Random-phase approximation approach to rotational symmetry restoration in a three-level Lipkin model

K. Hagino and G. F. Bertsch
Institute for Nuclear Theory, Department of Physics, University of Washington, Seattle, Washington 98195
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We study an extended Lipkin-Meshkov-Glick model that permits a transition to a deformed phase with a broken continuous symmetry. Unlike simpler models, one sees a persistent zero-frequency Goldstone mode past the transition point into the deformed phase. We found that the RPA formula for the correlation energy provides a useful correction to the Hartree-Fock energy when the number of particle N satisfies $N>3$, and becomes accurate for large N. We conclude that the RPA correlation energy formula offers a promising way to improve the Hartree-Fock energy in a systematic theory of nuclear binding energies.

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I. INTRODUCTION

Hartree-Fock (HF) theory is the fundamental starting point to understand the ground state properties of many-fermion systems. Its main assumption is that a particle independently moves in a mean field generated by other surrounding particles. In nuclear physics, with the adjustment of a few parameters of an effective interaction, the HF theory has described reasonably well the global properties of nuclei throughout the periodic table [1]. However, correlation effects which go beyond HF are also significant. They appear most dramatically when the HF ground state violates a symmetry of the Hamiltonian such as rotational invariance or number conservation. A global theory of nuclear binding must surely take these correlation into account, if it is to achieve an accuracy at the 1 MeV level. A recipe is often used which is based on the projection after variation method [2].

In this paper, we argue that the RPA correlation formula can provide a better method in correcting the broken symmetry in the HF theory. In the RPA, a restoration of the symmetry breaking appears as a zero energy solution of the RPA equations. The correlation energy associated with the several symmetries can be calculated using the RPA formula [2,3]

$$E_{\rm corr}=\frac{1}{2}\left(\sum_i \hbar\omega_i - Tr(A)\right), \tag{1}$$

where ω_i is the (positive) frequency of the RPA phonon for the ith mode and A is the A matrix in the RPA equations. Our aim in this paper is to construct a simple Hamiltonian model to study the effects of correlations on the ground state energy and to show that the RPA formula is adequate in principle. To this end, we employ a three-level version [4–7] of the Lipkin-Meshkov-Glick (LMG) model. The model describes N identical fermions in three single-particle levels, each of which is N-fold degenerate. Exact solutions can be obtained by explicitly diagonalizing the model Hamiltonian. The RPA correlation energy was discussed by Brito *et al.* [7], but their parameters did not leave a continuous symmetry to be broken, as is the case for the transition between spherical and deformed nuclei. In this paper, we shall use parameters which mimic quadrupole motions in nuclei. In such a way, the correlation associated with rotational motion is easily studied.

The paper is organized as follows. In Sec. II, we first show that the RPA formula is exact for a simple model with a two-body interaction, Eq. (2) below. We then introduce the three-level Lipkin model in Sec. III and solve it in the HF as well as in the RPA. We compare the RPA correlation energy with the exact solution of the model and show that the RPA formula works well even in the vicinity of the critical point of the phase transition. A summary of the paper is given in Sec. IV, together with further discussions on the RPA formula.

II. RPA CORRELATION FORMULA

Before we study the correlation in the three-level Lipkin model, we would like to demonstrate that the RPA correlation formula works well, using an analytically solvable model. Consider a two fermion system bound in a harmonic potential coupled by a linear interaction

$$H=H_0+V=\sum_{i=1,2}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2}+\frac{1}{2}m\omega_0^2 x_i^2\right)-Cx_1x_2. \tag{2}$$

This model was first introduced in Ref. [8] to discuss the effects of the RPA correlation on the ground state density. A similar model has been considered in Ref. [9] in connection with the paired Wigner crystal. Using the transformation $\xi=(x_1+x_2)/\sqrt{2}$ and $\eta=(x_1-x_2)/\sqrt{2}$, the Hamiltonian can be written in the form

$$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\xi^2}+\frac{1}{2}m\left(\omega_0^2-\frac{C}{m}\right)\xi^2-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\eta^2}+\frac{1}{2}m\left(\omega_0^2+\frac{C}{m}\right)\eta^2, \tag{3}$$

from which we obtain the exact ground state energy

$$E_{\rm exact}=\frac{1}{2}\hbar\omega_0\left(\sqrt{1-\frac{C}{m\omega_0^2}}+\sqrt{1+\frac{C}{m\omega_0^2}}\right). \quad (4)$$

