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# Study of Approximations in the Nuclear Pairing-Force Problem

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The solvable two-level pairing model is used to test two new number-conserving approximations. These approximations are compared with the exact results, with perturbation theory, with the BCS method, and with the projected BCS method of Kerman, Lawson, and Macfarlane. It is found that second-order perturbation theory and one of the tested approximations work rather well for not too high values of the pairing-force strength, while for higher values the other approximation turns out to be quite good.

## I. INTRODUCTION

The first step in many nuclear calculations is made by use of the BCS method. However, in this procedure an important symmetry of the system is broken; namely, the wave functions are not eigenfunctions of the number operator. The dispersion in the number is of the order of $N^{1/2}$, where $N$ is the number of the particles in the system. This is almost negligible in the theory of superconductivity, whence the BCS approximation originated, but its spurious effects may be quite considerable in the nuclear case. Another drawback inherent in the BCS approach is, as is well known (see, e.g., Hogaasen-Feldman,[1] Rho and Rasmussen,[2] Mang, Rasmussen, and Rho[3]), that there may be a critical value of the pairing-force strength below which there is no solution to the BCS equations, except for the trivial one that gives no configuration mixing at all. This aspect of the BCS approach is clearly unphysical and, again, may be traced to the dispersion in the number of the particles.

Some time ago, Unna and Weneser (UW)[4] put forward a method by which the spurious effects of the dispersion in the number of particles are

eliminated within the random-phase approximation (RPA). In a more recent work,[5] a variational approach to the nuclear many-body problem was suggested. This approach takes into account (approximately) two-body correlations in the ground state. In the present note we study these two methods by their application to the exactly solvable two-level pairing model (see e.g., Refs. 1, 2, and Brown[6]). The results of these methods are compared with the exact ones, with second-order perturbation theory, with the BCS method, and with (an approximate version of) the projected BCS method of Kerman, Lawson, and Macfarlane (KLM).[7] We find that perturbation theory (which to the best of our knowledge has not as yet been applied to this problem) yields surprisingly good results for not too high values of the pairing-force strength. This conclusion holds also for the variational approach ($F$). These two approximations, which are rather simple and by their nature number conserving, may be especially useful in those cases where there is no solution (except for the trivial one) to the BCS equations. The method of projection *before* variation,[3,8] which gives nontrivial solutions in those cases, is certainly more cumbersome than the above-mentioned methods. For higher values of the interaction we find that the UW method yields quite good results.

## II. BRIEF SURVEY OF MODEL AND APPROXIMATIONS

### A. Model

The pairing-force Hamiltonian is given by

$$H=\sum_j \epsilon_j N_j-\tfrac{1}{4}G\sum_{jj'mm'}(-1)^{j-m}(-1)^{j'-m'}\times a_{jm}^{\dagger}a_{j-m}^{\dagger}a_{j'-m'}a_{j'm'}. \tag{1}$$

Here

$$N_j=\sum_m a_{jm}^{\dagger}a_{jm}. \tag{2}$$

We restrict ourselves to the numerically solvable case of just two levels, which we designate by the indices 1 and 2. The degeneracy of the $i$th level ($i=1, 2$) is $g_i^2$, i.e.,

$$g_i^2=2j_i+1, \quad i=1, 2. \tag{3}$$

The energy difference between the two levels is $\epsilon$. We choose

$$\epsilon_1=0, \quad \epsilon_2=\epsilon. \tag{4}$$

Now, introduce the two sets of quasispin operators (see, e.g., Refs. 2 and 6):

$$S_+=\sum_{m>0}(-1)^{j_1-m}a_{j_1m}^{\dagger}a_{j_1-m}^{\dagger}=S_-^{\dagger}, \tag{5a}$$

$$S_z=\tfrac{1}{2}(N_1-\tfrac{1}{2}g_1^2), \tag{5b}$$

$$L_+=\sum_{m>0}(-1)^{j_2-m}a_{j_2m}^{\dagger}a_{j_2-m}^{\dagger}=L_-^{\dagger}, \tag{6a}$$

