Eur. Phys. J. A **7**, 155–165 (2000)

THE EUROPEAN PHYSICAL JOURNAL A

Occupation numbers in Self Consistent RPA

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Received: 10 September 1999
Communicated by B. Povh

Abstract. A method is proposed which allows to calculate within the SCRPA theory the occupation numbers via the single particle Green function. This scheme complies with the Hugenholtz van Hove theorem. In an application to the Lipkin model it is found that this prescription gives consistently better results than two other commonly used approximations: lowest order boson expansion and the number operator method.

PACS. 21.60.-n Nuclear-structure models and methods – 21.60.Jz Hartree-Fock and random phase approximations – 21.60.Fw Models based on group theory

1 Introduction

The solution of the many body problem beyond the mean-field level is not a very well settled problem. Though the meanfield approach for all kinds of many body problems is quite uniquely defined, the determination of the higher order correlation functions is not. Besides the usual partial resummation of Feynman graphs (e.g. ring summation in RPA) there also exist variational ansätze such as those introduced by Jastrow, Gutzwiller, together with the Resonating Valence Bond approach, etc. [1]. However only in rare cases these variational approaches can be worked through to the end by minimizing the groundstate energy so that any new route can have interesting perspectives. In most cases there remains the additional problem of how to determine the excited states. One of the attractive features of the Raleigh-Ritz variational Hartree-Fock (HF) theory is indeed that it yields, consistently within the same theory, groundstate and excited states (quasiparticle excitations).

Since some time we have elaborated on a theory for two body correlations functions which in a certain sense can be considered as an extension of HF theory to two body clusters. We for instance obtain selfconsistent nonlinear equations for the correlation functions which simultaneously determine the correlated groundstate energy and the spectrum of excitations. We named this approach Self - Consistent Random Phase Approximation (SCRPA) [2–6], since it is a consistent generalization of the standard linear RPA approach [7–10]. This formalism was also developed independently by a second group of authors which coined for it the name Cluster Hartree-Fock (CHF) which seems also very appropriate [11]. This type of theory took its roots several decades back starting with the work of Hara [8]. Considerable progress was achieved by D. Rowe using the equation of motion method which is summarized in [9]. Some years later the theory was rederived using the method of many body Green functions [12,2]. Since that time not much progress was made on the formal aspect of the theory until the more recent works cited above.

The SCRPA has lately given a series of interesting results for various many-body problems [13,4,5]. Nevertheless some open problems persisted in the past with this formalism concerning for instance the consistent evaluation of single particle quantities such as the single particle density matrix or the occupation numbers. An approximation which lately came very much in use in relating these quantities back to SCRPA (or to its poorer but numerically easier variant the so called Renormalized RPA (RRPA) [8]) is based on the particle number method which long time ago already was advocated by D. J.Rowe [10]. Very recently we have proposed and applied a different method which calculates these quantities via the single particle Green's function with a mass operator coupling back to the SCRPA [4,6]. In those works, however, neither a detailed derivation nor an assessment of its quality was given. On the other hand it has been pointed out that certain consistency relations are indeed fulfilled.

The purpose of the present paper is therefore to give a quite detailed derivation and to make a systematic investigation in a model case of the Green's function approach and to contrast it with other methods.

The paper is organized as follows: In section II the SCRPA equations are deduced, their coupling with the single particle Green's functions is presented in section III, the application to the Lipkin model is developed in section

IV, the numerical results in section V and the conclusions are given in section VI.

2 Outline of the problem

Self Consistent RPA can be derived in various ways, the best known being the equation of motion method [10], which is close to the Green's function method described below. The method which probably exhibits most clearly the analogy with ordinary HF theory is the one due to Baranger [14]. Let us first rederive in this way single particle HF. To this end we define a mean single particle energy in the following way (see (1) at bottom of this page), where E^N_ν and $|N,\nu\rangle$ are in principle exact eigenenergies and eigenstates of the Hamiltonian for a system with N particles. For the groundstate we have $\nu = 0$ and $a^\dagger_k$ is a single particle creation operator. Minimizing (1) with respect to the amplitudes φ^μ_k and $\varphi^{\mu *}_k$ leads directly to the following eigenvalue problem

$$\sum_{k'} \langle 0| \left\{ a_k, \left[H, a^\dagger_{k'} \right] \right\} |0\rangle \;\; \varphi^\nu_{k'} = \varepsilon_\nu \;\; \varphi^\nu_k \tag{2}$$

where $\{...,...\}$ is the anticommutator.

It is easy to verify that (2) is just one of the forms of the usual single particle HF equations, once $|0\rangle$ is chosen to be a Slater determinant.

Let us now in the same way find equations which describe another form of elementary excitations of the system such as density vibrations. To this purpose we define in analogy to (1) a mean excitation energy (see (3) at bottom of this page).

Minimization with respect to the amplitudes $X^\mu_{kk'}, Y^\mu_{kk'}$ leads to

$$\langle 0| \left[\delta Q, \left[H, Q^\dagger_\nu \right] \right] |0\rangle = E_\nu \;\; \langle 0| \left[\delta Q, Q^\dagger_\nu \right] |0\rangle \tag{4}$$

where

$$Q^\dagger_\nu = \sum_{k>k'} \left(X^\nu_{kk'} a^\dagger_k a_{k'} - Y^\nu_{kk'} a^\dagger_{k'} a_k \right) \tag{5}$$

and δQ is a variation (with respect to X or Y) of $Q^\dagger$. Equation (4) constitutes the SCRPA equations which are described in great detail elsewhere [3–6]. Explicitly

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \; \mathcal{N} \; \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} \tag{6}$$

where the matrices A and B are double commutators coming from the left hand side of (4) and $\mathcal{N}$ is the norm matrix to be discussed in the following section. If the ground state $|0\rangle$ is known as a functional of the amplitudes X, Y, then the expectation values needed to build to the matrices A, B and $\mathcal{N}$ can be expressed in terms of X, Y and (6) leads to a nonlinear eigenvalue problem for the RPA amplitudes which have to be determined iteratively very much like the HF equations (2). Ideally this would be the way in which the SCRPA equations are built. However, in most cases the dependence of the ground state, defined in (10) below, on X, Y is unknown and therefore one of the main purposes of the present paper is to show how the A, B and $\mathcal{N}$ matrices can be approximately expressed in terms of the X, Y amplitudes without this knowledge. To avoid a proliferation of names we will still call it SCRPA. This study will be performed in the frame of a simple model where in fact the ground state can be constructed explicitly in terms of X, Y allowing for a comparison with the approximate expressions for A, B and $\mathcal{N}$.

A further interesting property of (4), (5), (6) is that they are equivalent to

$$\langle 0| \left[Q_\nu, \left[H, Q^\dagger_{\nu'} \right] \right] |0\rangle = E_\nu \delta_{\nu,\nu'} \tag{7}$$

$$\langle 0| \left[Q^\dagger_\nu, \left[H, Q^\dagger_{\nu'} \right] \right] |0\rangle = 0 \tag{8}$$

This form is interesting since these equations have exactly the same structure as any mean field Hartree-Fock-Bogoliubov equations, be it for single Fermions or Bosons or, as here, for Fermion pairs.

