Self Consistent and Renormalized particle-particle RPA in a Schematic Model

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Abstract

The dynamical effects of ground state correlations for excitation energies and transition strengths near the superfluid phase transition are studied in the soluble two level pairing model, in the context of the particle-particle self consistent Random Phase Approximation (SCRPA). Exact results are well reproduced across the transition region, beyond the collapse of the standard particle-particle Random Phase Approximation. The effects of two-body correlation in the SCRPA are displayed explicitly.

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An extension of the self-consistent Random Phase Approximation (SCRPA) to the particle-particle case (pp-SCRPA) has been recently presented by Dukelsky, Röpke and Schuck [1]. The main concern there is with differences between ground state correlations due to pairing vibrations and Bruekner-Hartree-Fock ground state correlations. In this report we use the soluble schematic model used in [1] to study different aspects of the pp-SCRPA. Namely, we examine the behavior of the system as we approach the transition point from the normal to the superfluid phase and investigate the importance of the two-body ground state correlations for excitation energies and transition strengths in this domain.

The model is the standard two-level pairing model whose Hamiltonian is given by

$$H = \frac{\epsilon}{2} \sum_{\sigma} \sigma N_\sigma - g \Omega \sum_{\sigma,\sigma'} A^+_{\sigma} A_{\sigma'}$$

where $\sigma = \pm 1$ labels the upper and lower levels which have equal pair degeneracy $\Omega = j+1/2$ and $N_\sigma, A^+_{\sigma}$ are respectively the number and pair operators in the level $\sigma$, i.e.

$$N_\sigma = \sum_m a^{+}_{\sigma m} a_{\sigma m}, \quad A^+_{\sigma m} = \frac{1}{\sqrt{\Omega} 2} \sum_m (-)^{j-m} a^{+}_{\sigma m} a^{+}_{\sigma-m}.$$  

(2)

For each level $\sigma$ the operators

$$S^+_{\sigma} = \sqrt{\Omega} A^+_{\sigma}, \quad S^-_{\sigma} = S^+_{\sigma}^+, \quad S^0_{\sigma} = \frac{1}{2} (N_\sigma - \Omega)$$

(3)

satisfy an SU(2) algebra.

The addition, $P^+$, and removal, $R^+$, phonon creation operators of the pp-SCRPA for the model are [1]

$$P^+ = \lambda A^+_1 - \mu A^+_{-1}, \quad R^+ = \rho A^-_{-1} - \tau A^+_1$$

(4)

and the pp-SCRPA ground state $|0\rangle$ is defined as the vacuum of these phonons, i.e.

$$P |0\rangle = R |0\rangle = 0.$$  

(5)

Addition and removal excitations are normalized as

$$\langle 0 | [P, P^+] |0\rangle = 1, \quad \langle 0 | [R, R^+] |0\rangle = 1, \quad \langle 0 | [R^+, P^+] |0\rangle = 0$$

(6)
which gives, using Eqs. (4),
\[
\lambda^2 \langle 0 | \left(1 - \frac{N_1}{\Omega}\right) | 0 \rangle + \mu^2 \langle 0 | \left(1 - \frac{N_{-1}}{\Omega}\right) | 0 \rangle = 1
\]
\[
\tau^2 \langle 0 | \left(1 - \frac{N_1}{\Omega}\right) | 0 \rangle + \rho^2 \langle 0 | \left(1 - \frac{N_{-1}}{\Omega}\right) | 0 \rangle = -1
\] (7)
\[
\tau \lambda \langle 0 | \left(1 - \frac{N_1}{\Omega}\right) | 0 \rangle + \mu \rho \langle 0 | \left(1 - \frac{N_{-1}}{\Omega}\right) | 0 \rangle = 0
\]

The pp-SCRPA equations for the present model can be written in the form [1,2]
\[
\begin{pmatrix}
A & B \\
B^* & C
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix}
= \omega
\begin{pmatrix}
U & 0 \\
0 & V
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix}
\] (8)
where
\[
A = \langle 0 | \left[A_1, H, A_1^+\right] | 0 \rangle, \quad B = -\langle 0 | \left[A_1, H, A_{-1}^+\right] | 0 \rangle,
\]
\[
C = \langle 0 | \left[A_{-1}, H, A_{-1}^+\right] | 0 \rangle, \quad U = \langle 0 | \left[A_1, A_1^+\right] | 0 \rangle,
\]
\[
V = \langle 0 | \left[A_{-1}, A_{-1}^+\right] | 0 \rangle
\]
with the usual definition of the symmetrized double commutator
\[
[A, B, C] = \frac{1}{2} ([A, [B, C]] + [[A, B], C]).
\]