$$L_z=\tfrac{1}{2}(N_2-\tfrac{1}{2}g_2^2). \tag{6b}$$

The $S$ operators commute with the $L$ operators, and each set of operators by itself satisfies angular momentum commutation relations. In terms of these operators, the two-level pairing Hamiltonian reads

$$H=\tfrac{1}{2}\epsilon g_2^2+2\epsilon L_z-G(L_++S_+)(L_-+S_-). \tag{7}$$

It is also possible to introduce a total quasispin operator $\vec{J}$ by defining

$$\vec{J}=\vec{S}+\vec{L}. \tag{8}$$

In terms of $\vec{J}$, our Hamiltonian assumes the form

$$H=\tfrac{1}{2}\epsilon g_2^2+2\epsilon L_z-GJ_+J_-, \tag{9}$$

which is convenient for studying the strong-coupling limit.

We limit ourselves to a system with an even number of particles and to the study of the ground state and the first excited state $0^+$. The relevant unperturbed states in that case are

$$|SS_z, LL_z\rangle$$

with an obvious notation. Since the $S$ and $L$ operators do not change the quantum numbers $S$ and $L$, we shall omit $S$ and $L$ in the following, keeping in mind for calculational purposes that the relevant $(S, L)$ multiplet is defined by

$$S=\tfrac{1}{4}g_1^2, \quad L=\tfrac{1}{4}g_2^2. \tag{10}$$

The unperturbed ground state $|\Phi_0\rangle$ of the $N$-particle system ($N$ being an even integer) is

$$|\Phi_0\rangle=|-\tfrac{1}{4}g_1^2+\tfrac{1}{2}N, -\tfrac{1}{4}g_2^2\rangle. \tag{11}$$

The relevant states of the $N$-particle system are obtained by the application of the operator $L_+S_-$ to $|\Phi_0\rangle$. It is rather easy to calculate the matrix elements of $H$ between these states and then diagonalize the resulting matrix.

### B. BCS Approximation

The BCS theory is well known. For the present model, the BCS ground-state energy is

$$E_g=\epsilon g_2^2 v_2^2-\Delta^2/G-\tfrac{1}{2}G(g_1^2v_1^4+g_2^2v_2^4), \tag{12}$$

while the energy of the first excited state $0^+$ is given by

$$E(0^+)=E_g+2\min\{E_1, E_2\}. \tag{13}$$

Here,

$$E_1=(\lambda^2+\Delta^2)^{1/2}, \tag{14}$$

$$E_2=[(\epsilon-\lambda)^2+\Delta^2]^{1/2}. \tag{15}$$

### C. Projected BCS Method (KLM)

According to this method,[7] matrix elements of physical quantities should be calculated with wave functions obtained by projecting out and normalizing the part of the BCS wave function corresponding to the correct number of particles. Actually, in the present case we have not carried out the exact calculation in accordance with the above prescription, but have carried out the calculation only up to order $g^2$, as discussed in Ref. 4.

### D. Elimination of Number Dispersion in RPA (UW)

Within the framework of the RPA it is easy and straightforward to separate out explicitly any desired degree of freedom.[4,9-12] In our case, this is the number degree of freedom in the BCS treatment of pairing correlations. The method expounded in Ref. 4 (see also Refs. 9–12) identifies and removes the spurious effects of the BCS treatment (within the RPA).

### E. Second-Order Perturbation Theory (PERT.)

There is nothing novel here about second-order perturbation theory, except possibly for its application to the present problem. Its calculation for the two-level model is quite easy; the only states which may contribute to the perturbation of a state $|S_z, L_z\rangle$ are $|S_z, L_z\rangle$ itself (in first order) and $|S_z+1, L_z-1\rangle$, $|S_z-1, L_z+1\rangle$ (in second order).