For a hamiltonian with two body interactions one verifies easily that (4) contains at most one and two body density matrices. Roughly speaking the two body density matrices can be expressed as quadratic forms of the amplitudes X and Y (for more details see [3–6]).

An important point is to realize that (5) is **not** restricted to the particle-hole (ph) and (hp) subspaces as is of common use in the nuclear literature on the subject [1,10,15]. Here the only restriction in (5) is that it should not contain any diagonal (i.e. Hermitian) components. Therefore in $Q^\dagger_\nu = \sum_{k \neq k'} \chi^\nu_{kk'} a^\dagger_k a_{k'}$ the matrix χ is not Hermitian. The single particle basis in which (4,5,6) shall be solved is obtained from

$$\langle 0| \left[H, Q^\dagger_\nu \right] |0\rangle = \langle 0| \left[H, Q_\nu \right] |0\rangle = 0 \tag{9}$$

One can show that (9) is obtained from the minimization of the SCRPA ground state energy with respect to

$$\epsilon_\mu = \frac{\sum_{\nu,k} \left\{ (E^{N+1}_\nu - E^N_0) |\langle N,0| \varphi^\mu_k a_k |N+1,\nu\rangle|^2 + (E^N_0 - E^{N-1}_\nu) |\langle N,0| \varphi^{\mu *}_k a^\dagger_k |N-1,\nu\rangle|^2 \right\}}{\sum_{\nu,k} \left\{ |\langle N,0| \varphi^\mu_k a_k |N+1,\nu\rangle|^2 + |\langle N,0| \varphi^{\mu *}_k a^\dagger_k |N-1,\nu\rangle|^2 \right\}} \tag{1}$$

$$E_\mu = \frac{\sum_{\nu,k>k'} \left\{ (E^N_\nu - E^N_0) |\langle N,0| X^\mu_{kk'} a^\dagger_k a_{k'} |N,\nu\rangle|^2 - (E^N_\nu - E^N_0) |\langle N,0| Y^\mu_{kk'} a^\dagger_{k'} a_k |N,\nu\rangle|^2 \right\}}{\sum_{\nu,k>k'} \left\{ |\langle N,0| X^\mu_{kk'} a^\dagger_k a_{k'} |N,\nu\rangle|^2 - |\langle N,0| Y^\mu_{kk'} a^\dagger_{k'} a_k |N,\nu\rangle|^2 \right\}} \tag{3}$$

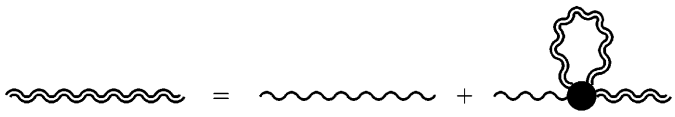

Fig. 1. Schematic graphical representation of the mean field equation for quantum fluctuations. The dot stands for the first order Born contribution to the mean field potential. A more elaborate graphical representation can be found in ref [5]

the basis [3,4,6] but one also directly realizes that (9) is consistent with the equations of motion (7,8), since it is well known [3,14] that they follow from the definition of the RPA groundstate as the vacuum of the excitation operator (5). i.e.

$$Q_\nu|0\rangle = 0. \tag{10}$$

Equation (10) demonstrates explicitly that the corresponding groundstate $|0\rangle$ will be a functional of the amplitudes X, Y. Actually (10) can be viewed as an eigenstate equation of the nonhermitian operator Q_ν with eigenvalue zero.

Expression (5) can be inverted as long as the amplitudes X, Y are normalized in the standard way

$$\sum_{k>k'} \left(X^\nu_{kk'} X^{\nu'*}_{kk'} - Y^\nu_{kk'} Y^{\nu'*}_{kk'} \right) = \delta_{\nu\nu'} \tag{11}$$

and one obtains

$$a^\dagger_k a_{k'} = \sum_\nu \left(X^\nu_{kk'} Q^\dagger_\nu + Y^\nu_{kk'} Q_\nu \right) k > k'. \tag{12}$$

Together with its hermitian conjugate and (10) one then can evaluate two body densities of the form $\langle 0|a^\dagger_{k_1} a_{k_2} a^\dagger_{k_{2'}} a_{k_{1'}}|0\rangle$ appearing in (6) in terms of X, Y and the single particle density matrix $\rho_{kk'} = \langle 0|a^\dagger_{k'} a_k|0\rangle$. In cases where one can explictely construct the groundstate from (10) also $\rho_{kk'}$ is known as a functional of X, Y. However, as stated already, the groundstate is generally not known and an independent scheme of how to express $\rho_{kk'}$ in terms of X, Y must be developed. This point has been a matter of debate in the past [15] and shall again be one of the main subjects here. It should be noted that, depending on the problem at hand, it can also happen that certain elements of the two body density matrix can not be explicitely expressed in terms of the X, Y amplitudes. In the Lipkin model studied below one particular matrix element of the two body density which belongs to this category will be exposed. We will, however, demonstrate that once a method to calculate the single particle density matrix is available, a reliable way to evaluate the missing two body matrix elements can be found. As mentioned above, in the Lipkin model the RPA groundstate can be constructed explicitly, allowing a comparison of the approximations against the fully consistent treatment of the SCRPA equations.

It is also possible to provide a more physical interpretation of (6). The matrix B contains the pair potential of the two fermion pairs whereas the matrix A contains the normal selfconsistent potential for fermion pairs. Qualitatively we can represent the selfconsistent equations (6) as in Fig. 1 [2] where the wiggly line stands for quantum fluctuations. Such a selfconsistent mean field potential for density fluctuations as shown in Fig. 1 seems quite natural, since the groundstate of an interacting Fermi system can be considered as a gas of quantal fluctuations. The presence of fluctuations also has a feedback on the single particle motion, an issue which we mainly want to consider in this paper. For example, to couple back consistently the single particle density matrix $\rho_{kk'} = \langle 0| a^\dagger_k a_{k'} |0\rangle$ to the amplitudes X and Y in order to close the system of equations, has been a matter of debate in the past [16]. As we mentioned already in the Lipkin model the RPA ground state can be constructed explicitly and then the approximations can be checked against the fully consistent treatment in this case.

3 Coupling the single particle Green's function to the Self Consistent RPA

The eigenvalue problem (4) has as usual a corresponding Green's Function (GF) formulation. For the following it is useful to also briefly outline this approach which, of course, is completely equivalent to the eigenvalue problem (4). The derivation with the GF scheme has been presented in detail before [5], but in order to make this article more selfcontained we will repeat here the main steps.

Let us therefore define the two time chronological Green's function at zero temperature which describe density fluctuations

$$G^{t-t'}_{k_1 k_2 k'_1 k'_2} = -i \langle 0| T \left(a^\dagger_{k_2} a_{k_1} \right)_t \left(a^\dagger_{k'_1} a_{k'_2} \right)_{t'} |0\rangle \tag{13}$$

where T is the chronological operator and

$$O_t = e^{iHt} O e^{-iHt} \tag{14}$$

with H the full Hamiltonian operator. In principle in (13) one should take only the fluctuating operator $a^\dagger a - \langle 0|a^\dagger a|0\rangle$ but since in the equations of motion (4,5) any c-number drops out we will stay with the definition given in (13).

