-level pairing model [1] this quantity can be expressed as an expression in the operators T^+ and T^- up to any order in a fast converging series according to

$$T^0 = -\frac{N}{2} + \frac{1}{N}T^+T^- + \frac{1}{N^2(N-1)}T^{+2}T^{-2} + \cdots. \tag{7}$$

With this relation the SCRPA equations are completely closed and we can proceed to the numerical solution. We notice that with respect to Ref. [4] the SCRPA, Eq. (5), is a (6×6)-dimensional problem whereas before it was 4×4.

We now come to the presentation and discussion of the results. In what follows, SCRPA(6) refers to the SCRPA method with RPA excitation operator quadratic in the bosons operators i.e., Eq. (2), while SCRPA(4) refers to the same method but with RPA excitation operator linear in the bosons operators, i.e., $U_\nu = V_\nu = 0$. In the following we also use the set of parameters $\alpha = 3$, $N = 30$ as in Ref. [4], for which in this model the phase transition point is localized at $x = 1.0$, where $x = G\sqrt{N/\alpha}$. SCRPA always shows a clear superiority over the standard RPA, though, besides some quantities, the differences are not very pronounced. Concerning the ground-state energy we do not give results but we only notice that we arrive practically at the same interpretations as in Ref. [4]. However, in order to test the accuracy of our approach it is instructive to calculate the differences of energies of the ground-state band with L values just one unit away from the absolute ground state. One such quantity is the "chemical potential" which should be identified with the Lagrange parameter used for restoring the symmetry,

$$\mu = \tfrac{1}{2}(E^0_{L+1} - E^0_{L-1}). \tag{8}$$

In Table I we show μ when we calculate separately $E^0_{L\pm1}$ (in the standard RPA and SCRPA) and then take the difference. We also give in Table I the L values which correspond for a given x value to the absolute ground state. In Table I we see a strong improvement of SCRPA(6) and SCRPA(4) over the standard RPA and the high quality of the results in comparison with the exact values in the region around the phase transition point. Also SCRPA(6) is still improved over SCRPA(4). We could also have taken the μ values found from adjusting the correct $L = \langle P\rangle$ values in the standard RPA and SCRPA calculations; we have checked numerically that the results are always practically identical.

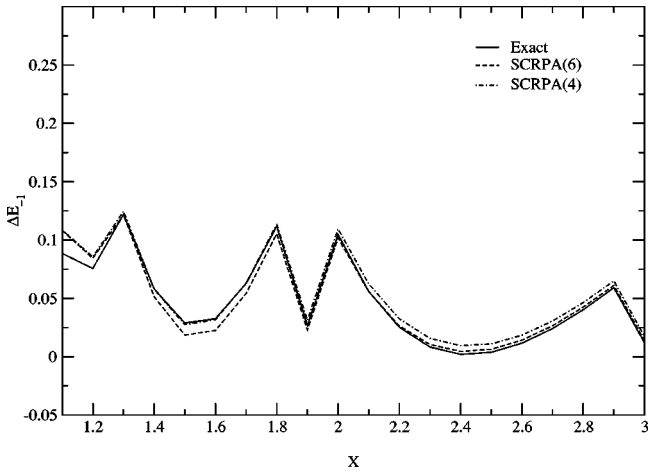

FIG. 1. Comparison between the exact, SCRPA(6), and SCRPA(4) results for the excitation energy $\Delta E_{-1} = E^0_L - E^0_{L-1}$ in the deformed region.

