Quasiparticle Random Phase Approximation with an optimal Ground State

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Abstract

A new Quasiparticle Random Phase Approximation approach is presented. The corresponding ground state is variationally determined and exhibits a minimum energy. New solutions for the ground state, some with spontaneously broken symmetry, of a solvable Hamiltonian are found. A non-iterative procedure to solve the non-linear QRPA equations is used and thus all possible solutions are found. These are compared with the exact results as well as with the solutions provided by other approaches.

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The random phase approximation (RPA) and its quasiparticle (qp) generalization (QRPA) are powerful tools for describing the collective degrees of freedom of many-fermion systems in various branches of physics like nuclear physics, solid state, plasma physics, atomic clusters.

Usually the RPA and QRPA are presented by making use of boson expansion techniques. If the one body transition operator is expressed linearly in bosons, the many body Hamiltonian with the two body interaction included becomes a quadratic polynomial in bosons
describing harmonic motion of the selected degree of freedom. For the evident reasons the resulting approach is called a quasiboson approximation (QBA). The main drawback of this approximation scheme is that the QRPA (henceforth called as the standard QRPA) exhibits a collapse for a critical value of the strength of the attractive particle-particle force, i.e. the lowest eigenvalue becomes imaginary. In the case of the many body Hamiltonians used for the description of the transition rates of single and double beta decays the realistic proton-neutron force is expected to be close to its critical value. Due to this feature many theoretical works have been devoted to improving the standard QRPA by removing the ground state instabilities [1–11].

It is a common practice to investigate the validity of different approximation schemes within exactly solvable models, which describe the gross properties of the fermion many-body systems [1–5,7,8,14,15]. Recently, it has been shown that the QRPA does not develop any collapse and is in good agreement with exact results, if the Pauli exclusion principle (PEP) is consistently implemented in this approach [1]. However, there is another group of studies saying that the collapse of the QRPA indicates a phase transition, i.e., a rearrangement of the nuclear ground state [2,3,5,15]. In Ref. [2], in order to avoid the QRPA collapse, a new static ground state is defined by means of a semiclassical approach. A new collective mode, for a many-body system with proton-neutron pairing interaction, has been found beyond the point where the QRPA breaks down. This new solution requires the restoration of the PEP, objective that can be touched through a boson expansion technique. We note that the main difference between the semiclassical and the QRPA solutions consists in the description of the ground state.

In this letter we point out new features for a many fermion system by improving the QRPA description of the ground state. A new ansatz for the QRPA wave functions is proposed, which allows us to minimize the QRPA ground state energy and, at the same time, to diagonalize the QRPA equations. The method proposed will be conventionally called as QRPA with an optimal ground state. One hopes that the present approach is a suitable tool for a realistic treatment of many body systems. It is worth mentioning that
the correct description of the ground state of a many-body system is a steady interesting subject which has attracted the efforts of many groups [3,10,13].

For the sake of simplicity we consider the proton-neutron monopole Lipkin Hamiltonian which is exactly solvable [1,2,4,8,10]

\[
H_F = \epsilon (\hat{N}_p + \hat{N}_n) + \lambda_1 A^\dagger A + \lambda_2 (A^\dagger A^\dagger + AA),
\]

where \(\hat{N}_p\) (\(\hat{N}_n\)) and \(A^\dagger\) are the proton (neutron) number and proton-neutron pair operators, respectively [2]. The spaces of single particle states associated to the proton and neutron systems, respectively, are restricted to a single j-shell. The model Hamiltonian can be obtained from a Hamiltonian which in the particle representation, consists of pairing interaction for alike nucleons, and a monopole-monopole proton-neutron two body interaction of particle–hole and particle–particle types [1,2,8,10]. For the single j-shell, considered here, one obtains:

\[
\begin{align*}
\lambda_1 &= 4\Omega [\chi (u_p^2 v_n^2 + v_p^2 u_n^2) - \kappa (u_p^2 u_n^2 + v_p^2 v_n^2)], \\
\lambda_2 &= 4\Omega (\chi + \kappa) u_p v_p u_n v_n \quad \Omega = j + \frac{1}{2},
\end{align*}
\]