The two-body GF in (13) depends only on one time difference exactly as in the one particle case. One can then establish a formally exact Dyson equation for it. Like in the single particle case the mass operator splits into an instantaneous part and a frequency dependent part. The first one contains the meanfield description of the quantal fluctuations and that is all we want to treat here. In the approximation of the instantaneous effective Hamiltonian the Dyson equation reads

$$\omega G^{SCRPA}_{k_1 k_2 k'_1 k'_2} = \mathcal{N}_{k_1 k_2 k'_1 k'_2} + \sum_{p_1 p_2 k_1 k_2 p_1 p_2} \mathcal{H}^{(0)} \, G^{SCRPA}_{p_1 p_2 k'_1 k'_2} \tag{15}$$

with

$$\mathcal{N}_{k_1 k_2 k'_1 k'_2} = \langle 0| \left[a^\dagger_{k_2} a_{k_1}, a^\dagger_{k'_1} a_{k'_2} \right] |0\rangle \tag{16}$$

and

$$\mathcal{H}^{(0)}_{k_1k_2k_1'k_2'} = \sum_{p_1p_2} \langle 0| \left[a^\dagger_{k_2}a_{k_1},\left[H,a^\dagger_{p_1}a_{p_2}\right]\right]|0\rangle \ \mathcal{N}^{-1}_{p_1p_2k_1'k_2'} \tag{17}$$

One easily recognizes from (15-17) the equivalence with (4) which explains the use of the superscript $SCRPA$. Since the (15), (16), (17) have been derived at length in several preceding articles [3,5] we will not represent them here in any detail.

For the coupling with the single particle Green's function it is useful to define a SCRPA T-matrix from (15) in the following way

$$G^{SCRPA}_{k_1k_2k_1'k_2'} = G^0_{k_1k_2k_1'k_2'} + G^0_{k_1k_2p_1p_2}T^{SCRPA}_{p_1p_2p_2'p_2'} \ G^0_{p_1'p_2'k_1'k_2'} \tag{18}$$

with

$$G^0_{k_1k_2k_1'k_2'} = \frac{n_{k_2}-n_{k_1}}{\omega-\varepsilon_1+\varepsilon_2}\delta_{k_1k_1'}\delta_{k_2k_2'} \tag{19}$$

where $n_k = \left\langle 0|a^\dagger_k a_k|0\right\rangle$ and $\varepsilon_k = \frac{k^2}{2m} + \sum_{k'} \overline{v}_{kk'kk'} \ n_{k'}$ are the occupation numbers and generalized single particle energies which we assumed without loss of generality to be diagonal and $\overline{v}_{k_1k_2k_3k_4}$ is the antisymmetrised matrix element of the two body interaction. With (15-17) the T-matrix in (18) is uniquely defined. Since this is quite standard procedure we do not further elaborate on the form of the T-matrix. A form equivalent to (18) is given by (we use summation convention)

$$G^{SCRPA}_{k_1k_2k_1'k_2'} = G^0_{k_1k_2k_1'k_2'} + G^0_{k_1k_2p_1p_2}K^{SCRPA}_{p_1p_2p_2'p_2'} \ G^{SCRPA}_{p_1'p_2'k_1'k_2'} \tag{20}$$

with

$$K^{SCRPA}_{k_1k_2k_1'k_2'} = \mathcal{H}^{(0)}_{k_1k_2k_1'k_2'} - (\varepsilon_{k_1}-\varepsilon_{k_2})\,\delta_{k_1k_1'}\delta_{k_2k_2'} \tag{21}$$

From (20-21) we also read off the equality

$$\sum_{k_3k_4} K^{SCRPA}_{k_1k_2k_3k_4}G^{SCRPA}_{k_3k_4k_1'k_2'} = \sum_{k_3k_4} T^{SCRPA}_{k_1k_2k_3k_4} \ G^0_{k_3k_4k_1'k_2'} \tag{22}$$

The important point to recognize is that the mass operator of the single particle Dyson equation

$$(\omega-\varepsilon_k) \ G^\omega_{kk'} = \delta_{kk'} + \sum_p \mathcal{M}^\omega_{kp} \ G^\omega_{pk'} \tag{23}$$

has a well known representation in terms of the full two body T-matrix [4]. For better visibility we present the relation graphically in Fig. 2.

At this point it has now become obvious what our interrelation of single particle GF and SCRPA shall be: we have to replace in Fig. 2 the full T-matrix by the approximate $T^{SCRPA}(\omega)$ defined in (18). In addition to this obvious construct there also exists a direct and strong consistency requirement. It stems from the fact that we have now two ways of calculating the correlation energy: the first uses the well known relation between the single particle GF and the ground state energy [5,17,18]

$$E_0 = -\frac{i}{2} \lim_{t'-t\to 0^+} Tr\left(i\frac{\partial}{\partial t}+\varepsilon_k\right) \ G^{t-t'}_{kk} \tag{24}$$

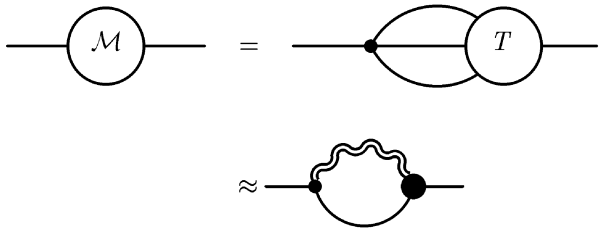

Fig. 2. The mass operator of the single particle Dyson equation represented in terms of the full two body T-matrix

The second expresses the correlation energy density via the two body GF (13):

$$E_{corr} = \frac{i}{4} \lim_{t'-t\to 0^+} Tr\left[\overline{v}_{k_1k_2'k_2k_1'}\left(G^{t-t'}_{k_1k_2k_1'k_2'} - G^{(0)t-t'}_{k_1k_2k_1'k_2'}\right)\right] \tag{25}$$

where again $\overline{v}_{k_1k_2'k_2k_1'}$ is the antisymmetrised two-body matrix element entering in the Hamiltonian H. One can also obtain the correlation energy from (24) via a suitable sustraction.

The requirement is now that both expressions for the correlation energy, that is, the one deduced from (24) and (25), agree. This is equivalent to the Hugenholtz-van Hove theorem which states that the chemical potential μ calculated via the single particle GF must be equal (at equilibrium) to the energy per particle when calculated from (25). It turns out that this only is achieved when expanding the GF in (23) to first order in the mass operator

$$G_k = G^0_k + G^0_k \ \mathcal{M}^\omega_k \ G^0_k \tag{26}$$

with

$$(\omega-\varepsilon_k) \ G^0_k = 1 \tag{27}$$

Of course one can use the iterated solution of the Dyson equation, *i.e.* $G_k = (\omega-\varepsilon_k-\mathcal{M}^\omega_k)^{-1}$ but for consistency then the particle-hole propagators of the SCRPA equation must be redefined accordingly. This has been discussed in [5] and may be elaborated in the future but for the moment we keep with the more restrictive consistency relation (26) together with (15-18).