Two other interesting quantities to be calculated within the SCRPA formalism and closely related to the chemical potential are the energy differences of the absolute ground state with its "left" and "right" neighbors just one unit away in L,

$$\Delta E_{\pm1} = \pm(E^0_{L\pm1} - E^0_L). \tag{9}$$

These quantities are interesting because, as we will explain below, they should be closely related to the lowest RPA eigenvalue Ω_1 in the symmetry broken phase. Because we obtain similar interpretation and conclusions for both $\Delta E_{\pm1}$, we will present and discuss only the result for ΔE_{-1}. In Fig. 1 we see a very good agreement with the exact results of both SCRPA(6) and SCRPA(4). However, we note that in this quantity no clear superiority of SCRPA(6) over SCRPA(4) can be detected, the results being at times in favor of the one or the other. The good quality of the results for $\Delta E_{\pm1}$ shows that the SCRPA method is able to reproduce the full spectrum. We also should notice that the smallness of $\Delta E_{\pm1}$ means that two neighboring ground states with L and $L\pm1$, respectively, are almost degenerate which indicates that the system is in the phase of spontaneously broken symmetry. Furthermore, one can check that in the large N limit $\Delta E_{\pm1}$ tends to zero. The zero eigenvalue (Goldstone mode) which is one of the solutions of the standard RPA in the deformed region corresponds to this degeneracy of the neighboring ground-state energies in the large N limit.

Let us now discuss the eigenvalues of RPA and SCRPA matrices. As it is well known [4,5], in the standard RPA the lowest eigenvalue corresponds in the symmetry broken (deformed) region to the spurious mode $\Omega_1 = 0$, whereas the sec-

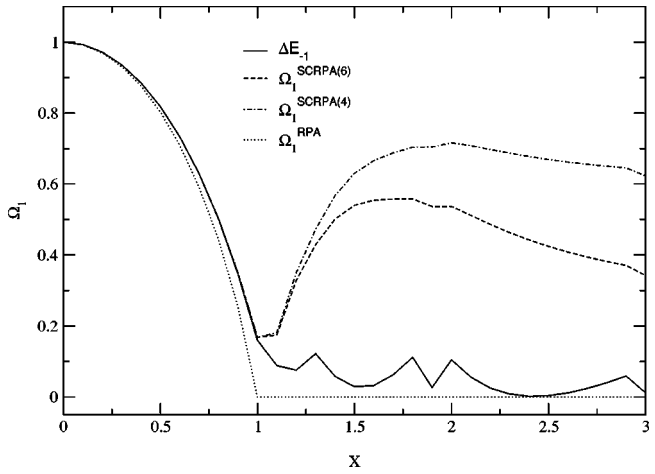

FIG. 2. The standard RPA, SCRPA(4), and SCRPA(6) results for the spurious mode Ω_1 compared with the exact energy of the excitation ΔE_{-1}.

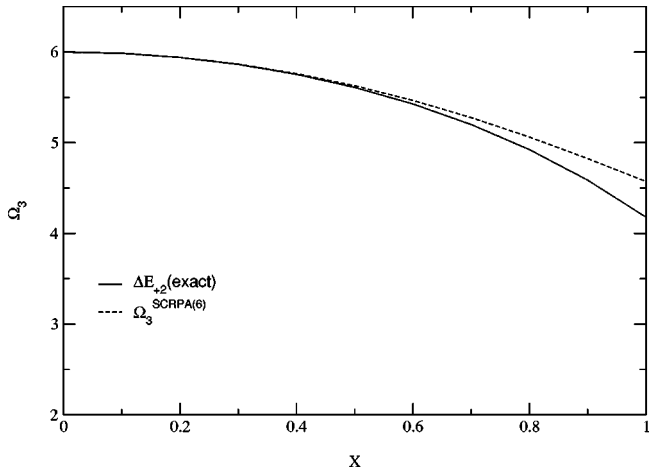

FIG. 3. The SCRPA(6) results of the energy of the excitation mode Ω_3 compared with the exact energy of the excitation ΔE_{+2} in the spherical region.

ond eigenvalue gives the excitation of the intrinsic system. Before coming to this point we should mention again that the RPA eigenvalues in the deformed region are calculated with the "intrinsic" Hamiltonian $H' = H - \mu P$. Therefore, when the symmetry is restored due to the appearance of the Goldstone mode, the RPA eigenvalues give the excitation energies of the system. The results for the mode Ω_2 are not shown in a figure because we obtain the same interpretation as already given in Ref. [4], however, with still improved results from SCRPA(6).