where \(u_p, v_p\) and \(u_n, v_n\) are the coefficients of the Bogoliubov-Valatin transformation for protons and neutrons, respectively. The parameters \(\chi\) and \(\kappa\) are the strengths of particle–hole and particle–particle proton-neutron interactions, respectively. We consider the boson mapping of the model Hamiltonian, following the Marumori recipe, i.e. the boson representation \(H_B\) is chosen so that its matrix elements (m.e.) between boson states are equal to the m.e. of \(H_F\) between the corresponding many fermion states [10]. The final result is [3,10]:

\[
H_B = \alpha_{11} B^+ B + \alpha_{02} (B^+ B^+ + B B) + \alpha_{22} B^+ B^+ B B
\]

\[
+ \alpha_{13} (B^+ B B B + B^+ B^+ B^+ B),
\]

with

\[
\begin{align*}
\alpha_{11} &= (2\epsilon + \lambda_1), \quad \alpha_{02} = \lambda_2 \sqrt{(1 - \frac{1}{2\Omega})}, \quad \alpha_{22} = -\frac{\lambda_1}{2\Omega}, \\
\alpha_{13} &= \lambda_2 \left[ \sqrt{(1 - \frac{1}{2\Omega}) (1 - \frac{1}{\Omega})} - \sqrt{(1 - \frac{1}{2\Omega})} \right].
\end{align*}
\]
The operator $B^\dagger$ is a creation boson operator, while $B$ is its hermitian conjugate operator.

The QRPA treatment of $H_F$ is determined by a RPA-like procedure applied to $H_B$. This consists in determining the phonon operator

$$Q^\dagger = X(B^\dagger + t) - Y(B + t^\dagger), \quad Q = (Q^\dagger)^\dagger$$

as well as the vacuum state $|rpa\rangle$ and the one phonon state $|Q\rangle$

$$|Q\rangle = Q^\dagger |rpa\rangle, \quad Q |rpa\rangle > 0.$$  

From the set of solutions depending on the parameters $(t, t^\dagger)$ one depicts that one for which the state $|rpa\rangle$ has a minimum energy. In contradistinction to the usual QRPA, here the phonon operator involves a C number which results in having a nonvanishing expected value for $Q$, in the state $|rpa\rangle$, i.e. a ”deformed ground state”.

The ansatz for the QRPA ground state $|rpa\rangle$, defined as vacuum state for $Q$ [see Eq. (6)], is taken as follows:

$$|rpa\rangle = e^{t^*B - tB^\dagger} e^{zB^\dagger B^\dagger - z^*BB} |\rangle.$$  

Here $|\rangle$ denotes the vacuum state for the boson operator $B$, which might be the mapping of the uncorrelated BCS ground state. $t, z$ are complex parameters: $t = re^{i\theta}$, $z = pe^{i\phi}$. The ansatz (7) obeys the second eq. (6) provided the following equation holds:

$$F(r, \theta, \rho, \phi) \equiv \sinh (2\rho) \frac{Y}{X} e^{-i\phi} \cosh (2\rho) = 0,$$

where the function $F$ depends implicitly on $r$ and $\theta$ variables, by means of $X$ and $Y$ amplitudes. It is worth to note that the functions describing the limiting cases $(\rho, \phi) = (0, 0)$ and $(r, \theta) = (0, 0)$ were earlier considered [2] as trial states in a time dependent formalism:

$$|rpa\rangle = e^{-r^2} e^{-tB^\dagger}, \quad |rpa\rangle = \frac{1}{\sqrt{\cosh (2\rho)}} e^{dB^\dagger B^\dagger} |\rangle.$$  

with $d = e^{i\phi} \tanh (2\rho)/2$. Due to this feature one expects that the present trial function accounts for new correlations in the ground state. The phonon amplitudes $X, Y$ satisfy the QRPA equations
\[ AX + BY = E_{rpa}UX, \]
\[ B^*X + AY = -E_{rpa}UY, \]