For space reasons we have been relatively short in this general section. We will, however, work out in some detail the model case of the next section so that the reader, by analogy, shall be able to reconstruct details also in the general case quite easily.

4 Application to the Lipkin Model

The Hamiltonian of the Lipkin [19] model is given by

$$H = \varepsilon J_0 - \frac{V}{2}(J^2_+ + J^2_-) \tag{28}$$

with

$$J_0 = \frac{1}{2}\sum_{m=1}^{\Omega}(c^\dagger_{1m}c_{1m} - c^\dagger_{0m}c_{0m}),$$
$$J_+ = \sum_{m=1}^{\Omega} c^\dagger_{1m}c_{0m}, J_- = \sum_{m=1}^{\Omega} c^\dagger_{0m}c_{1m} \tag{29}$$

The indices 0 and 1 denote the lower and upper levels respectively, separated by an energy ε, and m is the angular momentum projection in each shell with degeneracy Ω.

The commutation relations between these three operators, which are the generators of the SU(2) group, are

$$[J_+, J_-] = 2J_0, [J_0, J_\pm] = \pm J_\pm. \tag{30}$$

In the Lipkin model the number of particles is exactly that needed to completely fill the lower shell, i.e. $N = \Omega$.

4.1 SCRPA equations

The SCRPA solutions are built with the operators (we stay in the normal phase)

$$Q^\dagger = \frac{1}{\sqrt{-2\langle J_0\rangle}}[XJ_+ - YJ_-],$$
$$Q = \frac{1}{\sqrt{-2\langle J_0\rangle}}[XJ_- - YJ_+] \tag{31}$$

acting over a correlated vacuum $|0\rangle = |RPA\rangle$, which is defined by the equation

$$Q|RPA\rangle = 0 \tag{32}$$

to yield the excited state

$$|1\rangle = Q^\dagger|RPA\rangle. \tag{33}$$

The SCRPA equations (4) then take the following form

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = E\begin{pmatrix} X \\ Y \end{pmatrix} \tag{34}$$

with the matrix elements A and B defined by [10,20]

$$A = \left\langle [J_-, [H, J_{+\langle}]]\right\rangle / \langle [J_-, J_+]\rangle$$
$$B = \langle [J_+, [H, J_+]]\rangle / \langle [J_-, J_+]\rangle \tag{35}$$

where we used $\langle\cdots\rangle$ for $\langle RPA|\cdots|RPA\rangle$.

The normalization of the excited state $Q^\dagger|RPA\rangle$ is given by

$$\langle QQ^\dagger\rangle = \langle [Q, Q^\dagger]\rangle = X^2 - Y^2 = 1 \tag{36}$$

With (36) the inversion of (31) yields $J_+ = \sqrt{-2\langle J_0\rangle}\left(XQ^\dagger + YQ\right)$ and the matrix elements of the SCRPA matrices read

$$A_{SCRPA} = \varepsilon + 2VXY$$

$$B_{SCRPA} = 2V\frac{\langle J_0^2\rangle}{\langle J_0\rangle} + V(X^2 + Y^2) \tag{37}$$

From (37) we see that we face exactly the problem discussed in Sect. 3. The single particle occupation $\langle J_0\rangle$ and the square $\left\langle J_0^2\right\rangle$ can not directly be expressed in terms of X and Y. Of course as is well known in the present simple model it is possible to calculate the RPA groundstate via (32) explicitly [19,20] :

$$|RPA\rangle = \sum_{l=0}^{\Omega/2}\frac{(\Omega - 2l)!}{(\Omega/2 - l)!l!}\left(\frac{Y}{X}\right)^2 J_+^{2l}|HF\rangle \tag{38}$$

and therefore also $\langle J_0\rangle$ and $\left\langle J_0^2\right\rangle$ can explicitly be calculated [3]. However, this is not the usual situation and in general it will be very difficult if not impossible to solve the vacuum condition (32). We have therefore to develop other methods to get access to these quantities independently. As already mentioned this is the main objective of the present paper. The fact that (38) exists in this model makes the comparison with a full SCRPA based on a RPA wave function particularly instructive. As a word of caution we should mention again (see Sect. 2) that it is not possible to include J_0 as a further component into the definition of the RPA excitation operator $Q^\dagger$ (31) since J_0 is hermitian and it is then impossible to define the norm of the RPA excited state.

In the next section we will therefore elaborate on the evaluation of $\langle J_0\rangle$ via the single particle GF the way we have outlined it in the general section 3.

For later use we also introduce here the matrix elements renormalized of the RPA (RRPA) [8]

$$A_{RRPA} = \varepsilon, B_{RRPA} = 2V\langle J_0\rangle. \tag{39}$$

They will be used below when we will compare the results of the SCRPA not only to the exact solution but also to RRPA.

4.2 SCRPA and the single particle Green's function

As outlined above we have to construct a mass operator for the s. p. GF such that it yields exactly the same groundstate energy via (24) as when calculated directly from the two body GF (25). In order to explain the principle we first want to exemplify the procedure with standard RPA. In this case we have to put in (37) $X = 1$, $Y = 0$ and $\langle J_0\rangle = -\frac{\Omega}{2}$, $\left\langle J_0^2\right\rangle = \frac{\Omega^2}{4}$. Let us for example consider the interaction energy to RPA order

$$E_{pot} = -\frac{V}{2}\left(\left\langle J_+^2\right\rangle + \left\langle J_-^2\right\rangle\right) \Rightarrow E_{pot}^{RPA} = -V\ \Omega\ X\ Y \tag{40}$$

Using one of the RPA equations (dropping $1/\Omega$ corrections):

$$V\ \Omega\ X = (E + \varepsilon)\ Y \tag{41}$$

and multiplying this equation with X we obtain for E_{pot}:

$$E_{pot}^{RPA} = -V\ \Omega\ \frac{X^2}{E + \varepsilon}\ V\ \Omega \tag{42}$$

Expression (42) can be identified with the evaluation of the Feynman graph shown in Fig. 3 where the wiggly line represents the RPA phonon with energy E. The particle-hole bubble has energy $\varepsilon_{ph} = \varepsilon$ and together with

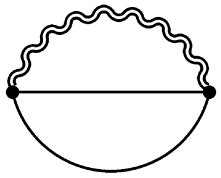

Fig. 3. Feynman graph representing E_{pot}^{RPA}

Fig. 4. Groundstate graph for the mass operator G_{1m}^{ω}

the phonon the vertical cut has energy $E+\varepsilon$ what corresponds to the energy denominator in (42). The amplitude of the phonon is X^2 and the two dots of the graph represents the interaction squared. As usual we can obtain the mass operator from the groundstate graph in cutting open the hole line. Therefore we obtain e. g. for the GF of the upper level ($G_{1m}^{t-t'} = -i\left\langle T\left(a_{1m}(t)\, a_{1m}^{\dagger}(t')\right)\right\rangle$) in the approximation of (26)

$$G_{1m}^{\omega} = \frac{1}{\omega - \frac{\varepsilon}{2}} + \frac{1}{\omega - \frac{\varepsilon}{2}}\, V\, \frac{\Omega^2 X^2}{\omega + E + \frac{\varepsilon}{2}}\, V\, \frac{1}{\omega - \frac{\varepsilon}{2}} \tag{43}$$

where the mass operator has the obvious graphical representation of Fig. 4

Using the (exact) relation (what is just a variant of (24)):

$$\frac{i}{2} \lim_{t'-t\to 0^+} \left(i\frac{\partial}{\partial t} - \frac{\varepsilon}{2}\right) G_{1m}^{t-t'} = -\frac{V}{2}\left\langle J_+^2\right\rangle \tag{44}$$

and inserting into the *lhs* expression (43) we obtain

$$-i \lim_{t'-t\to 0^+} \left(i\frac{\partial}{\partial t} - \frac{\varepsilon}{2}\right) G_{1m}^{t-t'} = -\frac{1}{2}\left(V\Omega\right)^2 \frac{X^2}{E+\varepsilon} \tag{45}$$

