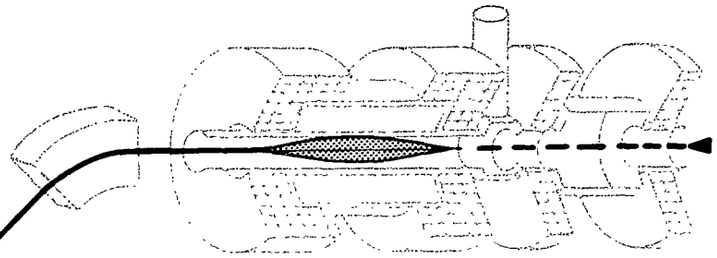

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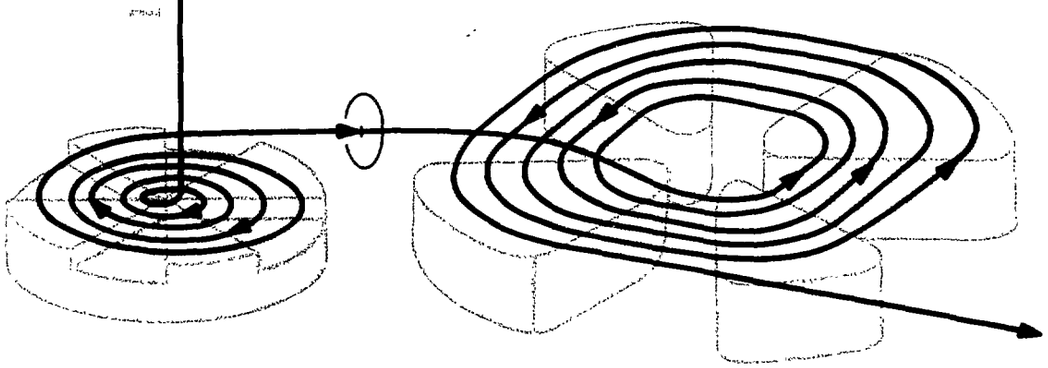

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Abstract

The recently derived Variational Random Phase Approximation is examined using the anharmonic oscillator model. Special attention is paid to the ground state RPA wave function and the convergence of the proposed truncation scheme to obtain the diagonal density matrix. Comparison with the standard Coupled Cluster method is made.

1 Introduction

In a recent paper [1] we presented a generalization of the Random Phase Approximation (RPA) which is in principle of Ritz variational character. We therefore want to call it hitherto Variational Random Phase Approximation (VRPA). It essentially consists in working with the true RPA ground state when setting up the RPA matrix rather than with the Hartree-Fock ground state [2]. In [1] we applied our theory to the Lipkin model [3] which is a well known testing ground for many body theories. The results were very encouraging and VRPA may represent an interesting variant to other well performing modern approaches to the many body problem such as Jastrow theory or the Coupled Cluster method (CCM). The appeal of VRPA lies in such features as its variational character and its applicability to finite temperature systems [1]. In many respects the anharmonic oscillator (AHO) represents a very stringent test of many body theories. An extensive study for this model case has recently been performed by Bishop and Flynn using the CCM technique [4]. We here therefore wanted to apply the VRPA to the AHO and compare our results to the ones obtained in [4].

Since the boson case represents its own specificities we will again be quite explicit in our formalism. For brevity we refrain from treating the most general case and thus rather give the formulas as they correspond to the model case only.

2 The anharmonic oscillator and the VRPA

The hamiltonian we will be using is of the form

$$H = \frac{1}{2}x^2 + \frac{1}{2}x^2 + \lambda x^4 \tag{1}$$

We will not treat here the asymmetric AHO nor the symmetric AHO with double well structure. We think that for these cases our theory will have to be specifically adapted and studies in this direction are under way.