Equation (8) has two solutions. We associate the solution of positive norm (normalized to +1) with the addition phonon, \(\lambda_+ = \lambda, \mu_+ = \mu\) and the corresponding eigenfrequency with \(\omega_+ = E_0(A + 2) - E_0(A)\). The negative norm solution (normalized to -1) we associate with the removal phonon \(\lambda_- = \tau, \mu_- = \rho\) and the corresponding eigenfrequency with \(\omega_- = E_0(A) - E_0(A - 2)\). This is the physical meaning of the first two Eqs. (7). The last one expresses the orthogonality of these two solutions.

From Eqs. (7) we get \(\tau\) and \(\rho\) in terms of \(\lambda\) and \(\mu\) and, choosing phases to agree with ref. [1], one has
\[
P^+ = \lambda A_1^+ - \mu A_{-1}^+
\]
\[
R^+ = \left(\frac{\langle 0 | \left(N_{-1} - \Omega\right) | 0 \rangle}{\langle 0 | \Omega - N_1 | 0 \rangle}\right)^{1/2} \mu A_1 - \left(\frac{\langle 0 | \Omega - N_1 | 0 \rangle}{\langle 0 | N_{-1} - \Omega | 0 \rangle}\right)^{1/2} \lambda A_{-1}.
\]
The model Hamiltonian (1) commutes with $S^{(2)}$, $S^{(-1)}$ and $S^{(1)} + S^{(-1)}$, where $S^{(2)} = \frac{1}{2} (S^{(σ)\dagger} S^{(σ)} + S^{(σ)} S^{(σ)}) + S^{(σ)^2}$. In particular, the ground states of even nuclei are defined in the $SU(2) \otimes SU(2)$ irreducible representation $\left(\frac{Ω}{2}, \frac{Ω}{2}\right)$. A basis of states in this subspace is given by

$$| m_1; m_2 \rangle = \left| \frac{Ω}{2} m_1 \right\rangle_1 \otimes \left| \frac{Ω}{2} m_2 \right\rangle_{-1}.$$  \hspace{1cm} (10)

The pp-SCRPA ground state of the $N = 2Ω$ system can therefore be expanded as

$$| 0 \rangle = \sum_{m=0}^{Ω} C_{m;-m} \left| -\frac{Ω}{2} + m, \frac{Ω}{2} - m \right\rangle$$

where $m$ is the number of particle pairs coupled to $J = 0$ in the upper-level.

The condition that $| 0 \rangle$ is the vacuum of the addition phonon, Eq. (5) gives the recursion relation

$$C_{m;-m} = \frac{μ}{λ} C_{m-1;-(m-1)}$$  \hspace{1cm} (11)

which allows for writing the normalized ground state explicitly as

$$| 0 \rangle = \frac{1}{\sqrt{\sum_{m=0}^{Ω} \left( \frac{μ}{λ}\right)^{2m}}} \left( \frac{μ}{λ}\right)^{m} \left| -\frac{Ω}{2} + m, \frac{Ω}{2} - m \right\rangle.$$  \hspace{1cm} (12)

Apparently we have a problem here, since the pp-SCRPA ground state has been determined by just one of Eqs. (5) and we still have the additional condition that $| 0 \rangle$ is also supposed to be the vacuum of the removal phonon. However, the second Eq. (5) gives for the coefficients of $| 0 \rangle$ the condition

$$C_{m;-m} = \frac{\langle 0 | (N_{-1} - Ω) | 0 \rangle \mu}{\langle 0 | Ω - N_1 | 0 \rangle \lambda} C_{m-1;-(m-1)}.$$  \hspace{1cm} (13)

This is consistent with Eq. (11) only if

$$\langle 0 | N_{-1} - Ω | 0 \rangle = \langle 0 | Ω - N_1 | 0 \rangle$$  \hspace{1cm} (14)

and that this is true follows from

4
\[ \langle 0 \mid N_1 + N_{-1} - 2\Omega \mid 0 \rangle = 0 \]

which can be interpreted as saying that the number of particles in the level +1 is equal to the number of holes in the level −1. Note that the above discussion uses the condition \[ N = 2\Omega \] (or \( S_0^{(1)} + S_0^{(-1)} = 0 \)) in an essential way.

