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Structure of the Phonon Vacuum State

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Abstract. The action of the long-range residual force on the the expectation value of observables in the nuclear ground-states is evaluated by finding optimal values for the coefficients of the canonical transformation which connects the phonon vacuum state with the (quasi-)particle ground-state. After estimating the improvements over the predictions of the independent particle approximation we compare the ground-state wave functions obtained using the presented approach with those obtained using the conventional random phase approximation (RPA) and its extended version. The problem with overbinding of the nuclear ground state calculated using the RPA is shown to be removed if one sticks to the prescriptions of the present approach. The reason being that the latter conforms to the original variational formulation. Calculations are performed within the two-level Lipkin model in which we present results for the binding energies.

1 Introduction

Approximating the correlated nuclear ground state has been receiving considerable attention since the early days of nuclear structure physics [1] and still represents a formidable challenge. This is an arduous task within the "beyond the mean-field" theories because of the action of the residual interaction which brings particle-hole admixtures into the ground states. In the present paper we focus on the effects of long-range part of this interaction. Unambiguously attributable to the latter is the quadrupole correlation energy, which, as shown by the findings in Ref. [2], is considerable and varies between 100keV and 5.5 MeV in different nuclei. The short-range residual forces on the other hand compete with the long-range ones in dominating the ground state shapes formation [3]. As a result of this competition in the beginning and the end of major shells the nucleons are paired giving rise to spherical shape while in the middle of the shell the nucleons are paired-off and they align to the field generating forces thus contributing to deformation. We conjecture that the present study can serve as a foundation to investigate the mechanism of the transition between these two regimes and in particular on the pairs decoupling process. The mechanism that we surmise was concocted in Ref. [4] and essentially implies that the long-range force breaks nucleon pairs which may further recouple due to the pairing force.

We approximate the nuclear ground state wave function with the phonon operators [5] vacuum state. A general form of the phonon vacuum was proposed by Sorensen [6] and later Goswami and Pal [7] estimated explicitly the correlation coefficients of the 2p-2h admixtures into the BCS wave function [8] relating them to the forward and backward phonon amplitudes. The expression they derived turned out to be also valid for higher order correlations [9] in the the random phase approximation (RPA) [10]. Being a small amplitude limit of the time-dependent Hartree-Fock approximation, however, RPA is known to be able to account only for small correlation effects. Since in open-shell nuclei the backward phonon amplitudes are by no means small, RPA is becoming questionable in describing the low-energy states of such nuclei. This problem was addressed by Hara [4, 12] who proposed an improvement over the RPA based on the Pauli blocking principle which plays a progressively important role with the increasing number of the valence nucleons. This extension has proven to be in better accord with the experimental data as demonstrated in a number of papers as for example in Refs. [13, 14]. Although its superiority over the standard RPA is undeniable, the variational character of the theory is violated as the ground state is found to be overbound. The strong argument that the variational property of a theory insures a converging succession of approximations to the exact solution fostered the formulation of a elaborate formalism, called self-consistent RPA [15], which as in the conventional particle-hole theory, allowed to take into account the nucleon correlations without explicitly constructing the ground state wave function.

In the present paper we keep using the explicit form of the fermionic many body vacuum [6] but depart from varying the excited state wave function. On the contrary we use the correlation coefficients as parameters which we fix by optimizing the ground state trial wave function using a variational procedure. This approach benefits from the findings in Ref. [16] where it was shown that this class of wave functions is a vacuum for a generalized phonon operator, adding to the standard one specific two-body operators correcting for the Pauli principle. By way of example using the two-level Lipkin-Meshkov-Glick(LMG) model [17] they showed that the additional terms improve the convergence substantially. In this way the phonon vacuum state absorbs additional correlations effects than of ones obtained using the equations-of-motion method for the standard phonon operator.

The paper proceeds as follows. In Section 2 we outline the problem and summarize the main obstacles towards the exact solution. Basic equations of several approximate methods including the RPA, ERPA and the explicit variation of the phonon vacuum state along with the exact solution within the LMG model are derived in Section 3. A comparison between them is performed on the basis of the ground state total energy. Summary and outlook is given in Section 5.

