Pairing correlations studied in the two-level model

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We study the pairing energy in the ground state of a system of N particles occupying a symmetric two-level model space with a level degeneracy Ω. Assuming a pairing Hamiltonian, we calculate the energies of the projected BCS states, using the exact, the Kamlah, and the Lipkin-Nogami particle number projection methods. We find that conclusions regarding the quality of the B.C.S. approximation as well as various approximate projection methods, drawn from studying the $N=\Omega$ case alone, are not valid in the more general $N \neq \Omega$ case when the pairing interaction is weak.

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I. INTRODUCTION

It is well known that pairing correlations are important in a nucleus with one or more open major shells. The Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity [1] is commonly applied to a nuclear system to simulate such correlations. The theory is quite satisfactory when the number of valence nucleons is large and the pairing interaction is strong compared to the level spacing. But in a nucleus with a relatively small number of valence nucleons or whose level gap is large, the BCS approximation either has no solution or introduces a non-negligible error to the pairing energy due to the particle number fluctuation in its wave function.

Various prescriptions have been introduced in the past to approximately project out a state with the right number of particles. These include the work of Kerman, Lawson, and Macfarlane (KLM) [2], Unna and Weneser (UW) [3], Kamlah [4], Lipkin [5], Nogami *et al.* [6, 7], and undoubtedly many others (see Ref. [8]). These projection methods were often validated by considering an exactly solvable symmetric two-level model [9] with the particle number N equal to the level degeneracy Ω [10–12]. In this special case, it was found that the BCS wave function has only a trivial minimum in energy when the pairing strength (G) is less than a critical value (G_c). In the strong pairing limit, the BCS pairing energy is a fraction $[(N-1)/N]$ of the exact result where the pairing energy is defined as the difference between the total energy and the Hartree–Fock energy for the ground state. It was also found [11] that the KLM and UW approximations are very accurate when the pairing strength is strong. However, since both the KLM and the UW are variation-before-projection (VBP) methods, they are not reliable when the pairing strength is close to or smaller than the critical value. On the other hand, second-order perturbation was found to be a very good approximation in this region [13]. Pradhan, Nogami, and Law [12] claimed, again by studying the special $N=\Omega$ case, that the Lipkin-Nogami prescription [5–7] works rather well for the entire range of the pairing force strength.

Interesting results can be obtained by considering the more general case in which $N \neq \Omega$. For example, Bishari, Unna, and Mann [11] showed that the critical behavior of the BCS solution is not present when $N \neq \Omega$ since the BCS wave function always has a nontrivial minimum (i.e., an extremum). They also examined the KLM and UM methods in this context.

In this work we will restrict ourselves to the symmetric two-level model but allowing for $N \neq \Omega$ as well as $N=\Omega$. We will focus on the variation-after-projection (VAP) method of Kamlah [4] and the Lipkin-Nogami prescription [5–7]. These two projection methods have been shown to yield a non-trivial minimum even in the $N=\Omega$ case for all values of the pairing strength. And, like the VBP methods of KLM [2] and UW [3], they are also very accurate when the pairing correlations are strong. For completeness, we will also include the independent pair approximation, the BCS approximation and, in the case of $N=\Omega$, the BCS solution with exact particle number projection.

We will concentrate on the ground-state pairing energy, which is the difference of the total energy and the Hartree-Fock (HF) energy for the ground state. This is justified because in the case of a weak pairing force, the pairing energy is only a small fraction of the total energy; even the HF energy is not a bad approximation to the total energy (i.e., the relative error is small). It would therefore be difficult to judge the quality of an approximate method if one were comparing the total energies only. In addition, one must not forget that low energy nuclear collective motion is influenced as strongly by the variation of pairing energy as by the HF energy although in medium and heavy nuclei the former is often at least three orders of magnitude smaller than the latter.

II. THE MODEL

As already stated, we consider a two-level model space with a degeneracy Ω (even) for each level. The pairing

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Hamiltonian for this model space is

$$\hat{H} = \sum_{k=1}^{\Omega} \epsilon_k \left(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}} \right) - G \sum_{k,l=1}^{\Omega} a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{l}} a_l, \qquad (1)$$

where $\epsilon_k = -\epsilon$ if $|k| \leq \Omega/2$ and $\epsilon_k = +\epsilon$ if $|k| > \Omega/2$. Thus the energy gap between the two levels is 2ϵ. To each state $|k\rangle$ there is a time reversed conjugate state $|\bar{k}\rangle$.

The exact solution can be obtained by introducing *two* sets of quasispin operators which satisfy the angular momentum commutation rules, as has been done by many others [8]:

$$\begin{aligned} J_{+,L} &= \sum_{k=1}^{\Omega/2} a_k^\dagger a_{\bar{k}}^\dagger, \quad J_{+,U} = \sum_{k=\Omega/2+1}^{\Omega} a_k^\dagger a_{\bar{k}}^\dagger, \\ J_{-,L} &= \sum_{k=1}^{\Omega/2} a_{\bar{k}} a_k, \quad J_{-,U} = \sum_{k=\Omega/2+1}^{\Omega} a_{\bar{k}} a_k, \\ J_{z,L} &= \frac{1}{2} \sum_{k=1}^{\Omega/2} \left(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}} \right) - \frac{\Omega}{4}, \\ J_{z,U} &= \frac{1}{2} \sum_{k=\Omega/2+1}^{\Omega} \left(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}} \right) - \frac{\Omega}{4}. \end{aligned} \qquad (2)$$