Defining the normalized amplitudes

\[ \lambda = \lambda \sqrt{\langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle}, \quad \mu = \mu \sqrt{\langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle}, \]

with \( \lambda^2 - \mu^2 = 1 \), we can write the pp-SCRPA equations as

\[
\begin{pmatrix}
\overline{A} & \overline{B} \\
\overline{B}^* & \overline{C}
\end{pmatrix}
\begin{pmatrix}
\overline{\lambda} \\
\overline{\mu}
\end{pmatrix} = \omega
\begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\begin{pmatrix}
\overline{\lambda} \\
\overline{\mu}
\end{pmatrix}
\]

(15)

where \( \overline{A}, \overline{B} \) and \( \overline{C} \) are now given by Eqs. (11) in terms of the normalized operators \( \overline{A}^+_1, \overline{A}^+_1 \) defined as

\[ \overline{A}^+_1 = \lambda \sqrt{\langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle}, \quad \overline{A}^-_1 = \lambda \sqrt{\langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle} \]

Evaluating the double commutators one obtains

\[
\overline{A} = \epsilon - g \frac{\langle 0 \mid (\Omega - N_1)^2 \mid 0 \rangle}{\langle 0 \mid (\Omega - N_1) \mid 0 \rangle} + g \langle 0 \mid 2\overline{A}^+_1 \overline{A}_1 + \overline{A}^+_1 \overline{A}_1 + \overline{A}^+_1 \overline{A}^+_1 \mid 0 \rangle
\]

(16)

\[
\overline{B} = g \frac{\langle 0 \mid (\Omega - N_1)(\Omega - N_{-1}) \mid 0 \rangle}{\langle 0 \mid (\Omega - N_1) \mid 0 \rangle}
\]

(17)

\[
\overline{C} = \epsilon - g \frac{\langle 0 \mid (\Omega - N_{-1})^2 \mid 0 \rangle}{\langle 0 \mid (\Omega - N_{-1}) \mid 0 \rangle} + g \langle 0 \mid 2\overline{A}^+_1 \overline{A}^-_1 + \overline{A}^+_1 \overline{A}^-_1 + \overline{A}^+_1 \overline{A}^+_1 \mid 0 \rangle.
\]

(18)

In order to calculate the expectation values appearing in these expressions we invert Eqs. (11) to find \( \overline{A}^+_1 = \overline{X}P^+ - \overline{\mu}R \) and \( \overline{A}^-_1 = \overline{\mu}P^+ - \overline{X}R \). From this we then obtain, using the vacuum condition (11), \( \langle 0 \mid \overline{X} \overline{A}^+_1 \mid 0 \rangle = \overline{\mu}^2 \), \( \langle 0 \mid \overline{A}^+_1 \overline{A}_1 \mid 0 \rangle = \overline{X}^2 \) and \( \langle 0 \mid \overline{A}^+_1 \overline{A}_1 \mid 0 \rangle = \overline{X} \overline{\mu} \). The matrices \( \overline{A}, \overline{B} \) and \( \overline{C} \) are thus functions of the pp-RPA amplitudes \( \overline{X} \) and \( \overline{\mu} \), of the one-body densities \( \langle 0 \mid N_1 \mid 0 \rangle, \langle 0 \mid N_{-1} \mid 0 \rangle \) and of the two-body densities \( \langle 0 \mid N_1^2 \mid 0 \rangle, \langle 0 \mid N_1 N_{-1} \mid 0 \rangle \) and \( \langle 0 \mid N_{-1}^2 \mid 0 \rangle \) and \( \langle 0 \mid N_1 N_{-1} \mid 0 \rangle \). Their final expressions are
\[
\begin{align*}
\mathcal{A} &= \epsilon - g \frac{\langle 0 | (\Omega - N_1)^2 | 0 \rangle}{\langle 0 | (\Omega - N_1) | 0 \rangle} + 2g \left( \mu^2 + \lambda \right) \tag{19} \\
\mathcal{B} &= g \frac{\langle 0 | (\Omega - N_1)(\Omega - N_{-1}) | 0 \rangle}{\langle 0 | \Omega - N_1 | 0 \rangle} \tag{20} \\
\mathcal{C} &= \epsilon - g \frac{\langle 0 | (\Omega - N_{-1})^2 | 0 \rangle}{\langle 0 | (\Omega - N_1) | 0 \rangle} + 2g \left( \lambda^2 + \lambda \right) \tag{21}
\end{align*}
\]