2 Formulation

Formally a wave function which contains quasiparticle admixtures into the independent quasiparticle wave function and is a vacuum for the phonon operators [5]

$$Q_{\lambda\mu i} = \frac{1}{2}\sum_{jj'}\left[\psi^{\lambda i}_{jj'} A(jj'|\lambda\mu) - (-1)^{\lambda-\mu}\varphi^{\lambda i}_{jj'} A^{\dagger}(jj'|\lambda-\mu)\right] \qquad (1)$$

can be expressed as [6]

$$|\rangle = N_0 . e^{\hat{S}}\rangle \qquad (2)$$

with

$$\hat{S} = -\frac{1}{2}\sum_{12;\lambda\mu} S_{\lambda}(j_1 j'_1|j_2 j'_2)(-)^{\lambda-\mu} A^{\dagger}(j_1 j'_1|\lambda\mu) A^{\dagger}(j_2 j'_2|\lambda-\mu). \qquad (3)$$

The coefficients $S_{\lambda}(j_1 j'_1|j_2 j'_2)$ are referred to as correlation coefficients and denote the amplitudes for the presence of zero, four, eight, ... quasiparticles in the ground state due to the virtual vibrations. These present a primary source of structure information for the ground states and make up a major part of our present research. The correlated and uncorrelated ground states are denoted as $|\rangle$ and $\rangle$ correspondingly. The quasiparticle-phonon nomenclature follows the one given in Ref. [5].

Using the ERPA, the correlation coefficients are found to satisfy the equations [4, 6]

$$\psi^{\lambda i}_{j_1 j'_1} = \sum_{j_2 j'_2}(1-\rho_{j_2 j'_2}) S_{\lambda}(j_1 j'_1|j_2 j'_2)\varphi^{\lambda i}_{j_2 j'_2}, \qquad (4)$$

where ρ_j is the quasiparticle occupation number on the level j.

In Eq.(2) N_0 is a normalization factor which in physical terms is the overlap between the independent-particle and the correlated wave functions. It is found to be

$$N_0^2 = \frac{1}{\langle e^{(S^{\dagger}+S)}\rangle} \qquad (5)$$

In RPA, suggesting small correlations so that higher order terms contribute relatively little, this constant is approximated as :

$$N_0^2 \approx \frac{1}{e^{\frac{1}{2}\sum_{j_1 j'_1 j_2 j'_2;\lambda}(2\lambda+1)S^2_{\lambda}(j_1 j'_1|j_2 j'_2)}}. \qquad (6)$$

An explicit solution to the system (4) was obtained by Hara [4].

Changing the frame of mind we shall try to obtain the correlation coefficients explicitly varying the wave function $|\rangle$ in the functional

$$\delta\langle|H|\rangle = 0 \qquad (7)$$

with $S_{\lambda}(j_1 j'_1|j_2 j'_2)$ being variational parameters, *i.e.* we shall try to solve the equation

$$\delta(N_0^2\langle e^{S^{\dagger}} H e^{S}\rangle) \equiv \langle e^{S^{\dagger}} H e^{S}\rangle\left(\delta N_0^2\right) + N_0^2\left(\delta\langle e^{S^{\dagger}} H e^{S}\rangle\right) = 0, \qquad (8)$$

with respect to $S_\lambda(j_1 j_1'|j_2 j_2')$. If one restricts the configuration space to 2p-2h admixtures only, the quantities that need to be evaluated are presented in the expression below

$$N_0^2\langle e^{S^\dagger} H e^S\rangle \approx \frac{\langle H\rangle + 2\langle HS\rangle + \langle S^\dagger HS\rangle}{1+\frac{1}{2}\langle S^\dagger S\rangle}. \tag{9}$$

Evaluating these quantities proves prohibitively laborious in the realistic case even within the restricted space and some approximate expressions for these will be given elsewhere. In order to assess the utility of our approach we have recourse to the widely used LMG model.

3 Solution within the Lipkin-Meshkov-Glick Model

In order to access the utility of different approaches and to prove the usefulness of the proposed scheme we limit the configuration space and simplify the inter-nucleon interaction to monopole-monopole one as suggested by Lipkin, Meshkov and Glick [17, 18] . This setting permits comparisons between the rates of convergence of different approximation methods, including the hereby described, to the exact solution.

