Coupled Self-Consistent RPA Equations for Even and Odd Particle Numbers.
Tests with Solvable Models.

M. Jemaï
Laboratoire des matériaux avancés et phénomènes quantiques, FST,
Université Tunis El-Manar 2092 El-Manar, Tunis, Tunisia. and
ISSATM, Université de Chartagne, Avenue de la République P.O. Box 77 - 1054 Amilcar, Tunis, Tunisia

P. Schuck
Institut de Physique Nucléaire d’Orsay, Université Paris-Sud, CNRS-IN2P3
15, Rue Georges Clemenceau, 91406 Orsay Cedex, France. and
Univ. Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

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Coupled equations for even and odd particle number correlation functions are set up via the
equation of motion method. For the even particle number case this leads to self-consistent RPA
(SCRPA) equations already known from the literature. From the equations of the odd particle
number case the single particle occupation probabilities are obtained in a self-consistent way. This
is the essential new procedure of this work. Both, even and odd particle number cases are based
on the same correlated vacuum and, thus, are coupled equations. Applications to the Lipkin model
and the 1D Hubbard model give very good results.

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I. INTRODUCTION

Developments of Many-Body approaches for strongly correlated systems is an active field of research. In the
past we developed an RPA theory which goes beyond the standard one and which is based on a correlated ground
state. To lowest order this leads to RPA equations where the single particle (s.p.) occupation numbers are not
the uncorrelated (Hartree-Fock (HF)) ones but correlated ones which are obtained in a self-consistent way from
the RPA solution. It is known as ‘re-normalized’ RPA (r-RPA) \[1, 2\]. However, in general the RPA equations contain additionally vertex (e.g., screening) corrections which also can be obtained self-consistently from the RPA solution. The whole procedure has been dubbed Self-Consistent RPA (SCRPA) \[3\] and references in there. SCRPA can also be seen as a sub-product of an even more
general approach which is the Time-Dependent Density Matrix (TDDM) theory based on a decoupling of the
BBGKY hierarchy of one, two, etc. correlation functions \[4, 5\]. In the past, there was always a certain
debate how to include the single particle (s.p.) occupations into the SCRPA scheme. Since the latter are
s.p. quantities and the RPA gives rise to two body correlations, it was not completely evident in which way to
close the system of equations. However, already Rowe promoted the so-called particle number operator method
to obtain self-consistent s.p. occupations \[6\]. Later this was further elaborated by F. Catara \[7\] and it has become known as the ‘Catara method’ since then. This
method mostly works quite well \[8\] but also fails more or less in particular cases \[9\]. It is for this reason that
in this work we elaborate a different scheme which seems to be more natural since it is also based on the equation
of motion (eom) method and employs the so-called odd particle number RPA (o-RPA) recently proposed by
one of the authors plus collaborators \[10\]. The latter can also be reformulated as a Dyson equation for the s.p.
Green’s function (GF) with a self-energy obtained from the con for the 2particle-1hole (2p-1h) and 2h-1p GF.
Since both, the SCRPA and o-RPA will be based on the same correlated vacuum, naturally even and odd particle
number channels become coupled. We may coin this scheme eo-SCRPA. We will apply this approach to two
exactly solvable model cases: the Lipkin model and the 1D Hubbard model. In both cases the results turn out
to be promising.

The paper is organized as follows: in section II we present the general theory. In section III, applications
to the Lipkin and Hubbard models are given. Section IV contains the conclusions and details of our procedures are presented in the Appendices.

II. GENERAL THEORY

As mentioned in the introduction, we will base our approach on the coupling of the even and odd particle number
eom. The latter will be obtained from the following ansatz

\[
q^\dagger_p = \sum_h x^\dagger_h^p a_h + \sum_{p' h'} U^{p h} p^{h'} a_h^p a_{p'}^h, \]

\[
q^\dagger_p = \sum_p x^\dagger_p^p a_p + \sum_{p' h'} U_{p'}^{h'} a_h^p a'_{p'}^h. \tag{1}
\]
where the indices 'p, h' refer to s.p. states 'above' and 'below' the Fermi surface, respectively, and \( a_{\mu}^\dagger, a_{\mu} \) are the fermion creation and annihilation operators. The equation for the s.p. basis in which the equations will be worked out will be given below. Our 'quasi-particle' operator in [10] has the good quality that its destructor exactly kills the so-called Coupled-Cluster-Doubles (CCD) wave function:

\[
q_{\mu} |Z\rangle = 0,
\]

with

\[
|Z\rangle = \exp \left( \sum_{pp'hh'} \frac{1}{4} Z_{pp'h'h'} a_{p}^\dagger a_{p'}^\dagger a_{h'} a_{h} \right) |HF\rangle,
\]

where |HF\rangle is the Hartree-Fock (HF) Slater determinant and the amplitudes must full-fill the following relations

\[
\sum_{h} x^{\mu}_{\alpha} Z_{pp'h'h'} = U^{\mu}_{pp'h'}, \quad \sum_{p} x^{\mu}_{\alpha} Z_{pp'h'h} = U^{\mu}_{pp'h'}. (4)
\]

The coefficients will be determined from the minimisation of a sum rule for the average s.p. energy

\[
\lambda_{\mu} = \frac{1}{2} \frac{\langle \{q_{\mu}, [H, q_{\mu}]\} \rangle}{\langle \{q_{\mu}, q_{\mu}\} \rangle} = \frac{1}{0 \langle \{q_{\mu}, q_{\mu}\} \rangle} \sum_{\alpha} (E_{\alpha}^{N+1} - E_{\alpha}^{N}) |\langle 0|q_{\mu}|\alpha\rangle|^2 (5)
\]

and equivalently for \( q_{\mu}^\dagger \). The even particle number equation relies on the usual RPA excitation operator [10]

\[
Q_{\nu} = \sum_{ph} X_{ph} a_{p}^\dagger a_{h} - Y_{ph} a_{h}^\dagger a_{p}. (6)
\]