Once we have the explicit expression (12) for the correlated ground state \( | 0 \rangle \), we can calculate the one- and two-body densities and solve the non-linear pp-SCRPA equations, Eqs. (15) and (19)-(21), for the pp-RPA amplitudes \( \lambda \) and \( \mu \). Results of such a calculation will be presented further on. Note that in the limit of standard pp-RPA, \( | 0 \rangle \) is replaced by the uncorrelated ground state and Eq. (15) reduces to the ordinary equation
\[
\begin{pmatrix}
\epsilon - g \Omega & -g \Omega \\
-g \Omega & \epsilon + 2g - g \Omega
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix} = \omega
\begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\begin{pmatrix}
\lambda \\
\mu
\end{pmatrix}. \tag{22}
\]

This illustrates the fact that, in practice, solving the SCRPA equations is rather demanding from a computational point of view, and in fact this has not been done so far in realistic cases. Several authors have therefore suggested alternate schemes to derive simpler equations which are more easily amenable to numerical treatment [1], [4]-[7]. In essence, the simplifying hypothesis consists in neglecting the two-body correlations in the pp-SCRPA equations of motion (15). These approximations are generically called renormalized RPA (RRPA). The pp-RRPA simplified version of the ingredients involved in Eqs. (10)-(18) reads
\[
\begin{align*}
\langle 0 | N_1^2 | 0 \rangle & \simeq \langle 0 | N_1 | 0 \rangle^2 + \left( 1 - \frac{\langle 0 | N_1 | 0 \rangle}{2\Omega} \right) \langle 0 | N_1 | 0 \rangle \\
\langle 0 | N_{-1}^2 | 0 \rangle & \simeq \langle 0 | N_{-1} | 0 \rangle^2 + \left( 1 - \frac{\langle 0 | N_{-1} | 0 \rangle}{2\Omega} \right) \langle 0 | N_{-1} | 0 \rangle \\
\langle 0 | N_1 N_{-1} | 0 \rangle & \simeq \langle 0 | N_1 | 0 \rangle \langle 0 | N_{-1} | 0 \rangle \\
\langle 0 | A_1^+ A_1 | 0 \rangle & \simeq \frac{1}{4\Omega^2} \langle 0 | N_1 | 0 \rangle^2 \\
\langle 0 | A_{-1}^+ A_{-1} | 0 \rangle & \simeq \frac{1}{4\Omega^2} \langle 0 | N_{-1} | 0 \rangle^2 \\
\langle 0 | A_1^+ A_{-1} | 0 \rangle & = \langle 0 | A_1^+ A_{-1} | 0 \rangle \simeq 0
\end{align*}
\]

and \( \mathcal{A}, \mathcal{B} \) and \( \mathcal{C} \) become respectively
\[
\bar{A} \simeq \epsilon - g \frac{\langle 0 \mid N_1 \mid 0 \rangle}{\Omega} - g\Omega \langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle
\]
\[
\bar{B} \simeq - g\Omega \langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle
\]
\[
\bar{C} \simeq \epsilon + 2g - g \frac{\langle 0 \mid N_1 \mid 0 \rangle}{\Omega} - g\Omega \langle 0 \mid (1 - \frac{N_1}{\Omega}) \mid 0 \rangle.
\]

The pp-RRPA equation is thus analogous to the pp-RPA equation (22), except that now \( g \) is renormalized by \( 1 - \frac{\langle 0 \mid N_1 \mid 0 \rangle}{\Omega} \) and the particle and hole energies are shifted respectively by \( -g \frac{\langle 0 \mid N_1 \mid 0 \rangle}{2\Omega} \) and \( g \frac{\langle 0 \mid N_1 \mid 0 \rangle}{2\Omega} \). In realistic cases [4] we have to make further approximations in the calculation of the one-body densities to avoid having to solve the vacuum condition, Eq. (5). For the calculations reported below we calculate \( \langle 0 \mid N_1 \mid 0 \rangle \) using the expression Eq. (12) for the phonon vacuum \( |0\rangle \). The difference between our pp-SCRPA and pp-RRPA results are thus solely due to neglecting two-body correlations in the pp-SCRPA equations of motion.