### F. Approach by Variationally Determined Transformation ($F$)

This approach[5] starts with an approximate calculation of two-body ground-state correlations, which are introduced by means of a unitary operator $e^{iF}$. The approximate ground state is written as

$$|\Psi_0\rangle = e^{iF}|\Phi_0\rangle . \tag{16}$$

Here $|\Phi_0\rangle$ is the unperturbed ground state, and $F$ is a one- and two-body Hermitian operator to be determined by minimizing $\langle\Psi_0|H|\Psi_0\rangle$. Assuming that higher powers of $F$ than the second may be neglected, the variation leads to a set of linear nonhomogeneous equations for the matrix elements of $F$. Then, we define $H'$ by

$$H' = e^{-iF} H e^{iF} . \tag{17}$$

In lowest order, the diagonal matrix elements of $H'$ are taken as the eigenenergies of the system. For reference purposes, we have dubbed this method the $F$ approximation.

For the present model, $F$ assumes the form

$$F = fL_+S_- + f^*S_+L_- . \tag{18}$$

The variation (up to second order in $f$) yields

$$f = -\tfrac{1}{2}iG/[\epsilon - \tfrac{1}{2}(\tfrac{1}{2}g_2^2 - \tfrac{1}{2}g_1^2 + N - 2)G] . \tag{19}$$

The ground-state energy in the present approximation is given by

$$E_g = \langle\Phi_0|H'|\Phi_0\rangle , \tag{20}$$

while the energy of the first excited state $0^+$ is given by

$$E(0^+) = \langle\Phi_0|S_+L_-H'L_+S_-|\Phi_0\rangle / \langle\Phi_0|S_+L_-L_+S_-|\Phi_0\rangle . \tag{21}$$

It should be noted that for the case

$$\tfrac{1}{2}g_2^2 - \tfrac{1}{2}g_1^2 + N - 2 > 0$$

we have a "natural" boundary for the validity of the present method, because $f$ as a function of $G$ has then a pole at

$$G = [\tfrac{1}{2}(\tfrac{1}{2}g_2^2 - \tfrac{1}{2}g_1^2 + N - 2)]^{-1} . \tag{22}$$

Obviously the assumption that $f$ is small goes wrong when one approaches the vicinity of the pole.

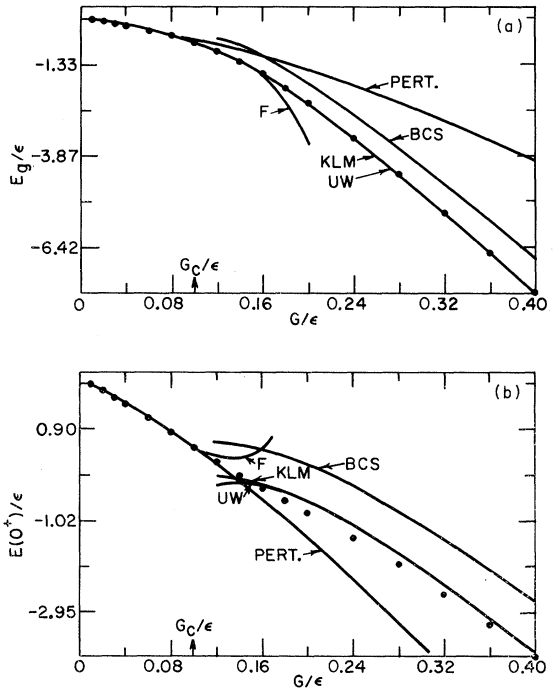


FIG. 1. (a) The ground-state energy $E_g/\epsilon$ for $N=10$, $g_2^2=10$, as a function of the pairing-interaction strength $G/\epsilon$. Dots denote the exact solution. The critical interaction strength below which there is only a trivial solution to the BCS equation is $G_c/\epsilon=0.1$. The results of the $F$ approximation are plotted up to the vicinity of the pole (see text). (b) The same as in Fig. 1(a) for the energy of the first excited state $E(0^+)/\epsilon$.