The \( X, Y \) amplitudes are the solutions of another sum-rule defining an average excitation energy of the even systems

\[
\Omega_{\nu} = \frac{1}{2} \frac{\langle 0|Q_{\nu}|H, Q_{\nu}\rangle|0\rangle}{\langle 0|Q_{\nu}, Q_{\nu}\rangle|0\rangle} = \frac{1}{0 \langle 0|Q_{\nu}, Q_{\nu}\rangle|0\rangle} \sum_{\mu} (E_{\mu} - E_{0}) |\langle 0|Q_{\nu}|\mu\rangle|^2 . (7)
\]

The destruction operator \( Q_{\nu} \) does not exactly kill the CCD ground state without introducing a generalization but it kills it to very good approximation as studies of model cases have shown. Therefore the even particle number equation (SCRPA) is the only point where the approach is not entirely consistent though the theory remains very performant as we will see below in the Application section. We, thus, will henceforth always suppose that

\[
Q|Z\rangle = 0 . \quad (8)
\]

The SCRPA equation corresponding to the minimisation of the mean excitation energy \( \Omega_{\nu} \) in (7) can be written as

\[
\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_{\nu} \\ Y_{\nu} \end{pmatrix} = \Omega_{\nu} \begin{pmatrix} X_{\nu} \\ Y_{\nu} \end{pmatrix} \quad (9)
\]

with the normalisation of the amplitude given as usual by

\[
\sum_{ph} (|X_{ph}|^2 - |Y_{ph}|^2) = 1 (10)
\]

and

\[
A_{ph,p'h'} = \frac{\langle a_{p}^\dagger a_{p}, [H, a_{p'}^\dagger a_{p'}]\rangle}{\sqrt{\eta_p - \eta_{p'} \eta_{p'h'} - \eta_{p'}}},
\]

\[
B_{ph,p'h'} = -\frac{\langle a_{p}^\dagger a_{p}, [H, a_{p'}^\dagger a_{p'}]\rangle}{\sqrt{\eta_p - \eta_{p'} \eta_{p'h'} - \eta_{p'}}} \quad (11)
\]

where \( \langle ... \rangle = \langle Z|...|Z\rangle / \langle Z|Z\rangle \). The SCRPA equations are well documented in the literature [1, 3, 5, 8] and we will not repeat their explicit form here. Let us simply say that \( A \) and \( B \) are functional of one and two particle density matrices when the Hamiltonian of the system is given by

\[
H = \sum_{kk'} t_{kk'} a_{k}^\dagger a_{k'} + \frac{1}{4} \sum_{klmn} \bar{v}_{klmn} a_{k}^\dagger a_{l}^\dagger a_{n} a_{m}. (12)
\]

The first part of the Hamiltonian represents the kinetic energy and the second part the two body interaction with the anti-symmetrized matrix element

\[
\bar{v}_{klmn} = \langle kl|v|mn\rangle - \langle kl|v|nm\rangle.
\]

From the minimisation of the sum-rule in eq. (5), we obtain two coupled equations

\[
\sum_{h'h'} \epsilon_{hh'} x_{h'}^\mu + \sum_{pp'h'} C_{h',pp'h} U_{pp'h'}^{\mu} = \lambda_{\mu} x_{h}^\mu (13)
\]

\[
\sum_{h'} C_{pp'h',h} x_{h'}^\mu + \sum_{p_{2}p_{1}h_{1}} D_{pp'h_{1},p_{2}p_{1}h_{1}} U_{pp'h_{1}}^{\mu} = \lambda_{\mu} U_{pp'h}^{\mu} (14)
\]

or written as a matrix eigenvalues equation

\[
\begin{pmatrix} \epsilon & C \\ C^\dagger & D \end{pmatrix} \begin{pmatrix} x_{\mu} \\ U_{\mu} \end{pmatrix} = \lambda_{\mu} \begin{pmatrix} x_{\mu} \\ U_{\mu} \end{pmatrix} \quad (15)
\]

with

\[
\epsilon_{hh'} = \langle a_{h}, [H, a_{h'}]\rangle = \epsilon_{h} \delta_{hh'} \quad (15)
\]

where we supposed that hitherto we work in the Mean-Field (MF) basis with diagonal s.p. MF energies \( \epsilon_{h}, \epsilon_{p} \).
The matrices $\mathcal{C}$ and $\mathcal{D}$ in (14) are obtained from the minimisation of the mean s.p. energy given in (5)

$$
\mathcal{C}_{pp'h',h} = \frac{\langle a_{p}'a_{p'}a_{p}, [H, a_{h}^\dagger] \rangle}{\sqrt{N_{pp'h}}}
$$

$$
\mathcal{D}_{pp'h',ppp'h} = \frac{\langle a_{p}'a_{p'}a_{p}, [H, a_{pp}^\dagger a_{p}, a_{h}] \rangle}{\sqrt{N_{pp'h}}\sqrt{N_{pp'h_1}}}
$$

$$
N_{pp'h'} = \langle a_{h}^\dagger a_{p'}a_{p}, a_{h}^\dagger a_{p'}a_{h} \rangle
$$

(16)

Equation (14) is essentially already given in (9). However, the way we solve this equation and, thus, couple it to the SCRPA of (13) is novel. Let us briefly describe the procedure. The coefficients $\mathcal{C}$ and $\mathcal{D}$ contain two and three body correlation functions. In particular they contain p-h operators which are given by the inversion of (16) valid because the $X, Y$ amplitudes in (9) form a complete orthonormal set of states

$$
a_{h}^\dagger a_{h} = \sqrt{n_{h} - n_{p}} \sum_{\nu} X_{ph}^\nu Q_{\nu}^\nu + Y_{ph}^\nu Q_{\nu}^\nu
$$

(17)

and its hermitian conjugate. All other correlation functions which do not contain those p-h operators and which are not of the pp′h type shall be discarded since they are supposedly less important. Commuting the destructor $Q$ to the right until they hit and kill the vacuum state $|Z\rangle$ leads to expressions of diverse correlation functions which only contain s.p. occupations $n_{h}$ and $n_{p}$ and RPA amplitudes $X, Y$. We want to call the coupled equations (9,11) and (14,16) ‘even-odd SCRPA’ (eo-SCRPA). One may find more details in the Application section below. This procedure to obtain the s.p. occupation numbers is the essential new point of this work. It is clear that in this way eqs. (9) and (14) become coupled. In our earlier publications the s.p. occupation numbers appearing in the SCRPA equations have always been obtained in a different, in our opinion less natural way. We should also say the the formal expressions of SCRPA are not altered, only the way how the s.p. occupation probabilities are calculated is new.