With $x = \frac{(a^\dagger + a)}{\sqrt{2}}$ and $p = i\frac{(a^\dagger - a)}{\sqrt{2}}$ one transforms (1) into

$$H = \frac{1}{2} + a^\dagger a + \lambda(a^\dagger + a)^4 \tag{2}$$

Where $a^\dagger$, a are the usual boson creation and annihilation operators. Since the above hamiltonian is boson number non-conserving and in order to optimize the basis it is useful to perform a Bogoliubov transformation among the $a^\dagger$, a :

$$\begin{aligned} b &= \frac{a - ta^\dagger}{\sqrt{1-t^2}} \\ b^\dagger &= \frac{a^\dagger - ta}{\sqrt{1-t^2}} \end{aligned} \tag{3}$$

and to express the Hamiltonian in the new operators (we follow the notation of ref. [4]) :

$$H = h_{00}+h_{11}b^\dagger b+h_{20}(b^\dagger b^\dagger+bb)+h_{22}b^\dagger b^\dagger bb+h_{31}(b^\dagger b^\dagger b^\dagger b+h.c.)+h_{40}(b^\dagger b^\dagger b^\dagger b^\dagger+h.c.) \quad (4)$$

with

$$\begin{aligned} h_{00} &= \frac{1+w^2}{4w}+\frac{\chi}{2} \\ h_{11} &= \frac{1+w^2}{2w}+2\chi \\ h_{20} &= \frac{1-w^2}{4w}+\chi \\ h_{22} &= \chi \\ h_{31} &= \frac{\lambda}{w^2} \\ h_{40} &= \frac{\lambda}{4w^2} \end{aligned} \quad (5)$$

where $\chi = \frac{3\lambda}{2w^2}$ and $w = \frac{1-t}{1+t}$

Our variational ansatz is given by the quasiparticle RPA [2] :

$$|\nu >= Q^\dagger|RPA > \quad (6)$$

with

$$\begin{aligned} Q^\dagger &= \frac{1}{\sqrt{2}}(\lambda b^\dagger b^\dagger - \mu bb) \\ Q &= \frac{1}{\sqrt{2}}(\lambda bb - \mu b^\dagger b^\dagger) \end{aligned} \quad (7)$$

with the normalization condition $\lambda^2 - \mu^2 = 1$.
The correlated RPA gound state is as usual defined by the implicit relation :

$$Q|RPA >= 0 \quad (8)$$

The variational principle then reads

$$\delta < \nu|H - E_\nu|\nu >= 0 \quad (9)$$

With (6) and (8) this leads in the usual way [2] to the following secular equation :

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix}\begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \omega \begin{pmatrix} \lambda \\ \mu \end{pmatrix} \quad (10)$$

with :

$$\begin{aligned} A &= \frac{< RPA|[bb,[H,b^\dagger b^\dagger]]|RPA >}{< RPA|[bb,b^\dagger b^\dagger]|RPA >} \\ B &= \frac{< RPA|[b^\dagger b^\dagger,[H,b^\dagger b^\dagger]]|RPA >}{< RPA|[bb,b^\dagger b^\dagger]|RPA >} \end{aligned} \quad (11)$$

As shown in [1] we have in addition to (10) a generalised mean field equation with inherent coupling to the RPA amplitudes λ, μ and which follows from minimizing the ground state energy.

$$< RPA|[H, Q^\dagger]|RPA >=< RPA|[H, Q]|RPA >=< RPA|[H, b^\dagger b^\dagger]|RPA >= 0 \quad (12)$$

The mean values in (11) and(12) are most readily evaluated in inverting (7)

$$\begin{aligned} b^\dagger b^\dagger &= \sqrt{2}(\lambda Q^\dagger + \mu Q) \\ b\, b &= \sqrt{2}(\lambda Q + \mu Q^\dagger) \end{aligned} \quad (13)$$

and using (8) ; this leads to

$$\begin{aligned} < b^\dagger b^\dagger b^\dagger b^\dagger > &= < b\, b\, b\, b >= 2\lambda\mu(1+W) \\ < b^\dagger b^\dagger b^\dagger b > &= < b^\dagger b\, b\, b >= 0 \\ < b^\dagger b^\dagger b\, b > &= 2\mu^2(1+W) \\ < b\, b\, b^\dagger b^\dagger > &= 2\lambda^2(1+W) \end{aligned} \quad (14)$$