The limit where the coupling constant C is equal to $m\omega_0^2$ corresponds to a translationally invariant Hamiltonian with an interaction $\frac{1}{2}m\omega_0^2(x_1-x_2)^2$, giving

$$E_{\rm exact}=\hbar\omega_0/\sqrt{2}. \quad (5)$$

Let us now solve the problem in the mean field approximation and then consider the RPA correlation energy. If the coupling constant C is small, one can regard V in the Hamiltonian (2) as a residual interaction. The mean field Hamiltonian H_0 then has already been decoupled and we immediately obtain

$$E_{\rm MF}=\hbar\omega_0/2+\hbar\omega_0/2=\hbar\omega_0. \quad (6)$$

We define the RPA excitation operator as

$$Q^\dagger=\sum_{i=1,2}(X_i a_i^\dagger-Y_i a_i), \quad (7)$$

where $a^\dagger$ and a are the creation and the annihilation operators of the unperturbative phonon, respectively. The RPA equation then reads

$$\begin{pmatrix} \hbar\omega_0 & -C\alpha_0^2 & 0 & -C\alpha_0^2 \\ -C\alpha_0^2 & \hbar\omega_0 & -C\alpha_0^2 & 0 \\ 0 & C\alpha_0^2 & -\hbar\omega_0 & C\alpha_0^2 \\ C\alpha_0^2 & 0 & C\alpha_0^2 & -\hbar\omega_0 \end{pmatrix}\begin{pmatrix} X_1 \\ X_2 \\ Y_1 \\ Y_2 \end{pmatrix}=\hbar\omega\begin{pmatrix} X_1 \\ X_2 \\ Y_1 \\ Y_2 \end{pmatrix}, \quad (8)$$

α_0 being the amplitude of the zero point motion defined as $\sqrt{\hbar/2m\omega_0}$. The solutions of this equation are found to be

$$\hbar\omega=\pm\left\{\hbar\omega_0\sqrt{1+\frac{C}{m\omega_0^2}},\quad \hbar\omega_0\sqrt{1-\frac{C}{m\omega_0^2}}\right\}. \quad (9)$$

We thus obtain

$$E_{\rm corr}=\frac{1}{2}\hbar\omega_0\left(\sqrt{1-\frac{C}{m\omega_0^2}}+\sqrt{1+\frac{C}{m\omega_0^2}}\right)-\hbar\omega_0, \quad (10)$$

which is precisely the needed correction to get the ground state energy, Eq. (4), starting from the mean field energy, Eq. (6). It reproduces Eq. (5) in the translationally invariant case.

It is interesting to compare the RPA approach with other ways of dealing with correlation energies associated with broken symmetries. In the case of center-of-mass motion, a recipe is often to subtract the expectation value of the center of mass operator from the mean field energy. With our Hamiltonian, this prescription gives

$$E_{\rm c.m.}=-\left\langle {\rm MF}\left|\frac{1}{2}\frac{(p_1+p_2)^2}{2m}\right|{\rm MF}\right\rangle=-\frac{1}{4}\hbar\omega_0. \quad (11)$$

The total $E_{\rm MF}+E_{\rm c.m.}=3\hbar\omega_0/4$ is not exact, although it is close to Eq. (5). This study clearly shows that the RPA formula provides a much better method to calculate correlation energies.

III. THREE-LEVEL LIPKIN MODEL

We now consider RPA correlations in a three-level Lipkin model. Labeling the levels 0, 1, and 2, we choose the Hamiltonian to be invariant under transformations between 1 and 2. The Hamiltonian we consider can be expressed

$$H=\epsilon(\hat{n}_1+\hat{n}_2)-\frac{V}{2}(K_1K_1+K_2K_2+K_1^\dagger K_1^\dagger+K_2^\dagger K_2^\dagger), \quad (12)$$

where

$$\hat{n}_\alpha=\sum_{i=1}^{N}c_{\alpha i}^\dagger c_{\alpha i},\quad \alpha=0,1,2, \quad (13)$$

$$K_\alpha=\sum_{i=1}^{N}c_{\alpha i}^\dagger c_{0i},\quad \alpha=1,2. \quad (14)$$