It may be helpful at this point to discuss for instance the matrix $\mathcal{D}$ in (14,16) a little more and give a graphical representation. From the double commutator in $\mathcal{D}$, we retain only those terms where a particle state of the triplet operator on the right connects to the interaction and the same for the triplet on the left. In doing so, what is left from the interaction is a density operator $a_{h}a_{h}$ for which we will make the diagonal approximation. Of course anti-symmetrization of the two particle indices will be fully respected. We then can make a graphical representation of the interaction process contained in $\mathcal{D}$ as shown in Fig. 1. After the diagonalization of the matrix which implies a self-consistency on the occupancies, we can find the occupation numbers $n_{h}$ as

$$
n_{h} = \langle a_{h}^\dagger a_{h} \rangle = \sum_{\mu} \langle \{ a_{h}^\dagger, g_{h,\mu} \} \rangle^2 = \sum_{\mu} |x_{h}^\mu|^2
$$

(18)

and

$$
n_{p} = \langle a_{p}'a_{p} \rangle = \sum_{\rho} |x_{p}^\rho|^2
$$

(19)

where the summation extends over all the amplitudes where $\lambda_{\mu} < E_{F}$ for hole state (or $\lambda_{\rho} > E_{F}$ for particle state). These simple expressions stem from the fact that, e.g., $a_{h}^\dagger$ commutes with $a_{h}^\dagger a_{h}a_{p}$. Please notice that these occupation numbers enter also the $A$ and $B$ matrices in Eq. (10). Again details of the procedure will become more clear in the applications we will give below.

Another way to find the same results for the occupancies is to define the Green Function (GF)

$$
\mathcal{G}_{h}(\omega) = \frac{1}{\omega - \epsilon_{h} - \mathcal{M}_{h}(\omega)}
$$

(20)

from where we find the resonances as

$$
\lambda_{\alpha} - \epsilon_{h} - \mathcal{M}_{h}(\lambda_{\alpha}) = 0
$$

(21)

The mass operator $\mathcal{M}_{h}$ is obtained from the eq. (14), eliminating the amplitude $U$,

$$
\mathcal{M}_{h} = \sum_{pp'h',ppp'h} \mathcal{C}_{pp'h'\omega}(\omega - \mathcal{D})^{-1}_{pp'h',ppp'h} \mathcal{C}_{ppp'h,pp'h_1}
$$

(22)

The solution of (21) has obviously the same eigenvalues as (14) and then $\mathcal{G}_{h}$ can be written as

$$
\mathcal{G}_{h}(\omega) = \sum_{\alpha} \frac{r_{\alpha}}{\omega - \lambda_{\alpha}}
$$

(23)

where

$$
r_{\alpha} = \frac{1}{1 - \mathcal{M}'|_{\omega=\lambda_{\alpha}}}
$$

(24)

and $\mathcal{M}'_{h} = d\mathcal{M}_{h}(\omega)/d\omega = -\mathcal{C}'(\omega - \mathcal{D})^{-2}\mathcal{C}$. We can easily check that $\sum_{\alpha} r_{\alpha} = 1$ (the sum over all residua) and we can write the Green function dependent on time as

$$
i\mathcal{G}_{h}(t-t') = -\theta(t-t') \sum_{\alpha(\lambda_{\alpha} < E_{F})} r_{\alpha} e^{-i\lambda_{\alpha}(t-t')}
$$

$$
+ \theta(t'-t) \sum_{\alpha(\lambda_{\alpha} > E_{F})} r_{\alpha} e^{-i\lambda_{\alpha}(t-t')}
$$

$$
i\mathcal{G}_{p}(t-t') = -\theta(t-t') \sum_{\rho(\lambda_{\rho} < E_{F})} r_{\rho} e^{-i\lambda_{\rho}(t-t')}
$$

$$
+ \theta(t'-t) \sum_{\rho(\lambda_{\rho} > E_{F})} r_{\rho} e^{-i\lambda_{\rho}(t-t')}
$$

(25)
Thus, we can find the s.p. occupation probabilities as
\[ n_h = -i \lim_{\nu' \rightarrow -0} \langle \mathcal{G}_h(t-t') \rangle \]
\[ n_p = -i \lim_{\nu' \rightarrow -0} \langle \mathcal{G}_p(t-t') \rangle \] (26)

Once we have the GF’s, we can calculate the ground state energy in the usual way via
\[ E_0 = -\frac{i}{2} \lim_{\nu' \rightarrow -0} \sum_k \left[ \frac{\partial}{\partial t} + \epsilon_k \right] \mathcal{G}_k(t-t') \] (27)

In order to test our idea, we chose two models where we know the exact solution. The first application concerns the Lipkin model as an orientation to nuclear physics. The second one focuses on solid state physics where the Hubbard model is chosen.