This is just half the potential energy (42) in the standard RPA approach. Proceeding analogously with G_{0m} and adding to (45) the corresponding expression yields the missing factor 2. This demonstrates that our construction of the mass operator in (43) is consistent with the RPA groundstate energy.

Since we now have the s. p. GF at hand it is straightforward to calculate the occupation numbers via

$$\left\langle a_{1m}^{\dagger} a_{1m}\right\rangle = -i \lim_{t'-t\to 0^+} G_{1m}^{t-t'} \tag{46}$$

Inserting into (46) the *rhs* of (43) yields

$$\sum_m \left\langle a_{1m}^{\dagger} a_{1m}\right\rangle = \left(V\Omega\right)^2 \frac{X^2}{\left(\varepsilon+E\right)^2} = Y^2 \tag{47}$$

where in the last equality we again made use of the RPA equations. It is easy to restore the value for $\langle J_0\rangle$ since $\sum_m \left\langle a_{0m}^{\dagger} a_{0m}\right\rangle = \Omega - \sum_m \left\langle a_{1m}^{\dagger} a_{1m}\right\rangle$ and therefore

$$\langle J_0\rangle = -\frac{\Omega}{2} + Y^2 \tag{48}$$

It is interesting to realize that (48) corresponds to the Holstein Primakoff boson expansion of $\langle J_0\rangle$ [15], a result which of course is consistent with RPA theory.

Let us now repeat the same procedure but with SCRPA. Using the SCRPA equations, in analogy to the steps above, we can write for E_{pot} :

$$E_{pot}^{SCRPA} = -2\,\langle J_0\rangle\, V \frac{\widetilde{A}\, XY + B\, X^2}{E+\varepsilon} \tag{49}$$

where $\widetilde{A} = A - \varepsilon$ and A, B are determined in (37). Again in cutting open the hole line we now find in analogy with (43) for the mass operator according to (26)

$$G_{1m}^{\omega} = \frac{1}{\omega - \frac{\varepsilon}{2}} - \frac{1}{\omega - \frac{\varepsilon}{2}}\, V \frac{\langle 0|\, J_-\, |1\rangle}{\omega + E + \frac{\varepsilon}{2}} \times \left[\langle 0|\, J_-\, |1\rangle\, \widetilde{A} + \langle 1|\, J_+\, |0\rangle\, B\right]\, \frac{1}{\omega - \frac{\varepsilon}{2}} \tag{50}$$

where $|1\rangle$ again is the excited state $Q^{\dagger}|0\rangle$. In the RPA limit we obtain (43). We immediately check that indeed we get back from G_{1m} (and G_{0m}) the correct expression (49) for E_{pot}^{SCRPA} inserting (50) into the *lhs* of (44) (and similar for G_{0m}).

Since we now have a consistent SCRPA expression for the single particle GF at hand we proceed, as this was our goal, to the calculation of $\langle J_0\rangle$. Inserting (50) into the *rhs* of (46) one directly obtains

$$\langle J_0\rangle = -\frac{\frac{\Omega}{2}}{1 - 2\left[\widetilde{A}\, XY + B\, X^2\right]\frac{V}{(\varepsilon+E)^2}} \tag{51}$$

$$= -\frac{\frac{\Omega}{2}}{1 + 2XY\,\frac{V}{(\varepsilon+E)}}$$

This is still an implicit equation for $\langle J_0\rangle$, since the SCRPA eigenvalue E depends on it. Before proceeding it is interesting to study several limits of (51). As expected for the interaction going to zero we recover the free gas limit $\langle J_0\rangle = -\frac{\Omega}{2}$. We already checked that (50) goes over into the RPA limit (43) when $\widetilde{A}$, B and the transition amplitudes are replaced by their RPA expressions. Therefore we also recover the boson expansion result.

One should note that in order to obtain the correct RPA, *i.e.* boson result one must not make the mistake to go over to the RPA limit, i. e. $X=1$, $Y=0$, $\left\langle J_0^2\right\rangle = \langle J_0\rangle^2 = \frac{\Omega^2}{4}$ only in (51) because to get (51) already the assumption has been used that $\langle J_0\rangle \neq -\frac{\Omega}{2}$ on the *rhs* of (50) what would not be consistent with the RPA groundstate energy then. Now if we nevertheless take the RPA limit, using directly (51), one obtains

$$\langle J_0\rangle = -\frac{\frac{\Omega}{2}}{1 + \frac{2}{\Omega}Y^2}. \tag{52}$$

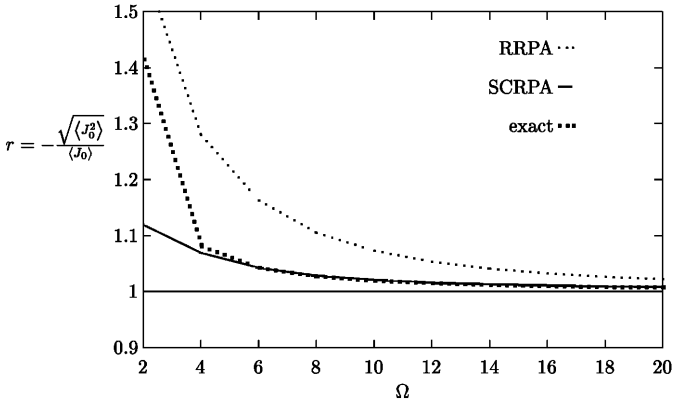

Fig. 5. The ratio $r = -\sqrt{\langle J_0^2 \rangle} / \langle J_0 \rangle$ for the fixed interaction strength $\chi = V(\Omega - 1)/\varepsilon = 1$ as a function of Ω. The exact results are represented by full squares, those obtained using the RPA vacuum (38) by a full line (SCRPA) and a dotted line (RRPA)

This result is interesting because it is precisely the lowest order result which one obtains with the number operator method [16,21]. In the light of our theory this formula (52) seems to be inconsistent because if on the rhs of (50) one keeps $\langle J_0 \rangle \neq -\frac{\Omega}{2}$, there is no reason to drop all the other terms going beyond standard RPA. So in this light the pure lowest order boson result (48) seems to be more consistent than the partially resummed series (52). We will see later that this is indeed confirmed by numerical results.