Where W is related to the single particle density by

$$W = 2 < b^\dagger b > \quad (15)$$

with (11) and (14) we then easily find for the elements of the RPA matrix in (10) :

$$\begin{aligned} A &= \frac{1}{1+W}[2h_{11} + 2h_{22} + (2h_{11} + 8h_{22})W + 24h_{22}\mu^2(1+W) + 16h_{40}\lambda\mu(1+W)] \\ B &= \frac{1}{1+W}[12h_{40}W + (12h_{40} + 8h_{22}\lambda\mu + 48h_{40}\mu^2)(1+W)] \end{aligned} \quad (16)$$

The mean field equation (12) reads :

$$2h_{20} + (2h_{20} + 3h_{31})W + 12h_{31}\mu^2(1+W) + 4h_{31}\lambda\mu(1+W) = 0 \quad (17)$$

The RPA equations (10) are so far not closed because A and B of (16) contain the density via the constant W defined in (15). Unfortunatly it is not completly trivial to express W as a function of the RPA amplitudes λ and μ. We encountered the same problem in our study on the fermionic VRPA in ref. [1]. We there proposed two different ways to solve this difficulty : either it is possible in specific cases to construct explicitly the ground state satisfying (8) or one has to evaluate W perturbatively using the definite truncation scheme proposed in [1].
As for the case of the Lipkin model [1] we can study both methods here. Indeed we obtain for the normalized RPA vacuum :

$$|RPA >= \frac{1}{\mathcal{N}} \sum_{l=0}^{\infty} \alpha_l \left(\frac{\mu}{\lambda}\right)^l b^{\dagger 4l}|0 > \quad (18)$$

where $|0>$ is the vacuum of the annihilation operator b and the α_l's are obtained from a recursion formula :

$$\alpha_l = \frac{\alpha_{l-1}}{4l(4l-1)} \tag{19}$$

The correctness of (18) can be checked by direct insertion into (8). The norm and the density can be expressed as follows :

$$\mathcal{N}^2 = \sum_{l=0}^{\infty} \alpha_l^2 \left(\frac{\mu}{\lambda}\right)^{2l} (4l)! \tag{20}$$

$$< b^\dagger b > = \frac{1}{\mathcal{N}} \sum_{l=0}^{\infty} \alpha_l^2 \left(\frac{\mu}{\lambda}\right)^{2l} 4l(4l)! \tag{21}$$

With (21), the VRPA equations (10) and (12) together with the expression (16) for the elements A and B form now a complete set of equations with the only unknowns λ and μ.
Solving these equations is equivalent to solving the Raleigh-Ritz variational problem (9) with the ansatz (6) assuring that we will get an upper bound for the groud state energy :

$$E_0 =< RPA|H|RPA >= h_{00} + \frac{1}{2}h_{11}W + 2h_{22}\mu^2(1+W) + 4h_{40}\lambda\mu(1+W) \tag{22}$$

However in more general cases it may not be very easy to calculate the ground sate wave function explicitly. We therefore proposed in [1] a truncation scheme for the determination of the diagonal density. In the study of the Lipkin model [1] this truncation scheme converged very rapidly . We therefore want to study it also in the present case. Our starting point is the identity :

$$< b^\dagger b\, b^\dagger b >=< b^\dagger b > + < b^\dagger b^\dagger b\, b >= \frac{W}{2} + 2\mu^2(1+W) \tag{23}$$

The lhs of (23) can also be evaluated in inserting a complete set of (unnormalized) multiphonon RPA states :

$$< b^\dagger b\, b^\dagger b >= \sum_{l=0}^{\infty} \frac{| < b^\dagger b\, Q^{\dagger 2l} > |^2}{< Q^{2l} Q^{\dagger 2l} >} \tag{24}$$

The proposed truncation takes into account up to two phonon states ($l=0$ and $l=1$) and with the above techniques for the evaluation of matrix elements (see (14)) we obtain

$$< b^\dagger b\, b^\dagger b > \cong \frac{W^2}{4} + \frac{16\mu^2(1+\mu^2)(1+W)^2}{(6+24\mu^2)+(12+24\mu^2)W} \tag{25}$$

Where the first term on the rhs corresponds to $l=0$ and the second to $l=1$. Equating (23) and (25) yields an equation for W in tems of λ and μ and again the system of equations is closed. This terminates the formal aspects of the theory and we now pass to the numerical analysis.