### III. APPLICATIONS

#### A. The Lipkin Model

The single-particle space of the Lipkin model consists of two fermion levels, each of which has a N-fold degeneracy see, e.g., [10]. The upper (lower) level has the energy of \( \frac{1}{2} (-\frac{1}{2}) \). The Hamiltonian of the Lipkin model is given by
\[ H = eJ_0 - \frac{V}{2}(J^2_+ + J^2_-) \] (28)

with \( e \) is the inter-shell spacing, \( V \) is the coupling constant and
\[ J_0 = \frac{1}{2} \sum_{m=1}^{N} \left( c^\dagger_{1m} c_{1m} - c^\dagger_{0m} c_{0m} \right) \]
\[ J_+ = \sum_{m=1}^{N} c^\dagger_{1m} c_{0m}, \quad J_- = (J_+)^\dagger \] (29)

with \( 2J_0 = \hat{n}_1 - \hat{n}_0, \hat{n}_i = \sum_m c^\dagger_{im} c_{im} \) and \( N \) is the number of particles equivalent to the degeneracies of the shells. We consider the odd excitation operator as [11], that is
\[ q^\dagger_\mu = \frac{1}{N} \sum_m x^\mu_{0m} c_{0m} + U^\mu_{0m} J_+ c^\dagger_{1m} \] (30)

with the minimisation of the sum rule in [5]. Based on the solution of the SCRPA equations [3, 10, 11] with the definition of the pair excitation operator as \( Q^+ = (XJ_+ - YJ_-)/\sqrt{(-2J_0)} \) (with \( J_+ = \sqrt{(-2J_0)}(XQ^+ - YQ) \), we obtain the \( X, Y \) amplitudes as being the solutions of SCRPA equations. From the minimisation of expression [5], we obtain a 2 x 2 matrix eigenvalue equation (see appendix A), with the Hamiltonian and norm matrices,
\[ \mathcal{H}_{ij} = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix} \quad \text{and} \quad \mathcal{N} = \begin{pmatrix} n_{00} & n_{01} \\ n_{10} & n_{11} \end{pmatrix} \] (31)

![FIG. 2: The difference between occupation number of the two level in Lipkin model, normalized by \( N \) as a function of \( \chi = V(N-1) \) for \( N = 4, 10, 20, 100 \). This with standard RPA (red dots), SCRPA (violet dashed-dot), eo-SCRPA (blue dashed line) with eom method for odd particle excitation and exact solution (full black line). Note that our approach gives the exact result for \( N = 4 \). Also, we present the results of Catara method for \( N = 10 \).](image-url)
FIG. 3: Same as Fig. 2 but for the square of the difference between occupation number of the two level in Lipkin model, normalized by $N^2$.

FIG. 4: Same as Fig. 2 but for the first excited state for $N = 4, 20, 100, 200$. Please note that one may make the hypothesis that the eo-SCRPA approach becomes exact in the $N \to \infty$ limit. Also, we present the results of Catara method for $N = 20$. 
FIG. 5: The correlation energy as a function of \( \chi = V(N - 1) \) for \( N = 4, 10, 20, 100 \) with eo-SCRPA (blue dashed line) compared to the exact solution (full black line). Note again that for \( N = 4 \) the exact result is obtained with our approach.

**FIG. 6:** Excitation energy between the system \( N + 1 \) and \( N \) particles as a function of \( \chi = V(N - 1) \) for \( N = 4, 10 \) with eo-SCRPA (blue dashed line) compared to the exact solution (full black line) \( \lambda_+ = E_{N+1}^N - E_N^N \).

where we define the elements of the two matrices as

\[
\begin{align*}
n_{00} & = \frac{1}{N} \sum_m \langle \{ c_{0m}, c^\dagger_{0m} \} \rangle \\
n_{01} & = n_{10} = \frac{1}{N} \sum_m \langle \{ c_{0m}, J^+ c^\dagger_{1m} \} \rangle \\
n_{11} & = \frac{1}{N} \sum_m \langle \{ c_{1m} J^-, J^+ c^\dagger_{1m} \} \rangle \\
H_{00} & = \frac{1}{N} \sum_m \langle \{ c_{0m}, [H, c^\dagger_{0m}] \} \rangle \\
H_{10} & = H_{01} = \frac{1}{N} \sum_m \langle \{ c_{1m} J^-, [H, c^\dagger_{0m}] \} \rangle \\
H_{11} & = \frac{1}{N} \sum_m \langle \{ c_{1m} J^-, [H, J^+ c^\dagger_{1m}] \} \rangle 
\end{align*}
\]

and the corresponding secular equation

\[
\det \left\{ \sum_{i'j'} N^{-1/2}_{i'i} H_{i'j'} N_{j'j}^{-1/2} - \lambda I \right\} = 0
\]
where the eigenvalues $\lambda$ are given in App. A. In the above equations (33) the correlation functions are expressed by the RPA amplitudes $X, Y$ in the way it is described in section III and App. A. The correlation functions which contain quadratic forms of occupation number operators as $\langle J_0 J_0 \rangle$ in above equation can in principle be expressed by the RPA amplitudes as well but leading to heavier expressions. Usually, we, therefore will employ the factorization approximation leading in the present case to $\langle J_0 J_0 \rangle \approx \langle J_0 \rangle^2$ what mostly turns out to be quite satisfactory. However, in the case of the Lipkin model one also can use the Casimir relation to close the system of equations, see App. A where also more details of the procedure are given. The results are shown in Figs. 2-7. They concern in the order: i) the expectation value $\langle J_0 \rangle$ of the difference of populations in upper and lower level, ii) the square of this quantity, iii) the first excitation energy, iv) the correlation energy, and v) the excitation energy between the system with the first excitation energy, upper and lower level, ii) the square of this quantity, iii) expectation value shown in Figs. 2-7. They concern in the order: i) the more details of the procedure are given. The results are close the system of equations, see App. A where also Lipkin model one also can use the Casimir relation to out to be quite satisfactory. However, in the case of the occupations even for $N = 4$ come out to be exact (as shown in Figs. 2, 5 and 7). In Fig.2, Fig.3 and Fig.4 in the panels with $N = 10$ and $N = 20$, we also show the results of the Catara method [7] for the calculation of the occupation numbers and first excited state (as a reminder, let us mention that using the Catara method for the occupation numbers has been named the SCRPA method in the past; we keep the same name while getting the occupations from the selfconsistent odd RPA). One can thus appreciate the important improvement obtained with the method of the present work where even and odd RPA’s are coupled.