4.3 Determination of $\langle J_0^2 \rangle$

In principle we are still short of the expectation value of the square of the occupation number. Eventually we could try to establish an analogous expression to what has been found for $\langle J_0 \rangle$ (51). However, at least in the present model the factorization relation

$$\langle J_0^2 \rangle \cong \langle J_0 \rangle^2 \tag{53}$$

seems to be extremely well fulfilled for the whole range of the interaction strength considered (see next section). Of course this may be a particularity of the model but we suppose that, as long as the operator J_0 or analogous operators in other problems are sufficiently collective, equation (53) should work quite reasonably. In order to check this we present the ratio $r = -\sqrt{\langle J_0^2 \rangle} / \langle J_0 \rangle$ for the fixed interaction strength $\chi = V(\Omega - 1)/\varepsilon = 1$. (i. e. at the mean-field transition point where fluctuations are expected to be maximal) as a function of Ω in Fig. 5. The exact results are represented by full squares, those obtained using the RPA vacuum (38) by a full line (SCRPA) and a dotted line (RRPA).

Only for Ω values lower than 4 one can see a significant deviation from unity. So definitely s-wave shells are difficult candidates. On the other hand should there be no degeneracy at all like in a rotating nucleus or in an electron system in a magnetic field there is no need to know the occupation number square since we have anyway

$$\left\langle a_k^\dagger a_k a_k^\dagger a_k \right\rangle = \left\langle a_k^\dagger a_k \right\rangle \tag{54}$$

So unless there is appearance of two fold degenerate levels in a problem one is probably well off with the factorization (53). In the former case a perturbative expansion of square operators in terms of linear operators as proposed in [3] using RPA excited states as intermediate states should adequately improve on (53) which represents the zero order approximation. This approximation is based on expanding the expectation value of any two body operator by inserting a complete set of RPA states. Specifically for the Lipkin model we have [3]

$$\langle J_0^2 \rangle = \sum_l \frac{\left| \langle J_0 Q^{\dagger 2l} \rangle \right|}{\langle Q^{2l} Q^{\dagger 2l} \rangle} \tag{55}$$

Truncating to first order and evaluating the expectation values using the vacuum condition we finally arrive to

$$\langle J_0^2 \rangle = \langle J_0 \rangle^2 + \frac{4XY \langle J_0 \rangle^2}{2 \langle J_0^2 \rangle + (X^2 + Y^2) \langle J_0 \rangle} \tag{56}$$

a relation which expresses $\langle J_0^2 \rangle$ in terms of $\langle J_0 \rangle$.

Let us next study the numerical results as they follow from our SCRPA theory described above.

5 Numerical results

In this section we mostly will present results for $\Omega = 14$. We will begin in first place to investigate the quality of the results for the correlation part of the groundstate energy, i. e. the correlation energy

$$E_{corr} = \langle H \rangle - \varepsilon \frac{N}{2} \tag{57}$$

with

$$\langle H \rangle = \langle J_0 \rangle [\varepsilon - V \; X \; Y] \tag{58}$$

We show E_{corr} as a function of $\chi = V(\Omega - 1)/\varepsilon$ in Fig. 6 for the RPA (dashed line), RRPA (small dots), SCRPA (full line) and the exact solution (full squares). In the first three cases the RPA vacuum (38) was used. For this reason this results represent the best possible correlation energies which can be obtained using each RPA formalism. It must be noticed that in the standard RPA calculations the RPA vacuum is replaced by the HF ground state [15]. Under this approximation one obtains $E_{corr} = 0$ for any value of the residual interaction. What we call the RPA and RRPA correlation energies in Fig. 6 are calculated introducing in (58) the X, Y amplitudes obtained using (39), both explicitly and in the evaluation of $\langle J_0 \rangle$ using the RPA vacuum. As it was mentioned many times, in most cases only approximate expressions for $\langle J_0 \rangle$, as those presented in (51) and (52), are available. Correlation energies calculated in this way are compared with the others in Table 1. It is a very well known fact that RPA due to the

Table 1. Correlation energy E_{corr}, (57), as a function of the interaction strength χ, listed in the first column. The energies listed in the second, third and fourth columns were evaluated using (38) for the RPA vacuum, and the X, Y obtained solving the RPA, RRPA and SCRPA equations, respectively. In the fifth and sixth columns the correlation energies were calculated using the approximations (51) and (52) for $\langle J_0 \rangle$ respectively. Exact results are shown in the last column

		RPA vacuum				
χ	RPA	RRPA	SCRPA	GF	(52)	exact
0.00	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.05	-0.00072	-0.00067	-0.00067	-0.00067	-0.00072	-0.00067
0.10	-0.00289	-0.00270	-0.00270	-0.00270	-0.00289	-0.00270
0.15	-0.00653	-0.00608	-0.00608	-0.00607	-0.00652	-0.00608
0.20	-0.01167	-0.01083	-0.01083	-0.01082	-0.01165	-0.01084
0.25	-0.01836	-0.01698	-0.01698	-0.01694	-0.01829	-0.01700
0.30	-0.02666	-0.02455	-0.02456	-0.02446	-0.02651	-0.02458
0.35	-0.03665	-0.03358	-0.03359	-0.03338	-0.03637	-0.03364
0.40	-0.04846	-0.04409	-0.04411	-0.04375	-0.04793	-0.04420
0.45	-0.06221	-0.05612	-0.05618	-0.05555	-0.06131	-0.05634
0.50	-0.07809	-0.06972	-0.06985	-0.06882	-0.07659	-0.07011
0.55	-0.09635	-0.08490	-0.08517	-0.08356	-0.09392	-0.08560
0.60	-0.11731	-0.10166	-0.10220	-0.09977	-0.11345	-0.10288
0.65	-0.14142	-0.11996	-0.12100	-0.11741	-0.13534	-0.12206
0.70	-0.16932	-0.13963	-0.14164	-0.13645	-0.15980	-0.14325
0.75	-0.20199	-0.16029	-0.16417	-0.15682	-0.18702	-0.16660
0.80	-0.24103	-0.18117	-0.18862	-0.17840	-0.21722	-0.19224
0.85	-0.28936	-0.20064	-0.21502	-0.20107	-0.25060	-0.22035
0.90	-0.35353	-0.21552	-0.24337	-0.22464	-0.28732	-0.25111
0.95	-0.45504	-0.21994	-0.27365	-0.24892	-0.32753	-0.28474
1.00		-0.20449	-0.30582	-0.27372	-0.37127	-0.32145
1.05		-0.15752	-0.33981	-0.29884	-0.41853	-0.36151
1.10		-0.07081	-0.37559	-0.32413	-0.46924	-0.40517
1.15		0.05370	-0.41308	-0.34944	-0.52326	-0.45271
1.20		0.20349	-0.45226	-0.37468	-0.58039	-0.50440
1.25		0.36207	-0.49306	-0.39978	-0.64044	-0.56051
1.30		0.51542	-0.53546	-0.42471	-0.70318	-0.62129