The interaction of N particles on 2 quantum levels is presented by the following Hamiltonian

$$H = H_0 + V;\ H_0 = \varepsilon J_0;\ V = \frac{G}{2}(J_+ + J_-)^2, \tag{10}$$

where

$$\begin{aligned} J_+ &= \sum_\alpha a^\dagger_{1\alpha} a_{-1\alpha}\,,\\ J_- &= \sum_\alpha a^\dagger_{-1\alpha} a_{1\alpha}\,,\\ J_0 &= \frac{1}{2}\sum_\alpha (a^\dagger_{1\alpha} a_{1\alpha} - a^\dagger_{-1\alpha} a_{-1\alpha}). \end{aligned} \tag{11}$$

are the analogous to the raising, lowering and angular momentum' z-component of the quasi-spin algebra respectively, $a^\dagger$ represents the particle creation operator, ± 1 in the subscript denote the upper or lower level, ε is the energy gap between the two levels and G is the interaction strength.

We shall also make use of the operators

$$s^+_\alpha = a^\dagger_{1\alpha} a_{-1\alpha};\, s^-_\alpha = a^\dagger_{-1\alpha} a_{1\alpha};\, s^0_\alpha = \frac{1}{2}(a^\dagger_{1\alpha} a_{1\alpha} - a^\dagger_{-1\alpha} a_{-1\alpha}). \tag{12}$$

The exact solution

$$|\Psi\rangle = \sum_i c_i |\Phi_i\rangle \tag{13}$$

is a superposition of states with $0, 1, 2 \ldots, N$ particles on the upper level ($|\Phi_0\rangle \equiv\rangle$). The weights c_i are readily obtained by solving the eigenvalue problem

$$\sum_{n'} \langle \Phi_n | H | \Phi_{n'} \rangle c_{n'} = E c_n. \tag{14}$$

The non-zero elements of the matrix on the left-hand side of the above equation evaluate to

$$\langle \Phi_n^* | H | \Phi_n \rangle = \left(-\frac{N}{2} + n \right) \varepsilon + G \left(-\frac{N}{2} + n + (n+1)(N-n) \right) \tag{15}$$

$$\langle \Phi_n^* | H | \Phi_{n+2} \rangle = \frac{G}{2} \sqrt{n(n-1)(N+2-n)(N+1-n)}. \tag{16}$$

For the ground state total energy we then obtain

$$E = \sum_i c_i^2 \langle \Phi_i^* H \Phi_i \rangle + 2 \sum_i c_i c_{i+2} \langle \Phi_i^* H \Phi_{i+2} \rangle. \tag{17}$$

We shall further present the solutions for exited states containing only one particle on the upper level and one hole on the lower one, *i.e.*

$$|1p1h\rangle_m = \left(\sum_\alpha (\psi_\alpha^{(m)} s_\alpha^+ - \varphi_\alpha^{(m)} s_\alpha^-) \right) \rangle \tag{18}$$

Employing the RPA, *i.e.*

$$\langle | s_\alpha^-, s_{\alpha'}^+ | \rangle = \delta_{\alpha\alpha'} \tag{19}$$

one obtains the well-known equation for the excitation energies and the forward and backward amplitudes:

$$\begin{pmatrix} \delta_{\alpha\beta}(\varepsilon - G) + G & -G(1-\delta_{\alpha\beta}) \\ -G(1-\delta_{\alpha\beta}) & \delta_{\alpha\beta}(\varepsilon - G) + G \end{pmatrix} \begin{pmatrix} \psi \\ \varphi \end{pmatrix} = \omega \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} \psi \\ \varphi \end{pmatrix} \tag{20}$$

which together with the normalization of the wave functions (18) yields

$$\begin{aligned} \psi^{(0)} &= \frac{1}{\sqrt{N}} \frac{1 + \chi/2 + \omega_0/\varepsilon}{\sqrt{\left(1 + \frac{\omega_0}{\varepsilon}\right)\left(1 + \chi + \frac{\omega_0}{\varepsilon}\right)}}\,, \\ \varphi^0 &= \frac{1}{\sqrt{N}} \frac{\chi/2}{\sqrt{\left(1 + \frac{\omega_0}{\varepsilon}\right)\left(1 + \chi + \frac{\omega_0}{\varepsilon}\right)}}\,, \end{aligned} \tag{21}$$

where

$$\chi = \frac{2G(N-1)}{\varepsilon}, \qquad \omega_0 = \varepsilon\sqrt{1+\chi}. \tag{22}$$