A. Exact solutions

Since the Hamiltonian given by Eq. (12) couples symmetric states with respect to interchange of particles only with other symmetric states, a suitable basis for the exact diagonalization of the Hamiltonian H is given by [5]

$$|n_1n_2\rangle=\sqrt{\frac{(N-n_1-n_2)!}{N!n_1!n_2!}}(K_1)^{n_1}(K_2)^{n_2}|00\rangle. \quad (15)$$

This is a simultaneous eigenstate of the number operators $\hat{n}_1$ and $\hat{n}_2$ with the eigenvalue of n_1 and n_2, respectively. The effect of the K operators on the states is given by relations such as

$$K_1|n_1n_2\rangle=\sqrt{(N-n_1-n_2)(n_1+1)}|n_1+1,n_2\rangle. \quad (16)$$

The matrix elements of H can easily be calculated and are given by

$$\langle n_1' n_2' | H | n_1 n_2 \rangle = \epsilon(n_1+n_2)\delta_{n_1',n_1}\delta_{n_2',n_2} - \frac{V}{2}\Big(\sqrt{(n_1+1)(n_1+2)(N-n_1-n_2)(N-n_1-n_2-1)}$$
$$\times \delta_{n_1',n_1+2}\delta_{n_2',n_2} + \sqrt{n_1(n_1-1)(N-n_1-n_2+1)(N-n_1-n_2+2)}\,\delta_{n_1',n_1-2}\delta_{n_2',n_2}$$
$$+ \sqrt{(n_2+1)(n_2+2)(N-n_1-n_2)(N-n_1-n_2-1)}\,\delta_{n_1',n_1}\delta_{n_2',n_2+2}$$
$$+ \sqrt{n_2(n_2-1)(N-n_1-n_2+1)(N-n_1-n_2+2)}\,\delta_{n_1',n_1}\delta_{n_2',n_2-2}\Big). \tag{17}$$

The dimension of the matrix to be diagonalized is $(N+1)(N+2)/2$. Further reduction can be achieved by considering that the Hamiltonian conserves the parity of each level [6].

B. Hartree-Fock approximation

Let us now solve the problem in the Hartree-Fock approximation. We consider a transformation of basis defined by operators $a_{\alpha i}$, with a_{0i} representing the occupied orbital. The HF state has the form

$$|\mathrm{HF}\rangle = \prod_{i=1}^{N} a_{0i}^{\dagger}|\rangle \tag{18}$$

and the transformation of basis is such as to minimize the expectation of the Hamiltonian. Let us write the transformation as

$$\begin{pmatrix} a_{0i}^{\dagger} \\ a_{1i}^{\dagger} \\ a_{2i}^{\dagger} \end{pmatrix} = \begin{pmatrix} \cos\alpha & \cos\beta\sin\alpha & \sin\beta\sin\alpha \\ -\sin\alpha & \cos\beta\cos\alpha & \sin\beta\cos\alpha \\ 0 & -\sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} c_{0i}^{\dagger} \\ c_{1i}^{\dagger} \\ c_{2i}^{\dagger} \end{pmatrix}. \tag{19}$$

Using these relations, it is straightforward to evaluate the energy surface $E(\alpha,\beta)=\langle \mathrm{HF}|H|\mathrm{HF}\rangle$ as

$$E(\alpha,\beta) = N\epsilon\sin^2\alpha - VN(N-1)\sin^2\alpha\cos^2\alpha. \tag{20}$$

Note that the potential surface $E(\alpha,\beta)$ is independent of β and thus totally flat in the β direction for the rotationally invariant Hamiltonian. For simplicity, we particularly choose $\beta=0$ in constructing the HF single particle operators, Eq. (19). The HF Hamiltonian thus spontaneously breaks the rotational symmetry, and the Goldstone mode will appear at zero excitation energy to restore the symmetry breaking, as we will show in the next subsection.

