Energy functional for the three-level Lipkin model

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We compute the energy functional of a three-level Lipkin model via a Legendre transform and compare exact numerical results with analytical solutions obtained from the random phase approximation (RPA). Except for the region of the phase transition, the RPA solutions perform very well. We also study the case of three non-degenerate levels and again find that the RPA solution agrees well with the exact numerical result. For this case, the analytical results give us insight into the form of the energy functional in the presence of symmetry-breaking one-body potentials.

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I. INTRODUCTION

Nuclear density functional theory (DFT) is applicable for a description of ground-state properties throughout the nuclear chart \cite{1, 2, 3, 4}. This theory is based on the theorem by Hohenberg and Kohn \cite{5}, and its practical applications are based on the self-consistent mean-field theory with density-dependent energy functionals \cite{6, 7, 8, 9}. Within nuclear DFT, the solution of the quantum nuclear many-body problem is relatively simple. The problem is, of course, with the construction of the energy functional.

Most approaches to the nuclear energy-density functional are empirical in nature, and the inclusion of pairing properties \cite{10, 11, 12, 13, 14, 15} is particularly important and challenging. There are only a few non-empirical approaches to the nuclear energy-density functional. The density-matrix expansion pioneered by Negele and Vautherin \cite{16} expands the non-diagonal one-body density matrix along its diagonal, and the expectation value of a Hamiltonian thus leads to an energy-density functional. In another formal approach \cite{17}, the energy-density functional is constructed as the Legendre transform of the ground-state energy as a functional of external one-body potentials. This approach is closely related to the Hohenberg-Kohn theorem \cite{5}. However, its starting point, i.e. the ground-state energy of a quantum many-body system as a functional of any external potential, is only available for a few solvable or weakly interacting systems. Furnstahl and co-workers \cite{18, 19} followed this path and derived energy-density functionals for dilute Fermi gases with short-ranged interactions. For Fermi gases in the unitary regime, simple scaling arguments suggest the form of the energy density functional \cite{20, 21, 22, 23}.

In nuclear physics, energy-density functional theory is a practical tool that is popular due to its computational simplicity and success. The universality of the functional, i.e. the possibility to study nucleons in external potentials, is seldom used. This distinguishes nuclear DFT from DFT in Coulomb systems and makes alternative formulations worth studying. For computational simplicity, we would like to maintain the framework of an energy functional. However, there is no need to focus on functionals of the density. The description and interpretation of nuclear systems is often based on shell-model orbitals rather than densities. For instance, in nuclear structure, one is often more interested in the occupation of a given shell-model orbital or the isospin-dependence of the effective single-particle energies than in the shape of the density distribution. This language is natural for shell-model Hamiltonians that are based on single-particle orbitals. It is the purpose of this paper to study and construct the energy functional of such a system.

Recently, the energy functional (in terms of occupation numbers) was constructed for the pairing Hamiltonian \cite{24}. In this paper we consider the three-level Lipkin model \cite{25, 26, 27, 28}. This is another solvable model that is relevant for nuclei. We will be able to gain insight into the formulations of energy functionals for two-body interactions that exhibit a continuous symmetry, and will study the effect of symmetry-breaking one-body potentials.

This paper is organized as follows. In Sect. II we construct the energy functional of the three-level Lipkin model with degenerate excited levels. We study the implications of symmetry-breaking one-body potentials in Sect. III and conclude with our Summary.

II. DEGENERATE ENERGY LEVELS

We consider the three-level Lipkin model \cite{25, 26, 27, 28} and follow the work by Hagino and Bertsch \cite{29}. This model consists of $N$ fermions that are distributed over three levels (labeled as 0, 1, and 2) consisting of $N$ degenerate, single-particle states each. The single-particle energies are $\varepsilon_0 = 0$, and the two excited levels are degenerate, $\varepsilon_1 = \varepsilon_2 \equiv \varepsilon$. The Hamiltonian is