The ground state total energy evaluates to

$$E = E_{HF} - N\omega_0(\varphi^0)^2, \tag{23}$$

where

$$E_{HF} = (G - \varepsilon)\frac{N}{2}. \tag{24}$$

The condition (19) disregards some aspects of the nature of the excited states (18), in particular the fact that the number of particle-hole state in the ground state may be non-negligible if sufficiently strong interaction is applied. In a broader context, than the hereby considered, Hara [4] suggested to include explicitly the number of quasiparticles on each level, which turned out to have dramatic effect on the collective properties of the low-lying states in even-even nuclei [13, 14]. Adapting it to the LMG model we can write

$$\langle|n_{+1}|\rangle = N\rho,\ \langle|n_{-1}|\rangle = N(1-\rho). \tag{25}$$

Equation (19) then transforms to

$$\langle|s^-_\alpha, s^+_{\alpha'}|\rangle = \delta_{\alpha\alpha'}(1-2\rho). \tag{26}$$

Analogous to the equation (20) in the current context is the following one

$$\begin{pmatrix} A_{\alpha_1\alpha_2} & B_{\alpha_1\alpha_2} \\ B^*_{\alpha_1\alpha_2} & A^*_{\alpha_1\alpha_2} \end{pmatrix}\begin{pmatrix} \psi^m_{\alpha_2} \\ \varphi^m_{\alpha_2} \end{pmatrix} = \omega\begin{pmatrix} U_{\alpha_1\alpha_2} & 0 \\ 0 & -U^*_{\alpha_1\alpha_2} \end{pmatrix}\begin{pmatrix} \psi^m_{\alpha_2} \\ \varphi^m_{\alpha_2} \end{pmatrix}, \tag{27}$$

where

$$A_{\alpha_1\alpha_2} = G(1-2\rho)^2 - \delta_{12}(1-2\rho)(G-\varepsilon), \tag{28}$$

$$B_{\alpha_1\alpha_2} = G(1-2\rho)(\delta_{\alpha_1\alpha_2} + 2\rho - 1), \tag{29}$$

and

$$U_{\alpha_1\alpha_2} = \delta_{\alpha_1\alpha_2}(1-2\rho). \tag{30}$$

The solution is

$$\psi^{(0)} = \frac{1}{\sqrt{N(1-2\rho)}}\frac{1+\chi/2+\omega_0/\varepsilon}{\sqrt{\left(1+\frac{\omega_0}{\varepsilon}\right)\left(1+\chi+\frac{\omega_0}{\varepsilon}\right)}}, \tag{31}$$

$$\varphi^0 = \frac{1}{\sqrt{N(1-2\rho)}}\frac{\chi/2}{\sqrt{\left(1+\frac{\omega_0}{\varepsilon}\right)\left(1+\chi+\frac{\omega_0}{\varepsilon}\right)}}, \tag{32}$$

where

$$\omega_0^2 = \varepsilon^2(1+\chi),\quad \chi = \frac{2G}{\varepsilon}[(1-2\rho)N - 1] \tag{33}$$

The system of equations closure is insured by adding the following one:

$$\rho = \frac{(\varphi^0)^2}{1+2(\varphi^0)^2}. \tag{34}$$

Finally, the featured method that we examine (conf. Sec. 2) translates in the language of the LMG model in the following way. The wave function (2) assumes the form

$$|\rangle = N_0 e^{\frac{1}{2}\sum_{\alpha_1\alpha_2} S_{\alpha_1\alpha_2} s^+_{\alpha_1} s^+_{\alpha_2}}\rangle. \tag{35}$$

If we truncate the exponent expansion to second order, *i.e.* allow for 2p-2h admixtures only into the ground-state wave function, we obtain

$$N_0^2 = \frac{1}{1 + \frac{1}{2}\sum_{\alpha_1\alpha_2}(1-\delta_{\alpha_1\alpha_2})S^2_{\alpha_1\alpha_2}}. \tag{36}$$