Concerning the low-lying eigenvalue of SCRPA which in the standard RPA corresponds to the zero-energy eigenvalue (Goldstone or spurious mode) in the deformed region, we present in Fig. 2 a comparison between the standard RPA, SCRPA(4), and SCRPA(6) with exact results. In the "spherical" phase we notice that the eigenvalue Ω_1 is identified with the exact "intraband" excitation ΔE_{-1}. Furthermore, we see the important improvement of the SCRPA results in both cases SCRPA(4) and SCRPA(6) with respect to the standard RPA result. After the phase transition ΔE_{-1} remains finite but very small, slowly decreasing for increasing x, while the lowest eigenvalue in the standard RPA corresponds to the spurious mode $\Omega_1 = 0$. Concerning the low-lying eigenvalue in SCRPA calculation we see that SCRPA(6) improves the result with respect to SCRPA(4) but it is still quite far from the exact result. We can notice that the Goldstone theorem is not correctly fulfilled in this case. Therefore, the problem of the identification of the low-lying eigenvalue is not yet solved in SCRPA in spite of the introduction of the quadratic boson terms in Eq. (2).

From the presence of the quadratic boson terms in the RPA excitation operator the SCRPA method produces a supplementary eigenvalue which is denoted as Ω_3. Let us now discuss the results for this mode, i.e., the third eigenvalue RPA of the SCRPA(6) which is presented in Fig. 3. In the spherical region we notice that this mode is identified with very good accuracy to the exact intraband excitation ΔE_{+2}. However, in the deformed region (not shown), the result obtained for this mode cannot be identified with one of the exact excitations of the system. At present we do not have an explanation of this fact. It is likely to be related to the failure of the Goldstone theorem mentioned above. See also further discussion of this point at the end of this paper. The difficulty may be of the same origin as with the Ω_1 mode.

A quantity which is particularly sensitive to the correct treatment of correlations in the ground state is the mean boson number (not shown in Ref. [4]). This expectation value can be obtained in terms of the RPA amplitudes according to

$$N_b = \langle b^\dagger b \rangle = \langle B^\dagger B \rangle + \sigma^2, \tag{10}$$

where $\langle B^\dagger B \rangle$ is given, in SCRPA(6), by $\langle B^\dagger B \rangle = \mu_1^2 + \mu_2^2 + \mu_3^2$. In Fig. 4 we show the results of the SCRPA(6), SCRPA(4), standard RPA, and mean-field methods for this quantity. Again with SCRPA(6) one notices a significant improvement over the standard RPA and HF method for which the agreement with the exact result is not satisfying. Also, we note in Fig. 4 that the SCRPA(6) improves slightly the result over

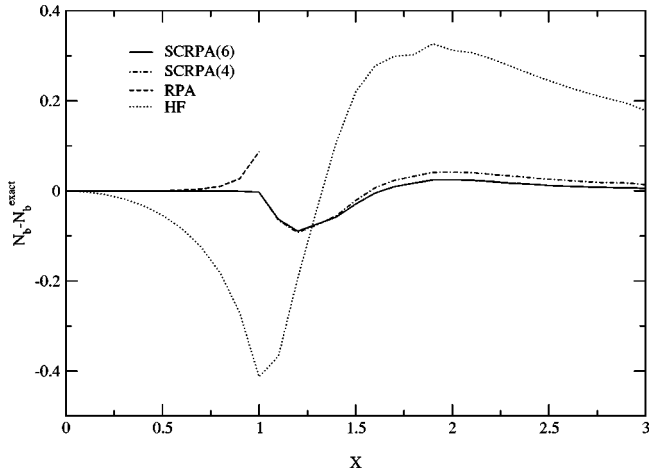

FIG. 4. The difference $[N_b - N_b^{\text{exact}}]$ calculated with SCRPA(6), SCRPA(4), RPA, and mean-field methods as a function of the interaction strength x.