The optimum choice of α is obtained by minimizing the potential surface $E(\alpha,\beta)$. It is convenient to express the solution in terms of the dimensionless parameter

$$\chi \equiv V(N-1)/\epsilon. \tag{21}$$

For $\chi<1$, the minimum appears at $\alpha=0$ (spherical phase). At $\chi=1$, the system undergoes a phase transition and, for $\chi>1$, the potential surface displays two symmetrical minima at $\cos 2\alpha = 1/\chi$ (deformed phase). The ground state energy in the HF approximation is thus given by

$$E_{HF} = \begin{cases} 0 & (\chi<1) \\ \dfrac{N\epsilon}{4}(2-\chi-1/\chi) & (\chi>1). \end{cases} \tag{22}$$

C. Random-phase approximation

We next solve the problem in the RPA in order to evaluate the correlation energy associated with the rotational motion. We define the RPA excitation operator as

$$Q^{\dagger} = X_1\tilde{K}_1 + X_2\tilde{K}_2 - Y_1\tilde{K}_1^{\dagger} - Y_2\tilde{K}_2^{\dagger}, \tag{23}$$

where

$$\tilde{K}_{\alpha} = \sum_{i=1}^{N} a_{\alpha i}^{\dagger} a_{0i}, \quad \alpha = 1,2. \tag{24}$$

The RPA equation is obtained from $\langle \mathrm{HF}|[\delta Q,[H,Q^{\dagger}] - \omega Q^{\dagger}]|\mathrm{HF}\rangle = 0$ for $\delta Q = \tilde{K}_1, \tilde{K}_2, \tilde{K}_1^{\dagger}$, and $\tilde{K}_2^{\dagger}$. The result is the well-known RPA matrix equation

$$\begin{pmatrix} A & B \\ -A & -B \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}, \tag{25}$$

where A and B are 2×2 matrices given by

$$A_{11} = \epsilon\cos 2\alpha + \frac{3}{2}\epsilon\chi\sin^2 2\alpha, \tag{26}$$

$$A_{12} = A_{21} = 0, \tag{27}$$

$$A_{22} = \epsilon(1-\sin^2\alpha) + \frac{1}{2}\epsilon\chi\sin^2 2\alpha, \tag{28}$$

$$B_{11} = -\epsilon\chi(\cos^4\alpha + \sin^4\alpha), \tag{29}$$

$$B_{12} = B_{21} = 0, \tag{30}$$

$$B_{22} = -\epsilon\chi\cos^2\alpha. \tag{31}$$

Because A and B are separately diagonal, the RPA matrix can be easily diagonalized. The RPA frequencies are found to be

$$\omega_1^2 = (A_{11}+B_{11})(A_{11}-B_{11}), \tag{32}$$

$$\omega_2^2 = (A_{22}+B_{22})(A_{22}-B_{22}). \tag{33}$$

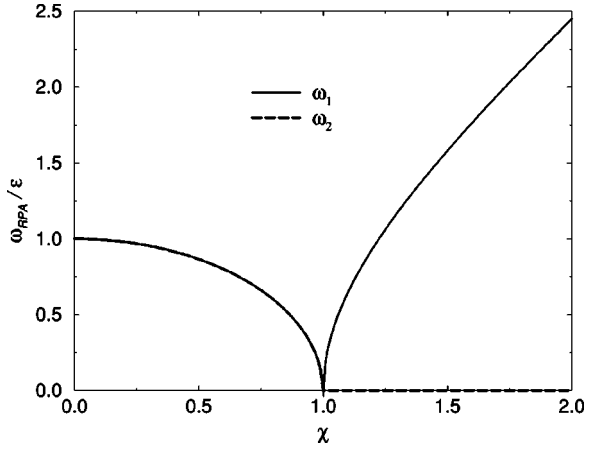

FIG. 1. RPA frequencies for collective vibrations as a function of $\chi \equiv V(N-1)/\epsilon$. The number of particle N is chosen to be 20.

Substituting the self-consistent value for α obtained in the previous subsection, we obtain

$$\omega_1^2 = \begin{cases} \epsilon^2(1+\chi)(1-\chi) & (\chi<1) \\ 2\epsilon^2(\chi+1)(\chi-1) & (\chi>1), \end{cases} \tag{34}$$

$$\omega_2^2 = \begin{cases} \epsilon^2(1+\chi)(1-\chi) & (\chi<1) \\ 0 \quad (\chi>1). \end{cases} \tag{35}$$

In the spherical phase, the RPA frequencies for the two modes are identical. In the deformed phase, on the other hand, the frequency for the second mode becomes zero. In this case, the first mode corresponds to the beta vibration, while the second mode corresponds to the rotational motion perpendicular to the symmetry axis. Figure 1 shows the RPA frequencies as a function of χ for $N=20$. One can clearly see the discontinuity at the critical point $\chi=1$.