$$H = \varepsilon (\hat{n}_1 + \hat{n}_2) - \frac{V}{2} (K_1 K_1 + K_2 K_2 + K_1^\dagger K_1^\dagger + K_2^\dagger K_2^\dagger).$$ (1)
Here, 
\[ \hat{n}_\alpha = \sum_{i=1}^{N} c_{\alpha i}^\dagger c_{\alpha i}, \quad \alpha = 0, 1, 2 \]  
(2)
is the number operator of level \( \alpha \), while 
\[ K_\alpha = \sum_{i=1}^{N} c_{\alpha i}^\dagger c_{\alpha i}, \quad \alpha = 1, 2 \]  
(3)
transfer fermions from the level 0 to the level \( \alpha > 0 \). We assume \( \varepsilon \geq 0 \) for the spacing to the degenerate levels 1 and 2. The operators \( c_{\alpha i}^\dagger \) and \( c_{\alpha i} \) create and annihilate a fermion in state \( i \) of level \( \alpha \). The Hamiltonian is invariant under the simultaneous orthogonal transformation of the \( N \) orbitals belonging to each level, and this symmetry facilitates the numerical solution of this problem [28]. Note that the Hamiltonian (1) is invariant under orthogonal transformations of states belonging to the degenerate levels 1 and 2, i.e.
\[ \begin{pmatrix} c_{11}^\dagger \\ c_{21}^\dagger \end{pmatrix} \rightarrow \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} c_{11}^\dagger \\ c_{21}^\dagger \end{pmatrix}. \]  
(4)
This symmetry will be broken by the Hartree-Fock (HF) solution (see below), and we will study the explicit breaking of this symmetry by additional one-body terms of the Hamiltonian in Sect. III.

The energy functional is the Legendre transform 
\[ F(n) = E(\varepsilon) - \varepsilon n(\varepsilon). \]  
(5)
Here 
\[ n(\varepsilon) = \partial E(\varepsilon) / \partial \varepsilon \]  
(6)
is the ground-state occupation of levels 1 and 2, while \( E(\varepsilon) \) is the ground-state energy as a function of the spacing \( \varepsilon \). The exact ground-state energy can be obtained numerically by diagonalizing a matrix of modest dimensions [28], and one can thus construct easily the exact energy functional. However, we are interested in gaining analytical insight into the problem. For this reason, we employ the analytical expression by Hagino and Bertsch [29] that expresses the ground-state energy in terms of the HF energy and corrections due to the RPA. The HF result depends on the size of the parameter \( \varepsilon/v \) where
\[ v \equiv V(N-1) \]  
(7)
is the effective strength of the two-body coupling \( V \) in the \( N \)-body system. The spherical phase is found for \( \varepsilon/v > 1 \), while one deals with a deformed phase for \( \varepsilon/v < 1 \). In the spherical (deformed) phase, the HF solution preserves (breaks) the symmetry (41) of the Hamiltonian. The results are [29]
\[ E = \sqrt{\varepsilon^2 - v^2} - \varepsilon \quad \text{for} \quad \varepsilon > v, \]  
(8)

Figure 1 compares the approximate ground-state energy to the RPA approximation for a system of \( N = 20 \) fermions. The RPA result shows a cusp at \( \varepsilon = v \equiv (N-1)V \), corresponding to the boundary between the spherical (\( \varepsilon > v \)) and the deformed phase (\( \varepsilon < v \)).

Let us start with the analytical construction of the energy functional (6) in the spherical phase. Here, the RPA solution is convex. We have
\[ n = \frac{\partial E}{\partial \varepsilon} = \frac{\varepsilon}{\sqrt{\varepsilon^2 - v^2}} - 1. \]  
(10)
This equation can easily be solved for \( \varepsilon(n) \), and the functional thus reads
\[ F(n) = -|v|\sqrt{n(n+2)}. \]  
(11)
Thus, for small occupation numbers (i.e. the weak coupling limit \( v \ll \varepsilon \)), the functional is nonanalytical and exhibits a square root singularity. This is a rather generic feature of energy functionals and is also seen in the energy functional for the pairing Hamiltonian.