B. The Hubbard Model

The Hubbard model is widely used to deal with the physics of strongly correlated electrons. Since the model can be solved exactly in one dimension (1D) and for small cluster sizes, it is very useful for theoretical investigations [8]. To be precise, our "Hubbard model" is a 6-site system at half filling with periodic boundary condition, described by the usual Hamiltonian [8, 13]:

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} + \frac{U}{2} \sum_{i, \sigma} \hat{n}_{i, \sigma} \hat{n}_{i, -\sigma}. \quad (34)$$

Here, $\hat{n}_{i, \sigma} = c_{i \sigma}^\dagger c_{i \sigma}$, $c_{i \sigma}^\dagger$ and $c_{i \sigma}$ are the creation and annihilation operators for an electron at site $i$ with spin $\sigma$, $U$ is the on-site (spin-independent) interaction, $-t$ is the hopping term of the kinetic energy. The eigenstates of the system can be expressed as linear combinations of Slater determinants. The Hamiltonian is rewritten in plane wave basis,

$$H = \sum_{k, \sigma} \varepsilon_k \hat{n}_{k \sigma} + \frac{U}{2N} \sum_{kk'q\sigma} a_{k\sigma}^\dagger a_{k+q\sigma} a_{k'\sigma}^\dagger a_{k'-q\sigma}. \quad (35)$$
with the transformation

\[ c_{j, \sigma} = \frac{1}{\sqrt{N}} \sum_{k} a_{k, \sigma} e^{-i k x_j} , \]  

(36)

where \( a_k = a_{k, \sigma}^\dagger a_{k, \sigma} \), and \( \xi_k = -2t \cos(k a) \), which are, respectively, the number operator of particles of the mode \((k, \sigma)\) and the energies of one particle on a lattice with a the parameter of the lattice which is taken as \( a = 1 \). For a problem with \( N \) sites, the condition of periodicity is given by \( c_{N+1, \sigma} = c_{1, \sigma} \). This implies that \( e^{-i k N} = 1 \), hence the values taken by \( k \) will be \( k = \frac{2\pi}{N} n \). In addition, the first Brillouin zone is defined on the field where \( -\pi < k < \pi \), which gives us the values of \( n \) as \( n = \frac{N}{2} \leq n < \frac{N}{2} \).

For the six sites, we have the possible states with the following wave vectors:

\[ k_1 = 0, \quad k_3 = -k_2 = \frac{\pi}{3}, \quad k_5 = -k_4 = \frac{2\pi}{3}, \quad k_6 = -\pi \]  

(37)

and with the kinetic energies (see Fig. 8), respectively,

\[ \varepsilon_{k_0} = -\varepsilon_{k_1} = t, \quad \varepsilon_{k_2} = \varepsilon_{k_3} = -\varepsilon_{k_4} = -\varepsilon_{k_5} = t \]  

(38)

The transfer wave vector \((q_{ph} = k_\sigma - k_h)\) takes the possible values as shown in the Table 1:

| \( q = \pm \frac{\pi}{3} \) | \( q = \pm \pi \) | \( q = \pm \frac{\pi}{6} \) |
|----------------|----------------|----------------|
| 51 \to q_31 = + | 61 \to q_31 = - | 42 \to q_32 = - |
| 63 \to q_32 = + | 52 \to q_32 = + | 53 \to q_33 = + |
| 41 \to q_34 = - | 43 \to q_34 = - | |
| 62 \to q_35 = - | |

TABLE I: The various momentum transfers in the 6 sites case.

At this point we proceed exactly as in the case of the Lipkin model: The excitation operator for the even system is given by

\[ Q_{\nu} = \sum_{ph\sigma} X_{ph\sigma}^\nu K_{ph\sigma}^+ - Y_{ph\sigma}^\nu K_{ph\sigma}^- \]  

(39)

with \( K_{ph\sigma}^+ = J_{ph\sigma}^+ / \sqrt{N_{ph\sigma}}, \quad J_{ph\sigma}^+ = a_{ph\sigma}^\dagger a_{h\sigma}, \quad N_{ph\sigma} = n_{h\sigma} - n_{p\sigma} \). With the inversion

\[ J_{h\sigma\rho}^- = \sqrt{N_{ph\sigma}} \sum_{\nu} \left( X_{ph\sigma}^\nu \nu_{\rho\sigma} + Y_{ph\sigma}^\nu \nu_{\rho\sigma} Q_{\nu}^\nu \right) \]

\[ J_{h\sigma\rho}^+ = \sqrt{N_{ph\sigma}} \sum_{\nu} \left( Y_{ph\sigma}^\nu \nu_{\rho\sigma} + X_{ph\sigma}^\nu \nu_{\rho\sigma} Q_{\nu}^\nu \right) \]  

(40)

we can calculate the mean values needed for the matrix elements of the SCRPA equations for the even particle number case

\[ \langle J_{p'h\sigma'}^+, J_{h\sigma\rho}^- \rangle = \sqrt{N_{p'h\sigma'} N_{ph\sigma}} \sum_{\nu} X_{p'h\sigma'}^\nu Y_{ph\sigma}^\nu, \]

\[ \langle J_{h\sigma\rho}^-, J_{p'h\sigma'}^+ \rangle = \sqrt{N_{p'h\sigma'} N_{ph\sigma}} \sum_{\nu} X_{p'h\sigma'}^\nu Y_{ph\sigma}^\nu, \]

\[ \langle J_{p'h\sigma'}^+, J_{p'h\sigma'}^+ \rangle = \sqrt{N_{p'h\sigma'} N_{ph\sigma}} \sum_{\nu} Y_{p'h\sigma'}^\nu X_{ph\sigma}^\nu, \]

\[ \langle J_{h\sigma\rho}^-, J_{h\sigma\rho}^- \rangle = \sqrt{N_{p'h\sigma'} N_{ph\sigma}} \sum_{\nu} Y_{p'h\sigma'}^\nu X_{ph\sigma}^\nu, \]  

(41)

where we replaced the "ph" operators by the RPA creation and destruction operators from the inversion (17) and then commute the \( Q \) operators to the right until they kill the ground state. All matrices become functional of the occupancies \( n_h \) and \( n_p \) and \( X, Y \) amplitudes in analogy to what was the case in the Lipkin model and, thus, the diagonalisation process implies at the same time an iteration on the occupancies and the amplitudes.