The variational problem then is rewritten as

$$\delta\Big(N_0^2\Big\langle(1+\frac{1}{2}\sum_{\alpha_1\alpha_2} S_{\alpha_1\alpha_2}s_{\alpha_2}s_{\alpha_1})H(1+\frac{1}{2}\sum_{\alpha_1\alpha_2} S_{\alpha_1\alpha_2}s^\dagger_{\alpha_1}s^\dagger_{\alpha_2})\Big\rangle\Big) = 0. \tag{37}$$

It can be rigorously proved, that in this simple model the correlation coefficients are all equal, *i.e.* $S_{ij} = S$. Then performing the variation (37) leads to the following simple quadratic equation for S:

$$1 + \Big(2\frac{\varepsilon}{G} + 2N - 4\Big)S - \frac{1}{2}(N^2 - N)S^2 = 0. \tag{38}$$

The ground-state energy in this case evaluates to

$$E = N_0^2\Big[E_{HF} + N(N-1)GS + \frac{1}{4}(\varepsilon - G)(-N+4)N(N-1)S^2 + GN(N-1)^2S^2\Big]. \tag{39}$$

Performing the variation (7) analytically in an extended configuration space represents a formidable challenge even in this simple model. With the aid of computers, however, we managed to evaluate the quantities of interest in a 4p-4h space for systems with up to 8 particles as will be shown in the last section.

4 Numerical Comparison

The three approximations presented in the previous section are compared with the exact solution based on the binding energies (Figure 1). From this figure one clearly designates the critical RPA strength

$$G_{crit} = -\frac{\varepsilon}{2(N-1)}, \tag{40}$$

which delineates the regions where a real solution exists and the one in which only a complex solution can be obtained. It is worthwhile to notice that the critical point stands just at the transition between the two nearly linear sections of the exact solution which are more distinguished in systems with a larger number

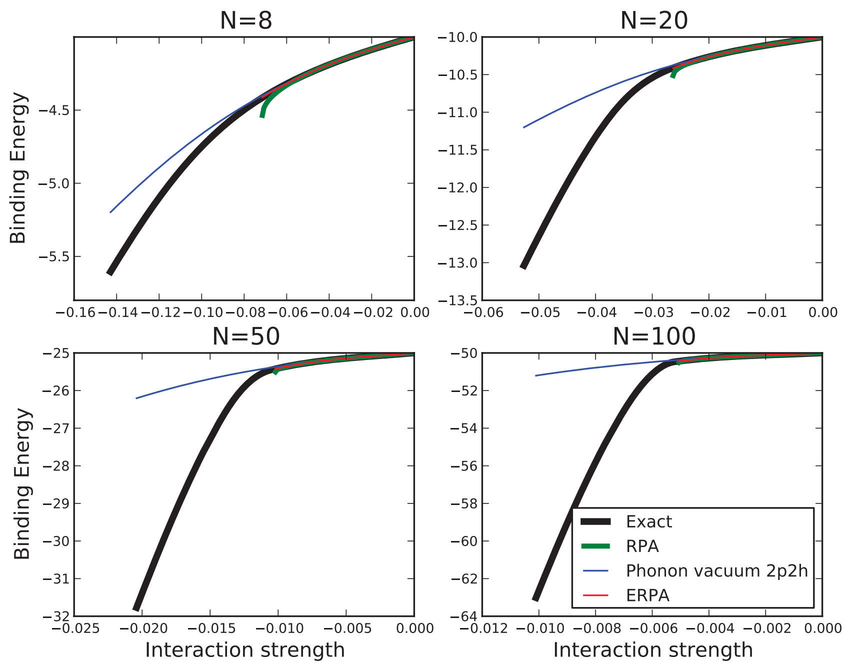

Figure 1. Binding energies (MeV) of two-level LMG model systems with $N = 8, 20, 50, 100$ particles as function of the interaction strength G(MeV). The energy gap between the two levels is set to 1 MeV.

of particles. The ERPA solution is also plotted in the same region as the RPA, *i.e.* $(G_{crit}, 0]$ and there ERPA performs much better than RPA as the former does not exhibit the overbinding near the critical point of the latter. Formally one can derive a critical strength for the ERPA as well as:

$$G_{crit} = -\frac{\varepsilon}{2\left[(1-2\rho)N - 1\right]}. \tag{41}$$

The simplicity of this formula, however, can be deceptive because the particle occupation ρ depends on the interaction strength, *i.e.* $\rho = \rho(G)$, which implies the self-consistent nature of the problem. We left this problem open for a future study.