(10)

where the RPA energy \( E_{rpa} \) is the excitation energy for the RPA state \(|Q\rangle\), i.e. \( E_{rpa} = E_1 - E_{g.s.} \). The RPA matrices \( A, B, U \), are determined in the usual manner and have the expressions:

\[
A \equiv < rpa | [B, H_B B^†] | rpa > \\
= a_{11} + 4a_{22}v^2 + 6a_{13}uv \cos \phi + r^2[4a_{22} + 6a_{13} \cos (2\theta)],
\]

(11)

\[
B \equiv < rpa | [B, H_B | rpa > \\
= 2a_{02} + 2a_{22}uv [\cos \phi + i \sin \phi] + 6a_{13}v^2 + r^2(2a_{22}[\cos (2\theta) + i \sin (2\theta)] + 6a_{13}),
\]

\[ U \equiv < rpa | [B, B^†] | rpa >= 1. \]

(12)

The double commutators are defined as \( 2[A, B, C] = [A, [B, C]] + [[A, B], C] \). Also, the notations \( u = \cosh (2\rho) \) and \( v = \sinh (2\rho) \) have been newly introduced. The matrix \( A \) is real, while \( B \) might be a complex number. In this letter we consider only situations where the solutions for the \( X, Y \) amplitudes are real. The arguments which support our choice is that the resulting phonon state should be the image, through the boson mapping, of a state in the fermionic space. However the amplitudes of the eigenstates of \( H_F \), in the basis \( \{ (A^\dagger)^n \} \), are real numbers. Thus the possible solutions for \( \theta \) and \( \phi \) are \( \theta = n\pi/2 \) and \( \phi = n\pi \) (\( n = 1, 2, \ldots \)). The additional parameters \( r \) and \( \theta \) entering the QRPA eigenvalue problem will be fixed by requiring that the expectation value of \( H_B \) in the RPA ground state reaches its minimum value \( E_{g.s.} \), in the space of these parameters. One finds

\[
H(r) \equiv < rpa | H_B | rpa >= C_0 + C_2r^2 + C_4r^4,
\]

(13)

\[
C_0 = a_{11}v^2 + 2a_{02}uv \cos \phi + a_{22}[u^2v^2 + 2v^4] \\
+ 6a_{13}uv^3 \cos \phi,
\]

\[
C_2 = a_{11} + 2a_{02} \cos (2\theta) + a_{22}[4v^2 + 2uv \cos (2\theta + \phi)] \\
+ 6a_{13}[uv \cos \phi + v^2 \cos (2\theta)],
\]
Several minima for $E_{g.s.}$ are to be mentioned:

(a) $r = 0$ and $\theta = \text{anything}$. This solution corresponds to the RPA ground state given by the second Eq. (9).

(b) $r = \sqrt{-C_2/2C_4}$, $\theta = 0$,

(c) $r = \sqrt{-C_2/2C_4}$, $\theta = \pi/2$,

(d) $r = \sqrt{-C_2/2C_4}$, $\theta \neq n\pi/2$ ($n=1,2,3...$).

The case d) yields a complex $B$ and therefore is not considered here. The solutions b), c) and d) are specific for the ansatz [7]. If only the quadratic terms in bosons are considered in $H_B$ (i.e., $a_{22}, a_{13} = 0$) then only the solution a) survives. The equations (10), (8) and one of a),b),c) are to be simultaneously solved. This non-linear problem is usually treated iteratively. However, this procedure does not guarantees that all solutions of this system of equations, are found. The procedure used in the present paper is as follows. First, we insert the solution for $r$ ($r = 0$ or $r^2 = -C_2/2C_4$) in the expressions defining the matrices $A$ and $B$ by Eqs.(11), (12). Determine the ratio $Y/X$ from any of equations (10) and insert the result in Eq. (8). Then Eq. (8) provides $\rho$ which is to be inserted in the equations for the RPA matrices. With the matrices $A, B$ fully known one determines the QRPA eigenvalue and eigenvectors, by solving the equations (10). This procedure is repeated for each minimum of $E_{g.s.}$ [the cases a), b) and c) mentioned above]. We note that solutions with $(\rho, \phi)$ and $(-\rho, \phi \pm \pi)$ are degenerate.