For the odd particle number case, we make again the following ansatz

\[ q_{h,\mu}^\nu = x_{h,\mu}^\nu a_{h,\mu} + \sum_{p'h} U_{p'h}^\nu a_{p'h}^\dagger + J_{p'h}^+ \]

\[ q_{p',\rho}^\nu = x_{p',\rho}^\nu a_{p',\rho} + \sum_{p'h'\rho} U_{p'h'}^\nu a_{p'h'}^\dagger + J_{p'h'}^+ - \]

(42)

From there, we can, as outlined in the general section II and as just now for the case of the Lipkin model calculate the occupation numbers. For more details, see App. 13

The results for the occupation numbers are again very satisfying, see Fig. 9. Also the excitation energies of the even particle number system, see Fig. 10, are very well reproduced. In Fig. 11 we show the ground state energies for the exact case compared to the eo-SCRPA solution. One should notice that there is barely an improvement using the eo-SCRPA versus the standard SCRPA because the latter produced already excellent results. So, we do not show the old SCRPA results again. It is not quite clear why there is this difference between the Lipkin and Hubbard models. Probably the fact that in Lipkin model, contrary to the Hubbard model, one uses collective ph operators makes it more difficult to fulfill the Pauli principle. So the performance of one or the other approach...
IV. CONCLUSION

In this work, we coupled even and odd particle number RPA self-consistently. Both systems are based on the same correlated RPA ground state. From the odd system, we get the occupation numbers, odd particle excitation energies, and the ground state energies whereas from the even SCRPA equations we get the excitation energies of the even system and transition probabilities. To make things clear, we should mention again that the SCRPA employed here has the same mathematical structure as the one used before \[8\], only the single particle occupation probabilities are now calculated via the odd selfconsistent RPA whereas they were obtained before via the so-called Catara method \[7\]. Both even and odd systems are coupled through non-linear equations which both contain the RPA amplitudes $X, Y$ and the s.p. occupation numbers $n_k$ in a non-linear way. We called this system of equations ‘even-odd’ SCRPA (eo-SCRPA). Applications to the Lipkin model and a six sites Hubbard ring at half filling gave very satisfying results for all quantities. The equations are relatively complex due to their non-linearity but they should be solvable with modern computers for realistic problems such as, e.g., the calculation of collective states in nuclei. The equations to be solved seem not to be of higher numerical complexity than, e.g., the Brueckner Hartree-Fock equations which have been solved a number of times for nuclei. The coupling of even and odd RPA’s has a couple of advantages: it gives richer results, i.e., excitation energies of even and odd particle number systems; there is a natural way how to obtain the ground state energy via the s.p. Green’s function and, last but not least, the results seem to be promising.
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Appendix A: Equation of Motion for odd particle number operator for Lipkin Model

We consider the odd excitation operator as

$$ q^\dagger_\mu = \frac{1}{N} \sum_m x^\mu_{0m} c_{0m} + U^\mu_{0m} J^+ c_{1m}^\dagger $$

(A1)

and the coefficients will be determined from minimisation of expression (5). Based on the solution of the SCRPA equations with the definition of the pair excitation operator as $Q^\dagger = (XJ_+ - YJ_-)/\sqrt{(-2J_0)}$ (with $J_+ = \sqrt{(-2J_0)}(XQ^\dagger - YQ)$), the $X$, $Y$ amplitudes are the solutions of the SCRPA equations with $H$ of the Lipkin Hamiltonian (28). From the minimisation of (5), we obtain a $2 \times 2$ matrix eigenvalue equation. The normal matrix is given by

$$ n_{00} = \frac{1}{N} \sum_m \langle c_{0m}, c_{0m}^\dagger \rangle = 1 $$

$$ n_{01} = n_{10} = \frac{1}{N} \sum_m \langle c_{0m}, J_+ c_{1m}^\dagger \rangle = 0 $$

$$ n_{11} = \frac{1}{N} \sum_m \langle c_{1m}, J_+ c_{1m}^\dagger \rangle $$

$$ = -\frac{1}{N} (N - 2) (1 + 2Y^2) \langle J_0 \rangle + \frac{2}{N} \langle J_0 J_0 \rangle $$

(A2)

where we have used the inversion (17) and the killing condition $Q|0\rangle = 0$. For the first Hamiltonian element we have

$$ \mathcal{H}_{00} = \frac{1}{N} \sum_m \langle c_{0m}, [H, c_{0m}^\dagger] \rangle = -\frac{e}{2} $$

(A3)

and for the off diagonal elements

$$ \mathcal{H}_{10} = \mathcal{H}_{01} = \frac{1}{N} \sum_m \langle c_{1m}, J_+, [H, c_{0m}^\dagger] \rangle $$

$$ = -\frac{e}{2N} \sum_m \langle c_{1m}, c_{0m}^\dagger \rangle $$

$$ -\frac{V}{N} \sum_m \langle c_{1m}, J_+ c_{1m}^\dagger \rangle $$

$$ = -V n_{11} $$

(A4)

And the anti-commutator for $\mathcal{H}_{11}$ is given by

$$ \mathcal{H}_{11} = \frac{1}{N} \sum_m \langle c_{1m}, [H, J_+ c_{1m}^\dagger] \rangle $$

$$ = \frac{3e}{2} n_{11} + V (2 - \frac{8}{N}) \langle J_0 J_- \rangle + \langle J_0 J_0 \rangle $$

$$ = \frac{3e}{2} n_{11} - 2VXY (2 - \frac{8}{N}) \langle J_0 \rangle + \langle J_0^2 \rangle $$

(A5)

with, for example

$$ \langle J_0 J_- \rangle = -4XY^2 \langle J_0 \rangle - 2XY \langle J_0 J_0 \rangle $$

(A6)

where we have again used the inversion (17) and the killing condition $Q|0\rangle = 0$.