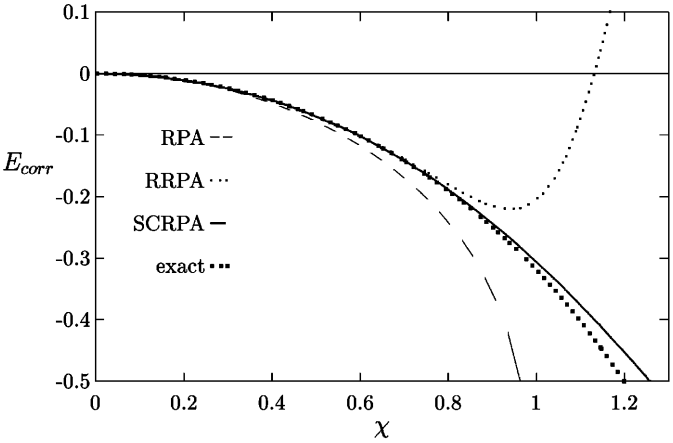

Fig. 6. Correlation energy E_{corr} vs. the interaction strength χ, using the exact solutions (full squares), the RPA (dashed line), the RRPA (small dots) and the SCRPA (full line). The last three were obtained using (38) for the RPA vacuum

quasiboson approximation, i. e. the violation of the Pauli principle, overestimates in general quite strongly the correlations and in fact overbinds in the groundstate energy. This the more, the closer one comes to the phase transition point where RPA collapses. This strong overbinding of the RPA was for example also found in a recent calculation [22] of the electronic binding energy of a metallic cluster. When compared with the exact results SCRPA performs extremely well for E_{corr} up to and even beyond the mean field phase transition point $\chi = 1$ whereas RRPA starts to deviate strongly from the exact result at $\chi \cong 1$.

Since it is not possible to distinguish in Fig. 6 that the SCRPA values of E_{corr} stays consistently above the exact ones, we also present the results in Table 1. In this Table we also include the results of the SCRPA but with $\langle J_0 \rangle$ calculated using the Green's function formalism, (51), labeled 'GF', and the number operator method, labeled '(52)'. As mentioned above, the SCRPA performs very well, better than the RRPA, when the RPA vacuum (38) is used. More important is the fact that correlation energies calculated through the Green's function formalism, (51), remain close to the exact energy, although not as close as the SCRPA, and are always larger than the exact energy, as expected from a variational result. At variance, correlation energies evaluted using (52) overbind the system far before the phase transition.

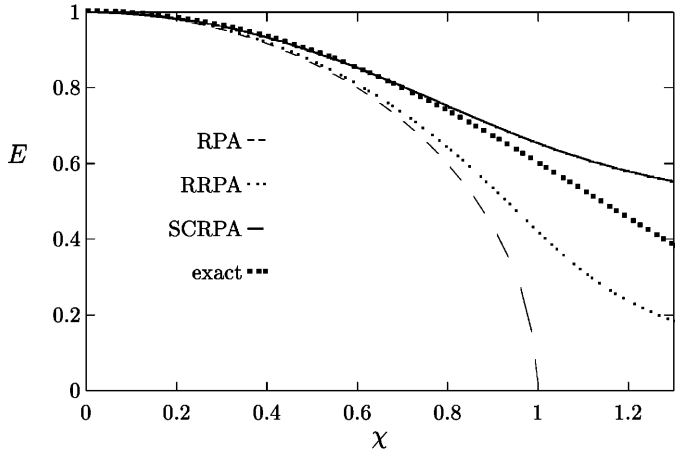

Fig. 7. Excitation energy E vs. the interaction strength χ, with the same convention of Fig. 6

Another interesting quantity is the excitation energy. We show E as a function of χ in Fig. 7. A similar scenario as in the previous figure prevails: SCRPA yields by far the best agreement with the exact results though the differences for $\chi \gtrsim 1$ are now more pronounced. It is also true here that the SCRPA excitation energy stays consistently above the exact results as can be seen from Table 2.

One could conclude from that that the SCRPA also leads to an upper bound for the excitation energy. This conjecture may be backed from the fact that we actually derived in Sect. 2 the SCRPA equations from a minimization within respect an average excitation energy. However, before drawing any definite conclusion in this respect, a more general model with more levels must be studied.

Let us now come to the investigation of the quality of the different expressions for $\langle J_0 \rangle$. There are essentially three: the one which we prefer on theoretical grounds is the one from the Green's function approach (51), since it is the only one which fulfills a strong consistency relation with SCRPA equations (i. e. the Hugenhotlz-van Hove theorem). The second is the quasiboson approximation (48) which represents the lowest order correction in $1/\Omega$ to the free gas results. The third comes from the so-called number operator expression (52) which has recently become very popular in the nuclear physics literature [16, 21, 23]. We have shown that it is as well obtainable from the GF approach in operating additional approximations to (51), and that those approximations are not consistent among them.

In Fig. 8 we show the quantity $\Omega/2 + \langle J_0 \rangle$ as a function of χ for the three approximations to $\langle J_0 \rangle$ when used in the SCRPA equations (of course only the one corresponding to GF method corresponds to our definition proper of SCRPA). In addition we show in Fig. 8 also the exact result (full squares). The solution of the GF method (and therefore the SCRPA proper) is shown by the full line. The quasiboson approximation is shown by the broken line and the number operator method by the dotted line. Not unexpectedly the GF results are closest to the exact ones. Somewhat a surprise is that the number operator method works no better than the quasiboson approximation. However in the light of our discussion in Sect. 4 where we argue that one passes from the GF expression (51) in an essentially uncontrolled way to the number operator expression (52) this outcome may seem less astonishing.

Table 2. Excitation energy E as a function of the interaction strength χ. The energies listed in the second, third and fourth columns were obtained solving the RPA, RRPA and SCRPA equations, respectively. Exact results are shown in the last column

χ	RPA	RRPA	SCRPA	exact
0.00	1.00000	1.00000	1.00000	1.00000
0.05	0.99875	0.99875	0.99894	0.99894
0.10	0.99499	0.99499	0.99577	0.99577
0.15	0.98869	0.98870	0.99048	0.99048
0.20	0.97980	0.97986	0.98308	0.98308
0.25	0.96825	0.96840	0.97359	0.97356
0.30	0.95394	0.95426	0.96202	0.96194
0.35	0.93675	0.93737	0.94840	0.94821
0.40	0.91652	0.91762	0.93290	0.93240
0.45	0.89303	0.89491	0.91539	0.91450
0.50	0.86603	0.86908	0.89605	0.89455
0.55	0.83516	0.83998	0.87500	0.87258
0.60	0.80000	0.80744	0.85242	0.84862
0.65	0.75993	0.77126	0.82852	0.82275
0.70	0.71414	0.73126	0.80358	0.79503
0.75	0.66144	0.68728	0.77795	0.76555
0.80	0.60000	0.63925	0.75200	0.73444
0.85	0.52678	0.58729	0.72616	0.70184
0.90	0.43589	0.53194	0.70088	0.66793
0.95	0.31225	0.47437	0.67658	0.63290
1.00		0.41663	0.65362	0.59701
1.05		0.36150	0.63226	0.56050
1.10		0.31175	0.61269	0.52369
1.15		0.26907	0.59499	0.48690
1.20		0.23372	0.57914	0.45046
1.25		0.20494	0.56507	0.41472
1.30		0.18157	0.55267	0.38001