3 Numerical results and discussion

The VRPA equations (10) can be solved by iteration in making a first guess for λ and μ in the set up of the matrix elements A and B. From the diagonalization we obtain new λ and μ. These are reinserted into A and B and so on until convergence is achieved. The matrix elements A and B are calculated in two ways: once exactly using (21) and once using the truncation scheme (25) for the determination of W. The corresponding ground state energies will be denoted E(RPA) and E(ARPA) respectively. They are represented in Table 1 together with the exact energies (from [4]) for various values of the interaction strengh. We also give in the table some results obtained by Bishop and Flynn [4] from the Coupled Cluster method. It is not completly unambiguos to which SUB(n) approximation of the CCM results we must compare ours. In principle only one and two body density matrices appear in our theory so one is tempted to take SUB(2) as the CCM partner; however for the calculation of the approximate W (eq. (24)) we also used a four body correlation, so probably it is fair to compare to SUB(4). For a more complete comparison we also included the results from SUB(8) into Table 1.
As we can see from Table 1 the results E(SUB(4)) when available and E(RPA) are extremly close to one another, apparently for all values of the coupling constant. We also see that the truncation scheme (25) works very well. The fact that the approximate values E(ARPA) are closer to the exact ones throughout is of course an accident. They also stay consistently above the exact values and thus E(ARPA) is still an upper bound in this example but it may of course be an accident (it was, however, the case of for the Lipkin model [1]). In any case we have no proof that the truncation scheme (24) does not violate the upper bound property of the Ritz variational procedure. On the other hand CCM is non variational from the outset. This manifests itself in the E(SUB(8)) values which lie below the exact ones. In Table 2 we make a convergence study of the truncation scheme (24)and (25). We present the values of W for three different cases. W(RPA) means the values obtained from (21), W(ARPA0) means the truncation at zeroth order and W(ARPA2) means our present truncation at the two phonon level ($l = 1$). We see that the convergence of the truncation is extremly rapid and the progression from $l = 0$ to $l = 1$ is very important.
In conclusion we may say that the variational RPA theory yields, for the anharmonic oscillator, ground state energies which are comparable to the ones obtained with the Coupled Cluster method [4].
We have restricted our investigation to the parity conserving phase because we think that before applying the VRPA to the double well oscillator we should incorporate important modifications to our theory. For instance projection techniques like the one proposed in [5] may be fruitful in this respect. Also the study of excited states needs further investigations. Studies on these subjects are in progress.

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λ	E_{exact}	E(SUB(2))	E(SUB(4)	E(SUB(8))	E(RPA)	E(ARPA)
0.1	0.55915	0.56031	0.55918	0.55915	0.55918	0.55917
1.0	0.8038	0.8125	—	0.8037	0.8047	0.8044
10.	1.5050	1.5313	—	1.5047	1.5087	1.5076
100.	3.1314	3.1924	—	3.1305	3.1406	3.1380
1000.	6.6942	6.8280	6.7109	6.6923	6.7146	6.7089

Table 1: Ground state energies of the anharmonic oscillator in various aproximations described in the text.

λ	W(RPA)	W(ARPA0)	W(ARPA2)
0.1	0.150×10^{-2}	0.451×10^{-2}	0.148×10^{-2}
1.0	0.525×10^{-2}	0.156×10^{-1}	0.495×10^{-2}
10.	0.703×10^{-2}	0.209×10^{-1}	0.641×10^{-2}
100.	0.749×10^{-2}	0.222×10^{-1}	0.689×10^{-2}
1000.	0.759×10^{-2}	0.225×10^{-1}	0.696×10^{-2}

Table 2: **Convergence of the density $W = 2 < b^{\dagger}b >$ as a function of the truncation . ARPA0 and ARPA2 are the first and second order of the truncation scheme in comparison with the exact RPA value.**