The correlation functions which contain quadratic forms of occupation number operators as $\langle J_0 J_0 \rangle$ in above equation can in principle be expressed by the RPA amplitudes as well but leading to heavier expressions. Usually, we, therefore will employ the factorization approximation leading in the present case to $\langle J_0 J_0 \rangle \approx \langle J_0 \rangle^2$. However, in the Lipkin model one also can use the Casimir relation

$$ \langle 4J_0 J_0 \rangle = N(N + 2) + 4 \langle J_0 \rangle - 4 \langle J_+ J_- \rangle $$

(A7)

Then all matrix elements $\mathcal{H}_{ij}$ become functions of $\langle J_0 \rangle$ and the RPA amplitudes $X, Y$. The eigenvalue problem can therefore be solved leading to a self-consistency problem for $\langle J_0 \rangle$ and the RPA amplitudes which are obtained from the SCRPA equations (11) (3). The occupation numbers are then given by

$$ n_0 = N \frac{\lambda_+ - \mathcal{H}_{11}/n_{11}}{\lambda_- - \lambda_+} $$

and $n_1 = N - n_0$ (A8)

where $\lambda_{\pm}$ are the eigenvalues of the $2 \times 2$ problem,

$$ \lambda_{\pm} = -\frac{e}{2} + \beta \pm \sqrt{\beta^2 + V^2 n_{11}} $$

(A9)

with $\beta = e - VXY(N - 4) - VXY(N - 4)(1 + 2Y^2) \langle J_0 \rangle_{n_{11}}$. Thus,

$$ \langle 2J_0 \rangle = n_0 - n_1 = 2n_0 - N $$

(A10)

Appendix B: Equation of Motion for Hubbard Model

For the Hubbard model (35) we define the odd excitation operator as in Eq. (11).

$$ q^\dagger_{h, \mu} = x^\mu_h a_{h+} + \sum_{p' h} U^\mu_{p' h} a_{p' +} J^+_{p' h} $$

$$ q^\dagger_{p, \rho} = x^\rho_p a_{p+} + \sum_{p' h} U^\rho_{p' h} a_{p+} J^+_{p' h} $$

(B1)

with $J^+_{p} = a^\dagger_{p} a_{h-}$ and $\sigma = \uparrow, \downarrow = +, -$. Remembering the notations for the occupation probabilities

$$ n_{k\rho} = \langle \hat{n}_{k\rho} \rangle = \langle a^\dagger_{k\rho} a_{k\rho} \rangle $$

(B2)

we have $n_{k_{\uparrow}} = n_{k_{\downarrow}}, n_{k_{\downarrow}} = n_{k_{\downarrow}}, n_{k_{\uparrow} \uparrow} = 1 - n_{k_{\uparrow}}$ and $n_{k_{\downarrow} \downarrow} = 1 - n_{k_{\downarrow}}$. This gives

$$ \mathcal{H}_{11} = \langle \{ a_{k_{\uparrow} +}, [H, a^\dagger_{k_{\uparrow} +}] \} \rangle = \epsilon_{k_{\uparrow}} - 2t + U/2 $$

(B3)

The term without interaction $H_0 = \sum_{k\rho} \epsilon_k \hat{n}_{k\rho}$ is given by

$$ \langle \{ a_{p_{\uparrow} +} J^+_{p_{\uparrow} +}, [H_0, a^\dagger_{p_{\uparrow} +} J^+_{p_{\uparrow} +}] \} \rangle = (\varepsilon_p - \varepsilon_h + \varepsilon_{p'}) N_{p' h} $$

(B4)
with \( N_{p'ph} = \langle (1 - \hat{n}_p) (2J_{ph,-}^0) \rangle + \langle J_{ph,-}^+ J_{ph,-}^- \rangle \). The term in the Hamiltonian for the transfer \( q \neq 0 \), \( H_{q=0} = \frac{U}{6} \sum_{kk'} \hat{n}_{k} \hat{n}_{k'} \) leads to

\[
\langle \{ a_{p'}^+ J_{hph}^+ \} \rangle \quad \text{for} \quad H_{q=0}, a_{p'}^+ J_{ph}^- \rangle = \frac{U}{2} \hat{N}_{p'ph} \quad \text{(B5)}
\]

\[
\sqrt{N_{p'ph} N_{p''p_1h_1}} D_{p'ph, p''p_1h_1} \rangle \{ a_{p''}^+ J_{h_{p_1h_1}^-} \} \rangle \quad \text{for} \quad H_{q=0}, a_{p'}^+ J_{ph}^- \rangle 
\]

\[
= \langle \{ a_{p''}^+ J_{h_{p_1h_1}^-} \} \rangle \quad \text{for} \quad H_{q=0}, a_{p'}^+ J_{ph}^- \rangle 
\]

\[
= \frac{U}{6} \left\{ \langle a_{h_1-q}^+ a_{p'}^+ a_{h+q}^+ a_{p}^- \rangle - \langle a_{h_1-q}^+ a_{p'}^+ a_{h}^- a_{p-q}^- \rangle + \sum_k \langle J_{hph}^- a_{k} a_{k+p'} \rangle \right\} \quad \text{(B6)}
\]

The elements of the matrix except the first row (or column) are given as follows.

\[
\sqrt{N_{p'ph} N_{p''p_1h_1}} D_{p'ph, p''p_1h_1} \rangle \{ a_{p''}^+ J_{h_{p_1h_1}^-} \} \rangle = \langle \{ a_{p''}^+ J_{h_{p_1h_1}^-} \} \rangle \quad \text{for} \quad H_{q=0}, a_{p'}^+ J_{ph}^- \rangle 
\]

\[
= \langle \{ a_{p''}^+ J_{h_{p_1h_1}^-} \} \rangle \quad \text{for} \quad H_{q=0}, a_{p'}^+ J_{ph}^- \rangle 
\]

\[
= \frac{U}{6} \left\{ \langle a_{h_1-q}^+ a_{p'}^+ a_{h+q}^+ a_{p}^- \rangle - \langle a_{h_1-q}^+ a_{p'}^+ a_{h}^- a_{p-q}^- \rangle + \sum_k \langle J_{hph}^- a_{k} a_{k+p'} \rangle \right\} \quad \text{(B7)}
\]