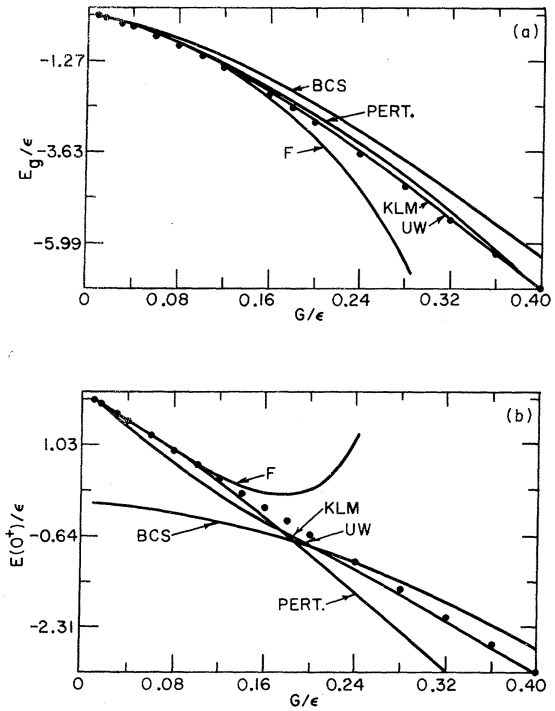


FIG. 2. (a) The same as in Fig. 1(a) for $N=6$. Note that in this case ($N<g_1^2$) there is no critical interaction strength. (b) As in Fig. 2(a) for $E(0^+)/\epsilon$.

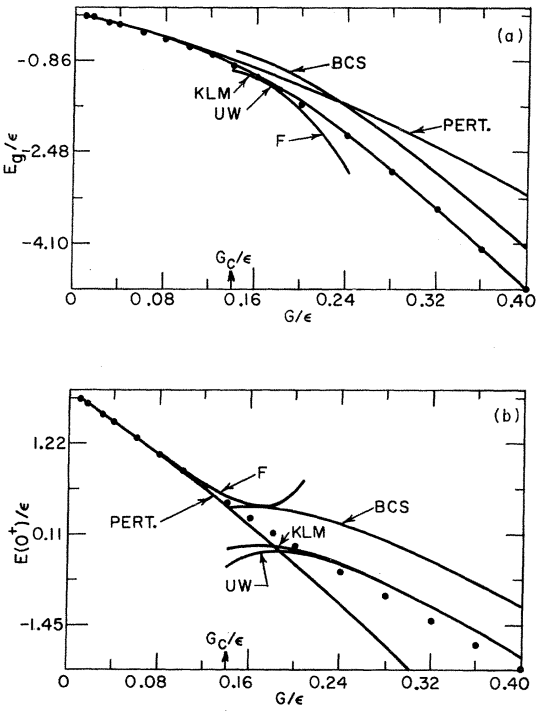


FIG. 3. (a) As in Fig. 1(a) for $g_2^2=6$. The critical interaction strength is $G_c/\epsilon=0.14$. (b) As in Fig. 3(a) for $E(0^+)/\epsilon$.