We next turn to the deformed case (\( \varepsilon < v \)). The occupation number is
\[ n(\varepsilon) = \frac{2N - 1}{4} - \frac{N - 1}{2} \frac{\varepsilon}{v} - \frac{\varepsilon}{\sqrt{2(v^2 - \varepsilon^2)}}. \]  
(12)
Equation (12) is difficult to invert analytically because of the term involving the square root. Note that this term also renders the occupation number negative as \( \varepsilon \) approaches \( v \). We avoid this problem by expanding Eq. (12) in powers of \( \varepsilon/v \), approximate \( \varepsilon/v \ll 1 \), and keep up to orders \( O(\varepsilon/v) \) in the resulting expression. The result is

\[
\varepsilon(n) = \frac{N - 2n - 1/2}{N - 1 + \sqrt{2}} v .
\]

Insertion of this result and Eq. (9) into Eq. (15) yields the density functional in the deformed phase.

Note that the energy functional is analytical in the strong coupling limit \( v \gg \varepsilon \). Again, this is a generic feature of energy functionals and was also exhibited in the pairing problem.

Figure 2 compares the exact energy functional with the RPA solutions obtained in the spherical and deformed phase for \( N = 20 \). Note that the spherical (deformed) phase corresponds to sufficiently small (large) occupation numbers. The inset shows that the RPA solution has a kink at the critical occupation number \( n \approx 0.7 \) at the phase transition. Note also that the solution of the deformed phase is a good approximation over the entire range \( n > 0.7 \), although its derivation employed the approximation \( \varepsilon \ll v \) corresponding to \( n \approx N/2 \), see Eq. (12).

How severe is the presence of the kink at \( n \approx 0.7 \) in the functional? To address this question, we employ the RPA functional in practical calculations. We add the one-body term \( \varepsilon n \) to the functional and numerically determine the occupation number \( n \) that minimizes the ground-state energy

\[
E(n) = F(n) + \varepsilon n .
\]

The energy taken at the minimum is plotted as a function of the minimizing occupation number \( n \) in Fig. 3. The result is also compared to the exact numerical result. We see that the energy functional, obtained via RPA, provides a good prediction of the ground state energy function of the three-level Lipkin model. At the phase transition, however, the functional predicts multiple values for the ground state energy, due to the discontinuity in the derivative at the phase transition. Thus, for external potentials \( \varepsilon \approx v \) the energy functional does not provide good predictive power, and the relatively small kink visible in the inset of Fig. 2 is, of course, the reason for this shortcoming.

### III. Non-degenerate energy levels and symmetry-breaking

The two-body interaction and the one-body terms of the Hamiltonian (11) are invariant under the symmetry transformation (4). In this section we study the breaking of this symmetry by a one-body potential, i.e. we lift the degeneracy of levels 1 and 2 in the Hamiltonian (11) and modify its one-body term as follows

\[
\varepsilon(\hat{n}_1 + \hat{n}_2) \rightarrow \varepsilon_1 \hat{n}_1 + \varepsilon_2 \hat{n}_2 .
\]

The two-body interaction remains the same. Technically it is convenient to substitute \( \varepsilon \rightarrow (\varepsilon_1 + \varepsilon_2)/2 \) in Eq. (1) and to add the term

\[
\frac{\varepsilon_1 - \varepsilon_2}{2}(\hat{n}_1 - \hat{n}_2)
\]

to the resulting expression. This approach is particularly convenient for the RPA calculation.

The question of symmetry-breaking is an important one. The energy functional corresponds to the symmetry-preserving two-body interaction that is probed by a symmetry-breaking one-body potential. Thus, the functional depends on two variables (the occupation numbers of levels 1 and 2), and we are interested in the form of this functional and in its relation to the functional of the symmetry-preserving case. We thereby hope to get insights into energy functionals for atomic nuclei. The
nuclear shell model, for instance, employs a spherically symmetric two-body interaction, but deformed nuclei are often described within a deformed mean-field basis that breaks the rotational invariance through one-body terms.