The numerical application is performed for a system of 4 protons and 6 neutrons moving in a $j = \frac{9}{2}$ shell. The strength parameters defining the model Hamiltonian are $\epsilon = 1 MeV$ while the two body interaction strengths $\kappa$ and $\chi$ are re-scaled as in Refs. [4,5]: $\kappa \rightarrow \kappa' \equiv 2\Omega \kappa$, $\chi \rightarrow \chi' \equiv 2\Omega \chi$. We adopt $\chi' = 0.5$ while $\kappa'$ is considered as a free parameter in the interval $(0,3) MeV$. In Table I we present the results for the QRPA and ground state energies corresponding to three values of $\kappa'$. If $\kappa' = 0.5$ there are only two solutions of type a), associated with the ansatz [4] (second equation). The solution a2) is similar to that obtained in [4] within the EPP QRPA formalism. The solution a1), with small QRPA
energy and a very large value of $E_{g.s}$, has not been seen before. Its finding is a merit of the adopted numerical procedure. For $\kappa' = 1.5, 2.5$ one finds solutions of type c) which are specific for the new ansatz of the RPA wave functions.

In Fig. 1 we present the potential energy surface as function of $r$ for the solutions a2), c1), c2) and c3), assuming $\kappa' = 2.5$. Note that for the solution c) $H(r)$ has two minima, at $r = \pm \sqrt{-C_2/(2C_4)}$.

The meaning of the negative $r$ consists of that the result for energy is not affected if we change the ansatz by replacing $t$ with $-t$.

In Fig. 2 the values of $\rho$ corresponding to different solutions are presented. Within the QBA, i.e. the quadratic bosonic Hamiltonian is considered, the value of $\rho$ is increasing rapidly in the vicinity of the QRPA collapse. The solution a2) does exist within the whole interval of $\kappa'$. This is caused by that the PEP principle included in the higher order bosonic expansion Hamiltonian prevents the collapse of the QRPA [1]. The solution a1) was found within the range $0.0 \leq \kappa' \leq 1.29$ and continues further as c1) solution. The solutions c2) and c3) start with $\kappa' = 1.53$ where they have equal values. For large value of $\kappa'$ the solution c2) is close to a2). It is worthwhile to notice that in the case of c3), with the lowest value of $E_{g.s}$ and large $\kappa'$ (see Table I), the corresponding values of $\rho$ are rather small. One may say that the corellations in the ground state are mainly induced by the "deformation" of the system, i.e. the stationary value of $r$. For $\kappa' > 2$, $\rho$ is slightly negative. This branch is obtained by shifting the phase $\phi$ with $\pi$ which is equivalent to changing the sign of $\rho$ but keeping $\phi$ unchanged.

In Fig. 3 we plotted the ground state energy $E_{g.s}$, the QRPA energy $E_{rpa}$ and the first excitation energy $E_1$ obtained by the standard QRPA, QRPA with an optimal ground state and by diagonalizing $H_F$, as function of $\kappa'$. Only solutions with low ground state energy are drawn. One remarks that by including the higher order boson terms in the Hamiltonian $H_B$ and considering the standard ansatz for $|rpa\rangle$ (see the second Eq. (9)) [solution a2)], there is no collapse of the QRPA solution. This solution coincides well with that provided by the EPP QRPA formalism [1]. However, for large values of $\kappa'$ ($\kappa' \geq 1.6$) this solution
approximates poorly the exact result for $E_{g.s}$. On other hand the new solution c3) is in an excellent agreement with the exact $E_{g.s}$ for this range of $\kappa'$. In fact, the exact result for $E_{g.s}$ is very well described by matching the approaches a2) and c3). Despite the fact the c3) approach simulates excellently the exact result for the ground state energy, the two treatments predict QRPA energies which deviate from each other by a large amount.