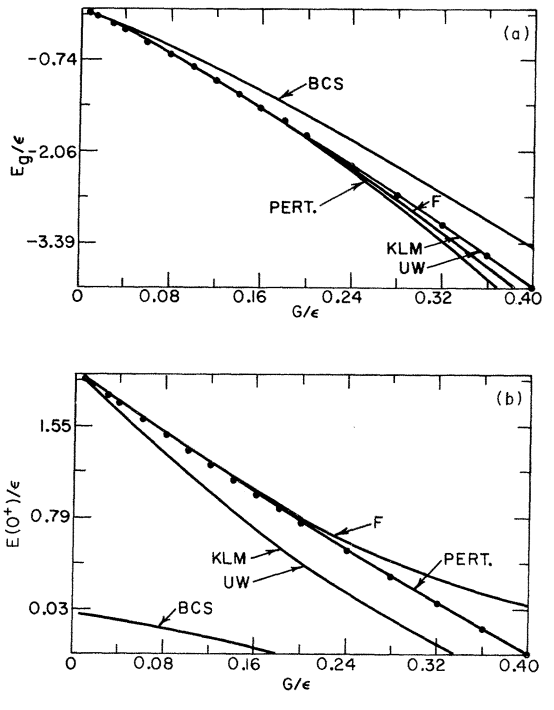


FIG. 4. (a) As in Fig. 1(a) for $N=4$, $g_2^2=4$. Note that in this case the $F$ approximation has no pole, and no critical interaction strength exists for the BCS approximation. (b) As in Fig. 4(a) for $E(0^+)/\epsilon$.

## III. RESULTS AND DISCUSSION

For a comparison of the various approximations we have fixed the degeneracy of the lower level to be

$$g_1^2=10$$

and have varied values of $g_2^2$ and $N$ as parameters. Typical results are presented in Figs. 1–4, where the exact values of the ground-state energy ($E_g$) and the energy of the first excited state [$E(0^+)$], together with the approximate results, are plotted as functions of the pairing interaction strength $G$.

The first conclusion to be drawn from the exact and approximate results is that the BCS approximation *proper* yields relatively poor results both for the ground state and for the first excited state energies. For the cases in which

$$N<g_1^2,$$

there is always a nontrivial solution to the BCS equations, but even in these cases the BCS results for $E_g$ and $E(0^+)$ are unsatisfactory. This is undoubtedly due to the spurious components contained in the BCS wave functions, which are not eigenfunctions of the particle-number operator. The (approximate) projected BCS method (KLM)

and the UW method aim to remedy this defect. In all the cases considered the (approximate) KLM and UW results are practically identical. In contrast to the BCS results, the KLM and UW results are very good for the ground-state energy and fairly good for the energy of the first excited state. Both energies improve with the increase of the pairing strength $G$. This latter aspect may also be verified directly in the symmetrical case ($g_1^2 = g_2^2 = N$) in which the BCS equations (and consequently the KLM and UW approximations) are solvable analytically,[2] and the approximate results may be compared with the exact ones in the strong-coupling limit. The fact that $E_g$ is better reproduced in the (approximate) KLM and UW methods than $E(0^+)$ is not really surprising, since both methods employ the BCS $u$'s and $v$'s which are determined from the variational principle for the ground state.

Being based on the BCS method, the KLM and UW approximations still suffer from the other drawback of the BCS method; namely, the existence of a critical value for the interaction strength, $G_c$, below which the BCS equations have only the trivial solution. Consequently, the KLM and UW methods yield only trivial results in this region. The existence of a $G_c$ does not imply any real phase transition in the model (as is evidenced by the exact results), but is merely a spurious effect of the BCS treatment. Nonetheless, it was pointed out in Ref. 1 that none of the approximations considered there were reliable in the neighborhood of $G_c$. The method of projection *before* variation[3,8] is devised to cope with this situation. However, it appears that much simpler methods may be adequate. Both second-order perturbation theory and the $F$ approximation are seen, in all the cases considered, to yield very good results both for $E_g$ and for $E(0^+)$ for not too high values of $G$. When there is a critical value $G_c$, second-order perturbation theory and the $F$ approximation work well up to $G_c$ and above it, at least until the KLM and UW approximations start to be reliable. This holds also in the cases when there is no critical value for the pairing-interaction strength.

In conclusion, it seems that whenever the BCS approximation, and especially its number-conserving extensions (KLM and UW), do not work due to the weakness of the interaction, perturbative or semiperturbative ($F$) methods may be successfully applied. In this sense, second-order perturbation theory and the $F$ approximation may be regarded as complementary to the KLM and UW approximations, the first pair of approximations being valid in the very same region where the second pair is invalid.

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