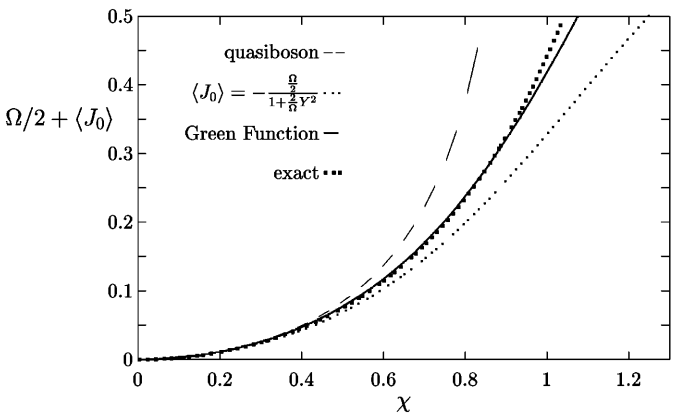

Fig. 8. Occupation numbers $\Omega/2 + \langle J_0 \rangle$ as a function of χ. The exact results are shown by full squares, the solution of the GF method by the full line, the quasiboson approximation by the broken line and the number operator method by the dotted line

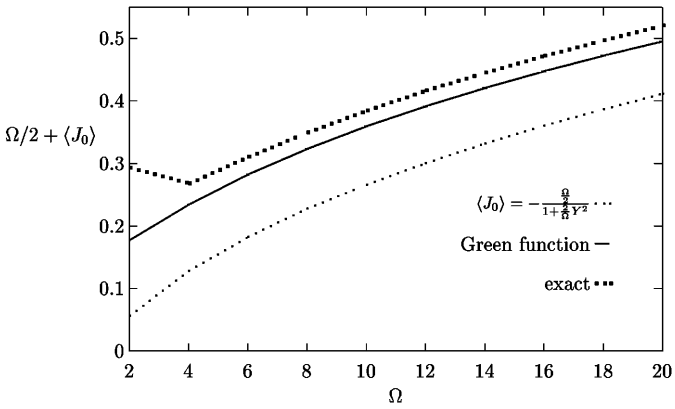

Fig. 9. Occupation numbers $\Omega/2 + \langle J_0 \rangle$ as a function of Ω for fixed $\chi = 1$, with the same convention of Fig. 8

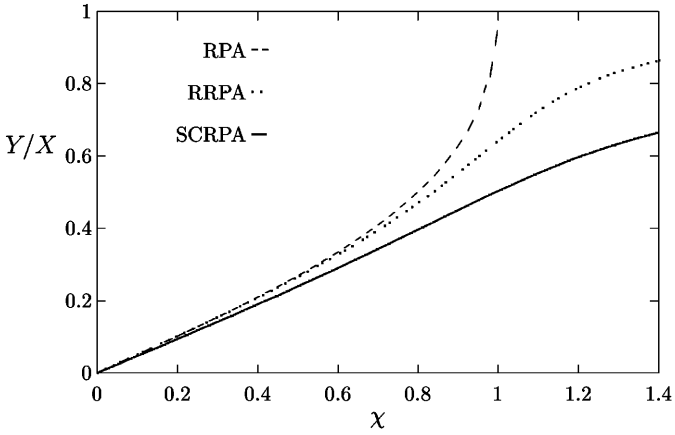

Fig. 10. RPA components of the wave function Y/X as function of the interaction strength. The lines follow the same convention as in Fig. 6

We should also say that the injection of $\langle J_0 \rangle$ and $\langle J_0^2 \rangle$ as expressed with the RPA groundstate wavefunction (38) into the SCRPA equation still improves the results in Fig. 8 with respect to GF. However, we do not show this result in order not to overload the figure and because it corresponds to a situation which in general is not realizable.

In Fig. 9 $\Omega/2 + \langle J_0 \rangle$ is shown not as a function of χ for fixed Ω but for fixed $\chi = 1$. as a function of Ω.

Again we see that $\Omega = 2$ appears as the worst case. It is, however, interesting to see that for this case the differences between the various approximations are also largely enhanced without, however, inverting their respective order.

One last interesting quantity is the ratio Y/X as a function of χ, shown in Fig. 10. It is well known that this ratio goes to 1 when approaching the phase transition point in RPA (as seen in th broken line) while the value of X and Y tend to ∞ individually. This then makes any RPA result close to a phase transition meaningless. On the other hand in SCRPA this ratio still stays of the order $1/2$ around the transition point and also X and Y remain within very reasonable limits ($X = 1.156, Y = 0.580$ at $\chi = 1$.)

A word of caution is worth here. While the energetics and the occupation numbers obtained with the SCRPA are very close to the exact ones, the wave functions around and beyond $\chi = 1$ (the value at which standard RPA collapses), being far better than those obtained with RPA or RRPA, can nontheless have an overlap with the exact wave function of less than 50% [24]. In this case the SCRPA must be extended to the deformed basis [3].

6 Conclusions

In this work we addressed the question of how to close the SCRPA equations in a consistent way and, in particular, of how to calculate single particle quantities such as occupation numbers in this formalism. We showed in detail how to couple back SCRPA into the single particle propagator consistently. The consistency criterion was based on the fulfillment of the Hugenholtz-van Hove theorem which states that the chemical potential obtained from the single particle propagator must be equal (at equilibrium) to the energy per particle when directly calculated via the correlation function. For some problems (for instance in such schematic models as considered here) there may also be correlation functions which involve the expectation value of the square of the occupation number operator, which fall out of the SCRPA space. We, however, showed that in general it seems to be an excellent approximation to replace the expectation values of these operators squared by the product of expectation values of the individual operators. Only for the very special case of $\Omega = 2$ we found that some caution has to prevail, though a perturbative expansion has been already proposed (55) to improve this approximation when needed.

Concerning the numerical results we found that SCRPA yields for this model case excellent results (besides $\Omega = 2$, see above). For instance we found that groundstate as well as excited energies are always close but consistently above the exact values. We also calculated the occupation numbers from the proposed form of the single particle propagator and found that they are closest to the exact values in comparison with other proposed approximate forms for the occupation numbers. Somewhat as a surprise comes the fact that the so called number operator method yields results not better than the quasiboson approximation. We give reasons which may back that this is in fact a generic feature. One should say, however, that the numerical differences for the occupation numbers using the different methods are, at least for the model considered, not very pronounced.

We also should mention that it is not very difficult to obtain good results for the Lipkin model in incorporating groundstate correlations in one way or the other. However, at comparable numerical complexity, the SCRPA equations do at least equally well, if not better, than any other theory on the market. In this respect we refer the reader to our earlier study of ref. [3]. A more severe test would be

to apply the present SCRPA scheme to other more realistic models like for example the multilevel pairing model for which, in the superfluid phase, the number operator approximation is not anymore valid. Such studies shall be presented in future work.

This work was supported in part by Conacyt (México) and by the DIGICYT (Spain) under contract No PB95/0123. J.G.H. thanks the warm hospitality received during his visit at the IEM, CSIC, Madrid, where part of this work was done.

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