In summary, a new ansatz for the QRPA wave functions was proposed. The additional new factor in this ansatz depends on a complex parameter $t$ which is fixed by requiring that the corresponding expectation value of the model Hamiltonian $H_B$ is minimum. The present paper constitute the first attempt in the literature, to determine the QRPA ground state (the vacuum state for the Q operator) as a solution of a variational equation. The numerical application shows clearly new effects caused by the presence of higher order boson terms in $H_B$ and by the complex structure of the ansatz for the state $|\text{rpa}\rangle$. Both features mentioned above prevent the QRPA to collapse. Several solutions are found in the interval of the interaction strength $\kappa'$ beyond the critical value. Each solution corresponds to a certain type of minimum in the $(r, \theta)$ variable and by that to a certain symmetry of the wave function. One may say that the present approach accounts, in an unified fashion, for the complementary features described by the EPP QRPA and the semiclassical formalism, which defines a new ground state for those $\kappa'$ where the standard QRPA fails.
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TABLE I. The predicted QRPA \( (E_{rpa}) \) and ground state \( (E_{g.s.}) \) energies for \( \kappa' = 0.5, 1.5 \) and \( 2.5, \chi' = 0.5 \) and \( j = 9/2 \). The parameters determining the RPA wave functions and the ground state energy are listed as well.

| Type | \( \rho \) | \( \phi \) | \( r^2 \) | \( 2\theta \) | \( C_0 \) | \( C_2 \) | \( C_4 \) | \( E_{g.s.} \) | \( E_{rpa} \) |
|------|----------|----------|---------|----------|--------|--------|--------|---------|---------|
|      |          |          |         |          |        |        |        | [MeV]   | [MeV]   |
| \( \kappa' = 0.5, E_{g.s.}^{exact} = -0.104 \text{ MeV} \) |
| a1   | 0.757    | 0        | 0       | -        | 7.001  | 0.002  | -0.100 | 7.001   | 0.046   |
| a2   | 0.114    | \( \pi \) | 0       | -        | -0.104 | 3.004  | -0.100 | -0.104  | 1.906   |
| \( \kappa' = 1.5, E_{g.s.}^{exact} = -0.823 \text{ MeV} \) |
| a2   | 0.308    | \( \pi \) | 0       | -        | -0.679 | 3.120  | -0.100 | -0.679  | 0.908   |
| c1   | 0.755    | 0        | 0.438   | \( \pi \) | 7.004  | -0.249 | 0.284  | 6.950   | 0.024   |
| \( \kappa' = 2.5, E_{g.s.}^{exact} = -3.638 \text{ MeV} \) |
| a2   | 0.400    | \( \pi \) | 0       | -        | -1.841 | 3.344  | -0.100 | -1.841  | 0.675   |
| c1   | 0.780    | 0        | 1.326   | \( \pi \) | 6.834  | -1.264 | 0.476  | 5.996   | 0.112   |
| c2   | 0.384    | \( \pi \) | 0.081   | \( \pi \) | -1.832 | -0.077 | 0.476  | -1.835  | 0.719   |
| c3   | 0.041    | 0        | 2.838   | \( \pi \) | 0.230  | -2.705 | 0.476  | -3.609  | 4.580   |
FIG. 1. Expectation value of the Hamiltonian $H_B$ as a function of the parameter $r$. The solutions labeled by a) and c) are those presented in the text below Eq. (14). The adopted values of $\chi'$ and $\kappa'$ are 0.5 and 2.5, respectively.
FIG. 2. The parameter $\rho$ of the RPA wave function [see Eqs. (7) and (9)] associated with the solutions a) and c) is plotted versus $\kappa'$. 
FIG. 3. Energies of the ground state $E_{g.s.}$, of the first excited state $E_1$ and the excitation energies $E_{rpa}(= E_1 - E_{g.s.})$ provided by diagonalizing $H_F$, by the standard QRPA and by the QRPA with an optimal ground state [a1), c2) and c3)], respectively, are plotted as function of $\kappa'$. 