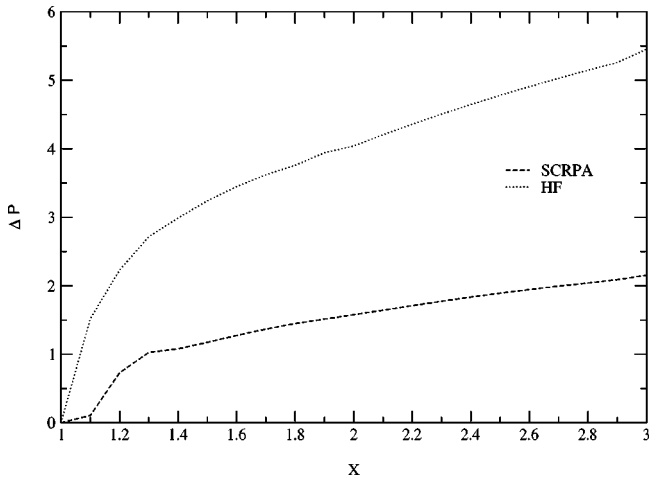

FIG. 5. Variance as a function of the interaction strength x.

the SCRPA(4) specially in the deformed region. Furthermore, we note that in standard RPA method, because we have a Goldstone mode in the deformed region, we cannot calculate this quantity.

Another quantity which is very interesting to investigate in the SCRPA method is the variance of the symmetry operator P given by

$$\Delta P^2 = \langle P^2 \rangle - \langle P \rangle^2. \tag{11}$$

In Fig. 5 we present the results corresponding to this quantity calculated with SCRPA and HF methods. This is a new result which was not elaborated in Ref. [4]. We see that the variance is strongly reduced compared to HF values. We, however, see that ΔP even in the SCRPA acquires sizable nonvanishing values. This simply means that the symmetry P, broken at the level of the mean-field theory, is not completely restored. Furthermore, we do not present the standard RPA results concerning this quantity in Fig. 5 because the RPA amplitudes originating from the Goldstone mode are divergent. This constitutes the same kind of situation as that for the boson number in the ground-state calculation for which we also have not given the standard RPA results in the deformed region.

In conclusion we reconsidered the work of Bertrand *et al.* [4] who treated the schematic Schütte-Da-Providencia model for interacting bosons and fermions within the SCRPA scheme. In Ref. [4] the RPA operator consisted only of one boson and fermions pair. Here we extended this configuration space and included in addition bosons pairs. One of the motivations to do this was to see whether the Goldstone theorem which was quite strongly violated in Ref. [4] is improved. It was found that the low-lying mode in the deformed zone, i.e., symmetry broken region, indeed is lowered by $\sim$30% when boson pair terms are added to the RPA operator. However, with respect to the first physical state, the position of the spurious mode is still too high and one therefore cannot say that it decouples to a good approximation from the physical spectrum. However, in spite of this somewhat disappointing result, the introduction of the extra terms allowed to reproduce very well a further excited state of the spectrum in the symmetry conserved phase and additionally the quantities which had already been calculated in Ref. [4] without the boson pair operators are still improved. We also calculated further quantities as the number of bosons in the ground state and the fluctuation of the symmetry operator. For instance the latter becomes strongly reduced with respect to its mean-field value. However, also for this quantity a substantial nonvanishing value remains. All in all we can say that the inclusion of the extra two boson pieces to the RPA operator allowed to calculate one more state in the spherical region, improve existing results from calculations without these terms, and lower the spurious state. However, with respect to the latter feature no real breakthrough could be observed and further ideas are needed to substantially improve the situation in the symmetry broken region whereas the "spherical" region seems to be well under control. In this respect this may be similar with other approaches treating correlations beyond mean-field-like coupled cluster theory, Jastrow, correlated basis function, etc.

We are specially grateful to Guy Chanfray and Peter Schuck for many interesting discussions and stimulating comments. We thank Raouf Bennaceur and Jorge Dukelsky for criticism and helpful comments. We gratefully acknowledge stimulating discussions with M. Oertel, D. Davesne, and H. Hansen.

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