The explicit variation of the phonon vacuum with 2p-2h admixtures on the other side yields solution for any G. Increasing the interaction beyond the RPA critical point causes progressive divergence of this solution from the exact one. This divergence exacerbates incrementing the number of particles in the system which elucidates the fact that in the strong interaction regime multi-particle-hole admixtures start to play a dominant role. Our endevours to take into account 4p-4h configurations have been impeded by the calculation of the following average

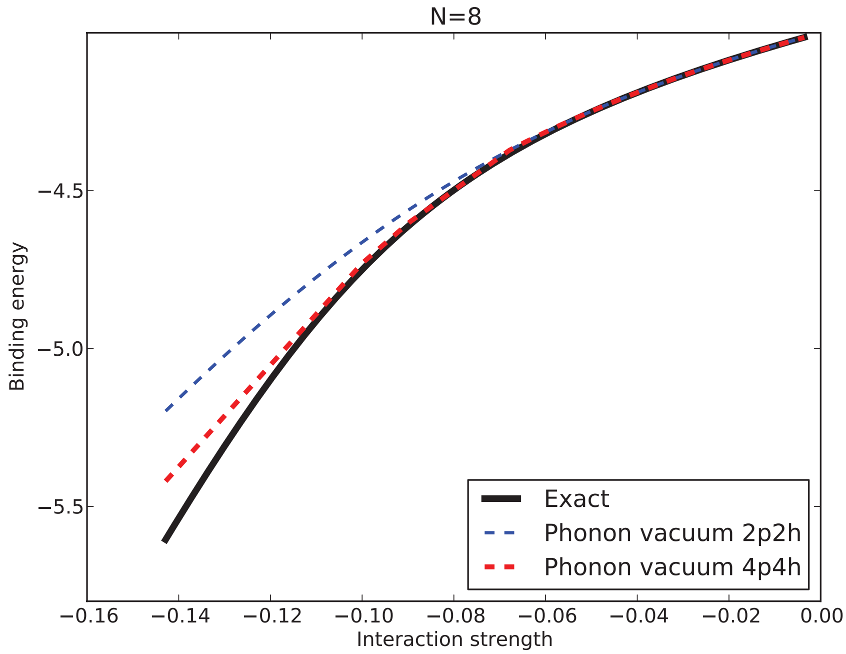

Figure 2. Same as in Figure 1 but for $N = 8$ particles only with 4p4h configurations included.

values

$$\langle s_2 s_1 s_3 s_4 J_- J_+ s_5^\dagger s_6^\dagger s_7^\dagger s_8^\dagger \rangle, \tag{42}$$

which we managed to handle with the aid of a computer for systems of up to 8 particles. The result is presented in Figure 2 which exhibits the fact that the 4p-4h solution is closer to the exact one than the 2p-2h solution which vindicates the prescription of the variational principle for monotonic convergence.

5 Conclusion and Outlook

In this work we initiated the development of a variational approach for approximating the ground state of nuclei tailored to take into account the action of the long-range residual forces. Essentially it is an attempt to provide a controlled succession of approximations for estimating the contributions from different multi-particle-hole admixtures. Applying our idea to the uncomplicated LMG model we showed its superiority over the RPA based on comparison with the exact solution for the binding energy. One drawback of the present development is that the complexity of calculating analytically higher order terms, which as shown in Sec. 4 play increasing important role in systems with larger number (> 10) of particles, escalates rapidly. For that purpose specific summation methods might prove very helpful. Being a many-body wave function the present development is expected to excel in describing phenomena involving many-particle correlations as, for example, cluster configurations. The influence of the long-range residual forces on the mean-field and the pairing correlations is another perspective which is currently progressing.

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