The numerical calculations are simple and require only a minor modification of the matrix elements corresponding to the one-body terms. For the analytical construction of the functional, we have to perform the HF and RPA calculations. We adapt the HF calculation of Ref. [29] to the case of non-degenerate levels and obtain the HF-energy surface

\[ E(\alpha, \beta) = N \sin^2 \alpha (\varepsilon_1 \cos^2 \beta + \varepsilon_2 \sin^2 \beta) \]

\[ -vN \sin^2 \alpha \cos^2 \beta \]

as a function of the two angles \(\alpha\) and \(\beta\) of the HF transformation. In the case \(\varepsilon_1 = \varepsilon_2\) of degenerate levels, the energy surface \(17\) becomes independent of \(\beta\).

In what follows, we assume \(\varepsilon_1 \leq \varepsilon_2\). The minimum of the energy surface \(17\) occurs at \(\alpha = 0\) (where \(\beta\) is arbitrary and can be chosen as zero) for \(\varepsilon_1 > v\), and at \(\cos 2\alpha = \varepsilon_1/v\) and \(\beta = 0\) for \(\varepsilon_1 < v\). Again, we refer to these cases as the weak-coupling regime and the strong-coupling regime, respectively. The Hartree-Fock energy thus becomes

\[ E_{HF} = \begin{cases} 0, & \varepsilon_1 > v, \\ -vN + \frac{\varepsilon_1^2 - v^2}{v}, & \varepsilon_1 < v. \end{cases} \]

Thus, within the HF approximation, all particles stay in level 0 in the weak-coupling regime, while the fermions occupy level 0 and level 1 in the strong-coupling regime. The RPA equation takes the well-known form

\[ \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}. \]

The nonzero matrix elements of the \(2 \times 2\) matrices \(A\) and \(B\) are

\[ A_{11} = \varepsilon_1 \cos 2\alpha + \frac{3}{2} v \sin^2 2\alpha, \]

\[ A_{22} = \varepsilon_2 - \varepsilon_1 \sin^2 2\alpha + \frac{v}{2} \sin^2 2\alpha, \]

\[ B_{11} = -v (\cos^4 \alpha + \sin^4 \alpha), \]

\[ B_{22} = -v \cos^2 \alpha. \]

Solving for the eigenfrequencies \(\omega\) yields

\[ \omega_1^2 = \begin{cases} \varepsilon_1^2 - v^2, & \varepsilon_1 > v \\ 2(v^2 - \varepsilon_1^2), & \varepsilon_1 < v \end{cases} \]

\[ \omega_2^2 = \begin{cases} \varepsilon_2^2 - v^2, & \varepsilon_1 > v \\ (\varepsilon_2 - \varepsilon_1)(\varepsilon_2 + v), & \varepsilon_1 < v \end{cases} \]

The total energy is

\[ E = E_{HF} + \frac{1}{2} \left( \sum_{i=1}^{2} \omega_i - \text{Tr} A \right), \]

and the result thus becomes

\[ E = \frac{1}{2} \sum_{j=1}^{2} \left( \sqrt{\varepsilon_{1,j}^2 - v^2} - \varepsilon_{1,j} \right) \text{ for } \varepsilon_1 > v, \]

\[ E = -\frac{N+4}{4} v + \frac{1}{2} \sqrt{\varepsilon_2 - \varepsilon_1} \sqrt{v + \varepsilon_2} + \frac{N+1}{4} \varepsilon_1 \]

\[ -\frac{\varepsilon_2}{2} - \frac{N-1}{4} \frac{\varepsilon_1^2}{v} \text{ for } \varepsilon_1 < v. \]

In the weak-coupling regime, the energy \(23\) is very simply related to the energy \(8\) for the spherical phase, while the energy of the strong-coupling regime differs mainly from its deformed counterpart \(9\) through the term that is nonanalytical in the level splitting \(\varepsilon_2 - \varepsilon_1\). It seems that the non-analyticity is an artifact of the RPA approximation.

Fig. 4 compares this analytical expressions \(23\) and \(24\) with the exact energy for a system of \(N = 10\) fermions. Again, the RPA fails at the boundary between the regime of strong and weak coupling, and the energy is not a convex function of the single-particle energies.