In the following, as already discussed several times, we retain from (B7) only those terms where the particle states of the left and right triple operators in \( D \) connect to the interaction. The remaining density operator from the interaction is approximated by its diagonal form. This leads to expressions evaluated in (B8) below. First let us discuss what kind of terms we are neglecting in this way. It should be noted that the terms of type \( \langle J_{p_{h}h_{p}'} J_{p_{h}h_{p}''} \rangle \) are probably small (with \( S_{p_1p_2} = a_{p_1} a_{p_2} \) for \( p_1 \neq p_2 \)) and \( \langle J_{ph}^+ S_{h_1h_2} J_{ph}^+ \rangle \) also small (with \( S_{h_1h_2} = a_{h_1} a_{h_2} \) for \( h_1 \neq h_2 \)) in eq. (B7). As shown in (3), the term \( \langle SJ \rangle = 0 \) and \( \langle SS \rangle \) are small. Only the terms non-zero in eq. (B7) like \( \langle J_{ph}^+ n_{k} J_{ph}^+ \rangle \) which can be calculated as shown in (B8) are kept. With the short hand notation \( ph_{\sigma} \equiv i, k \sigma \equiv k, N_1 = \hat{n}_{h_{\sigma}} - \hat{n}_{p_{\sigma}} \) and \( N_1 = n_{h_{\sigma}} - n_{p_{\sigma}} \), we can evaluate the following terms.
\( \langle J_i^- \hat{n}_k J_j^- \rangle = \sqrt{N_i N_j} \sum_{\nu, \nu'} X_i^\nu X_j^{\nu'} \langle Q_{\nu'} \hat{n}_k Q_{\nu'} \rangle \)

\( = \sqrt{N_i N_j} \sum_{\nu, \nu'} X_i^\nu X_j^{\nu'} \left( X_i^\nu X_j^{\nu'} - Y_i^{\nu'} Y_j^{\nu} \right) + \sum_{\nu} X_i^\nu X_j^{\nu} \sum_l \left( |X_i^\nu|^2 - |Y_i^{\nu'}|^2 \right) \langle \hat{n}_k \hat{N}_l \rangle \)

\( \langle J_i^+ \hat{n}_k J_j^+ \rangle = \sqrt{N_i N_j} \sum_{\nu, \nu'} Y_i^\nu Y_j^{\nu'} \langle Q_{\nu'} \hat{n}_k Q_{\nu'} \rangle \)

\( = \sqrt{N_i N_j} \sum_{\nu, \nu'} Y_i^\nu Y_j^{\nu'} \left( X_i^\nu X_j^{\nu'} - Y_i^{\nu'} Y_j^{\nu} \right) + \sum_{\nu} Y_i^\nu Y_j^{\nu} \sum_l \left( |X_i^\nu|^2 - |Y_i^{\nu'}|^2 \right) \langle \hat{n}_k \hat{N}_l \rangle \)

\( \langle J_i^- \hat{n}_k J_j^+ \rangle = \sqrt{N_i N_j} \sum_{\nu, \nu'} X_i^\nu X_j^{\nu'} \langle Q_{\nu'} \hat{n}_k Q_{\nu'} \rangle \)

\( = \sqrt{N_i N_j} \sum_{\nu, \nu'} X_i^\nu X_j^{\nu'} \left( X_i^\nu X_j^{\nu'} - Y_i^{\nu'} Y_j^{\nu} \right) + \sum_{\nu} X_i^\nu X_j^{\nu} \sum_l \left( |X_i^\nu|^2 - |Y_i^{\nu'}|^2 \right) \langle \hat{n}_k \hat{N}_l \rangle \)  \( \text{(B8)} \)

where we used \( Q_{\nu'} = \sum_l (X_i^\nu J_j^+ + Y_i^\nu J_j^-) \hat{N}_l^{-1/2} \) and the commutators

\[
\begin{align*}
\left[ Q_{\nu'}, \hat{n}_k \right] &= +N_l^{-1/2} \left( X_i^\nu J_j^- - Y_i^\nu J_j^+ \right) \\
\left[ Q_{\nu'}, \hat{n}_k \right] &= -N_l^{-1/2} \left( X_i^\nu J_j^- - Y_i^\nu J_j^+ \right) \\
\left[ Q_{\nu'}, Q_{\nu''} \right] &= \sum_l \left( X_i^\nu X_l^{\nu'} - Y_i^{\nu'} Y_l^{\nu} \right) \hat{N}_l N_l^{-1} \\
&= \delta_{\nu, \nu'} \sum_l \left( |X_i^\nu|^2 - |Y_i^{\nu'}|^2 \right) \hat{N}_l N_l^{-1}. \quad \text{(B9)}
\end{align*}
\]

This entails, \( \langle |Q_{\nu}, Q_{\nu'}| \rangle = 1 \) and

\[
\begin{align*}
\langle Q_{\nu'} \hat{n}_k Q_{\nu'} \rangle &= N_l^{-1/2} \left( X_i^\nu \langle J_i^- Q_{\nu'} \rangle - Y_i^{\nu'} \langle J_i^+ Q_{\nu'} \rangle \right) + \langle \hat{n}_k Q_{\nu} Q_{\nu'} \rangle \\
&= \left( X_i^\nu X_l^{\nu'} - Y_i^{\nu'} Y_l^{\nu} \right) + \delta_{\nu, \nu'} \sum_l N_l^{-1} \left( X_i^\nu X_l^{\nu'} - Y_i^{\nu'} Y_l^{\nu} \right) \langle \hat{n}_k \hat{N}_l \rangle \quad \text{(B10)}
\end{align*}
\]