We next present numerical results obtained for the two-level pairing model. They correspond to a case in which twenty particles distribute themselves in two \( \Omega = 10 \) levels separated by \( \epsilon = 2 \). In Fig. 1 we plot the energies \( \omega_+ \) and \( \omega_- \) as functions of the coupling strength \( g \). The pp-RPA collapses at \( g_{\text{crit}} = \frac{\epsilon}{2\Omega - 1} \), at which point the corresponding energies become equal, \( \omega_+ = \omega_- = -g_{\text{crit}} \). Since \( \omega_+ \) and \( \omega_- \) have the physical interpretation of (minus) two-nucleon removal energies respectively from the closed-shell-plus-two and from the closed-shell nuclei, this equality signals the breakdown of shell structure. On the other hand, neither the SCRPA nor the RRPA collapse, but instead follow closely the exact values in the neighborhood of the phase transition point. As \( g \) increases, however, the agreement with the exact energies deteriorates. In particular, the pp-SCRPA, and even more markedly the pp-RRPA energies approach values that differ from the exact strong coupling limits \( \omega_+ \to 0 \) and \( \omega_- \to -2g \) for large values of \( g \). In Fig. 2 we plot the occupation of the upper level in the ground state of the closed shell nuclei. Again we see that in the neighborhood of the phase transition point both approximations yield values close to the exact ones, whereas the pp-RPA value diverges. However, when \( g \) increases, the pp-SCRPA value lags consid-
erably behind the exact one, which agrees well with the pp-RRPA result almost up to the
strong coupling limit of \( \langle 0 | N_1 | 0 \rangle \rightarrow \Omega \). Fig. 3 shows, also as a function of \( g \), the square
of the two-particle transfer matrix element to the upper level:

\[
| \langle N + 2 | A_1^+ | N \rangle |^2 = \lambda^2 \left( 1 - \frac{\langle 0 | N_1 | 0 \rangle}{\Omega} \Omega \right).
\]

We find again the same behavior, with agreement near the phase transition point and dis-
agreement when \( g \) increases approaching the strong coupling limit \( \frac{\Omega + 1}{4} \).

In conclusion, we find that correlations introduced by the pp-SCRPA or by the pp-
RRPA allow for following the system across of the phase transition point associated with the
collapse of the ordinary RPA. However, it should be stressed that the pp-RRPA, which
is in fact an approximate treatment of the full pp-SCRPA performs even better than the
full theory for some observables. The pp-RRPA values for the occupancy of the upper level
agree with the exact values all the way up to the strong coupling regime, and pp-RRPA
values for the two-particle transfer matrix elements also perform somewhat better than the
pp-SCPRA values. Only for the excitation energies are the pp-SCRPA results better than
the corresponding pp-RRPA results. A possible perspective concerning these results could
be formed by recalling the well known fact that the standard RPA tends to overestimate
collectivity. In the present schematic model, on the other hand, the full pp-SCRPA seems
to underestimate it, whereas the omission of two-body correlations in the pp-RRPA gives
improved occupancy and transfer results. In general, when \( g \) increases towards the strong
coupling limit, pp-SCRPA and pp-RRPA correlations are not adequate to reproduce exact
values, indicating that we should consider the system as a pairing-deformed (superfluid)
system. This is consistent with the fact that the pair-coupling model is asymptotically
exact in the strong coupling limit.
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Figure captions

**Figure 1.** Excitation energies $\omega_+$ (upper points and curves) and $\omega_-$ as functions of the coupling strength $g$ for the two-level pairing model with $\epsilon = 2$, $\Omega = 10$ and $N = 20$.

**Figure 2.** Number of particles in the upper level for the ground state of the two-level pairing model. Same parameters as for Fig. 1.

**Figure 3.** Absolute square of the two particle addition matrix element to the ground state of the two-level pairing model. Same parameters as for Fig. 1.
de Passos et al.: Self Consistent... Fig. 1

![Graph showing energy (e/2) as a function of g with various approximations: RPA, RRPA, SCRPA, and Exact.](image_url)
de Passos et al.: Self Consistent... Fig. 3