The energy functional results from the Legendre transform

\[ F(n_1, n_2) = E(\varepsilon_1, \varepsilon_2) - \sum_{j=1}^{2} n_j \varepsilon_j, \]

and it is understood that \(\varepsilon_j = \varepsilon_j(n_1, n_2)\) results from the inversion of the occupation numbers

\[ n_j = \frac{\partial E}{\partial \varepsilon_j}. \]
We start with the weak-coupling regime \( \varepsilon_1 > v \) and find

\[
n_j = \frac{1}{2} \left( \frac{\varepsilon_j}{\sqrt{\varepsilon_j^2 - v^2}} - 1 \right).
\]  

(27)

Thus, the occupation number of the two energy levels depends only on the energy of the level itself, and the strength of the two-body interaction. Note that the occupation numbers are symmetric under exchange of level 1 and level 2. The inversion of Eq. (27) is straightforward, and we obtain the energy functional

\[
F(n_1, n_2) = -|v| \sum_{j=1}^{2} n_j (n_j + 1).
\]

(28)

Note that the functional (28) is symmetric under exchange of level 1 and level 2, and that it is simply the sum of two functionals. Its form could have almost been guessed from the functional (11) for degenerate levels.

We turn to the strong-coupling regime \( \varepsilon_1 < v \) which once again proves more difficult. The occupation numbers

\[
n_1 = \frac{2N + 1}{4} - \frac{x}{4} - \frac{N - 1}{2} \frac{\varepsilon_1}{v} - \frac{\varepsilon_1}{\sqrt{2(v^2 - \varepsilon_1^2)}}
\]

(29)

\[
n_2 = \frac{1}{4} (x + x^{-1} - 2)
\]

(30)
do not decouple as in the weak-coupling limit. Here, we employed the shorthand

\[
x \equiv \frac{\varepsilon_2 + v}{\varepsilon_2 - \varepsilon_1}.
\]

(31)

We solve Eq. (30) for \( x \) and obtain

\[
x(n_2) = 2n_2 + 1 + 2\sqrt{n_2(n_2 + 1)}.
\]

(32)

We insert this result into Eq. (29), approximate \( \varepsilon_1 \ll v \) and solve for \( \varepsilon_1 \). This expansion again renders the resulting functional convex, and we obtain

\[
\varepsilon_1(n_1, n_2) = \frac{N - 2n_1 + 1/2 - x/2}{N - 1 + \sqrt{2}} v.
\]

(33)

Finally, we insert this result into Eq. (31) and find

\[
\varepsilon_2(n_1, n_2) = \frac{v + x^2 \varepsilon_1}{x^2 - 1}.
\]

(34)

The insertion of the expressions (33) and (34) into the functional (25) thus yields the desired expression. Figure 5 shows the resulting functional and compares it to the exact solution. The agreement between the exact result and the RPA result is quite satisfactory. Note that the boundary between the regimes of strong and weak coupling is a one-dimensional line in the region of small occupation numbers \( n_{1,2} < 1 \).

IV. SUMMARY

We constructed the energy functional for the three-level Lipkin model with degenerate and non-degenerate excited levels. Our analytical results are based on RPA calculations and subsequent Legendre transformations. They agree well with exact numerical results in the limits of strong and weak coupling, respectively, but the RPA fails at the boundary between both regimes. In particular, the RPA energy is not a convex function of the single-particle energies in the strong-coupling regime.

In the case of non-degenerate excited levels, a continuous symmetry is broken by single-particle terms of the Hamiltonian while the two-body interaction alone preserves this symmetry. In the weak-coupling regime, the energy functional obtained from non-degenerate levels is simply related to the functional obtained for degenerate excited levels. Both exhibit a square-root singularity for small occupation numbers. The relationship is more complicated in the strong-coupling regime. However, the derived results should be useful in the construction of an occupation-number based energy functional for nuclear masses. Recall that the occupation-number-based mass formula by Duflo and Zuker [30] is superior to mass table calculations that employ nuclear energy-density functionals [3]. This gives prospect to the development of a global nuclear energy functional based on shell model occupations.

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