Figure 2 compares the ground state energy as a function of χ obtained by several methods. The number of particle N is set to be 20. The solid line is the exact solution obtained by numerically diagonalizing the Hamiltonian. The dashed line is the ground state energy in the Hartree-Fock approximation given by Eq. (22). It considerably deviates from the exact solution through the entire range of χ shown in the figure. The dot-dashed line takes into account the RPA correlation energy in addition to the HF energy. The improvement is apparent and significant. It is remarkable that the RPA formula works well even in the vicinity of the critical point of the phase transition $\chi=1$.

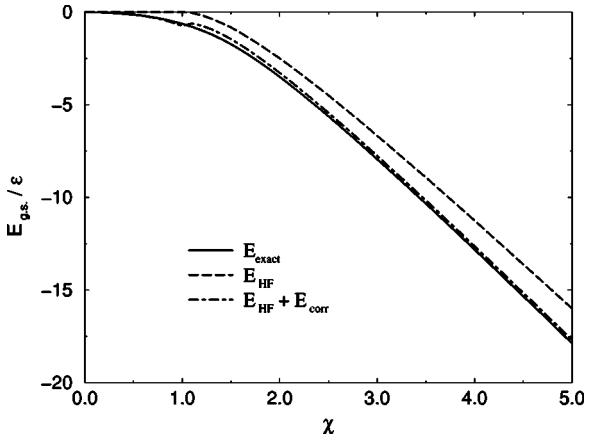

FIG. 2. Comparison of the ground state energy obtained by several methods. The solid line is the exact numerical solution. The ground state energy in the Hartree-Fock approximation is denoted by the dashed line, while the dot-dashed line takes into account the RPA correlation energy in addition to that.

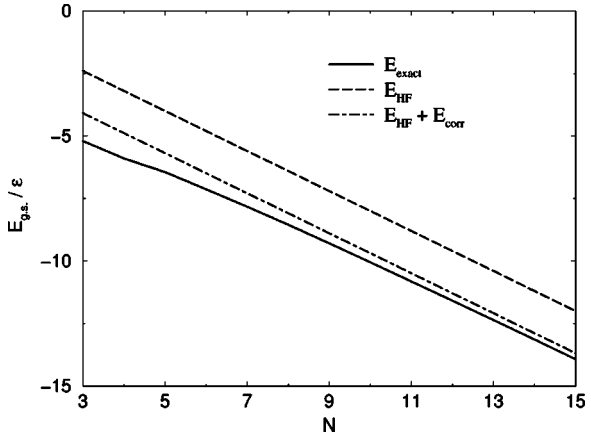

FIG. 3. The ground state energy as a function of N for $\chi=5.0$. The meaning of each line is the same as in Fig. 2.

It is expected that the RPA should be accurate for a large number of particles, and $N=20$ seems to fulfil that condition. We also would like to apply the approximation to nuclei with just a few valence nucleons. Figure 3 compares the exact energy with the HF + RPA as a function of N, for $\chi=5.0$. The RPA correction may be considered useful if it is within a factor of 2 of the exact. We see from the figure that this is satisfied for $N \geqslant 4$. For $N=2$, the exact correlation energy is several times RPA, and such near-magic nuclei would require a more elaborate way.

IV. SUMMARY AND DISCUSSIONS

We discussed the role played by the RPA correlation in the ground state energy. To this end, we used simple Hamiltonian models, like a bilinear interaction between two fermions as well as a three-level Lipkin model. The former is for the correlation associated with the center of mass motion, while the latter for the rotational motion. We showed that the ground state energy is well described in the mean field theory once the ground state correlations are taken into account in the RPA. We also showed that the RPA formula works well for a wide region of an order parameter, including in the vicinity of the critical point of the phase transition. Evidently, the RPA formula provides a powerful method to calculate energies for long range correlations, which are not included in the HF approximation.

Up to now, microscopic theory based on the mean field theory has not been as successful as other approaches in making a global fit to nuclear binding energies. The most

accurate theory of nuclear binding systematics [10] starts from the liquid drop model, and treats shell effects perturbatively. It fits the binding energies with an rms deviation of 0.67 MeV, a factor of 3 better than the Gogny or the published Skyrme functional. We believe that there are good prospects to develop a better microscopic global theory, treating correlation energies systematically by the RPA. Work towards this direction is now in progress [11].

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