In terms of these operators, the Hamiltonian and the particle number operator can be expressed as

$$\hat{H} = 2\epsilon(J_{z,U} - J_{z,L}) - G\left(J_{+,L} + J_{+,U}\right)\left(J_{-,L} + J_{-,U}\right), \qquad (3)$$

$$\hat{N} = \Omega + 2(J_{z,L} + J_{z,U}). \qquad (4)$$

The ground state of the system belongs to the subspace generated by the tensor product of multiplets of J_L and J_U having maximal J. Since each level has a degeneracy Ω, the maximal "total angular momentum" value J of either J_L or J_U is equal to $\Omega/4$. The solution is an eigenstate of the third component of the total quasispin in the space generated by the kets $|M_L, M_U\rangle$ which are eigenstates of $J_{z,L}$ and $J_{z,U}$ with eigenvalues M_L and M_U, respectively. Here M_L and M_U are related to each other by $M_L + M_U = (N - \Omega)/2$ where M_L takes the values

$$M_L = \begin{cases} -\frac{\Omega}{4}, \frac{2-\Omega}{4}, \ldots, \frac{2N_a-\Omega}{4} & (\text{for } N \leq \Omega), \\ \frac{\Omega-2N_a}{4}, \frac{2+\Omega-2N_a}{4}, \ldots, \frac{\Omega}{4} & (\text{for } N \geq \Omega), \end{cases}$$

where N_a=N for $N \leq \Omega$ and N_a=$2\Omega - N$ for $N > \Omega$. The problem is thus reduced to the diagonalization of a tridiagonal matrix of dimension $(N_a/2+1)$ whose matrix elements are given by [recall that $M_L+M_U = M'_L+M'_U = (N-\Omega)/2$]

$$\begin{aligned} H_{M_L,M'_L} &= \langle M_L, M_U | \hat{H} | M'_L, M'_U \rangle \\ &= \{2\epsilon(M_U - M_L) - G[(J + M_L)(J - M_L + 1) + (J + M_U)(J - M_U + 1)]\}\, \delta_{M_L,M'_L} \\ &\quad - G\sqrt{(J - M_L)(J + M_L + 1)(J + M_U)(J - M_U + 1)}\, \delta_{M_L,M'_L-1} \\ &\quad - G\sqrt{(J + M_L)(J - M_L + 1)(J - M_U)(J + M_U + 1)}\, \delta_{M_L,M'_L+1}. \end{aligned} \qquad (5)$$

We will concentrate on the pairing energy which is defined as

$$E_p \equiv E - E_{\rm HF}, \qquad (6)$$

where $E = \langle \psi_g | H | \psi_g \rangle$ is the total ground-state energy of the system and $E_{\rm HF}$ the HF energy which is given by

$$E_{\rm HF} = (N_U - N_L)\epsilon - \frac{NG}{2}, \qquad (7)$$

where N_L=N and N_U=0 if $N \leq \Omega$; and N_L=Ω and N_U=$N - \Omega$ if $N > \Omega$.

We will also consider the independent pair approximation (IPA) for which all pairs occupy the lowest possible level. The IPA state is an eigenstate of the one-body term in Eq. (1); its energy expectation value is

$$E_{\rm IPA} = (N_U - N_L)\epsilon - [N(\Omega + 2 - N) + 2N_L N_U]\frac{G}{4}. \qquad (8)$$

Note that in the case of N=Ω, the IPA energy is equal to the HF energy but otherwise it is lower than the HF energy. For Ω=10, the IPA and HF energies for different N are as follows:

N	4	6	8	10	12	14	16
$E_{\rm IPA}$	$-4\epsilon-8G$	$-6\epsilon-9G$	$-8\epsilon-8G$	$-10\epsilon-5G$	$-8\epsilon-10G$	$-6\epsilon-13G$	$-4\epsilon-14G$
$E_{\rm HF}$	$-4\epsilon-2G$	$-6\epsilon-3G$	$-8\epsilon-4G$	$-10\epsilon-5G$	$-8\epsilon-6G$	$-6\epsilon-7G$	$-4\epsilon-8G$

In the special case of $N=\Omega$, the following expressions for the pairing energy hold in the small (Nx) and large (Nx) limits, respectively [$x \equiv G/(2\epsilon)$]:

$$E_p^{\text{exact}} \simeq -\frac{N^2Gx}{8} - \frac{N^2(N-2)Gx^2}{16} \quad (N=\Omega,\ Nx \ll 1), \tag{9}$$

$$E_p^{\text{exact}} \simeq -\frac{N^2G}{4} + N\epsilon - \frac{N\epsilon}{2(N-1)x} \quad (N=\Omega,\ Nx \gg 1). \tag{10}$$

III. BCS APPROXIMATION

The BCS ground-state wave function is

$$|\text{BCS}\rangle = \prod_{k=1}^{\Omega}(u_k + v_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle, \tag{11}$$

where $|-\rangle$ is the bare vacuum state, $u_k^2+v_k^2=1$ with v_k^2 the probability that the states $|k\rangle$ and $|\bar{k}\rangle$ are occupied. In the two-level model space, one can identify all u_k and v_k for $k \le \Omega/2$ as u_L and v_L for the lower level and all u_k and v_k for $k > \Omega/2$ as u_U and v_U for the upper level. Since v_U can be related to v_L by $(v_L^2 + v_U^2)\Omega = N$, there is only one free parameter, which we choose to be v_L. The BCS energy is then

$$\begin{aligned} E_{\text{BCS}} &= \langle \text{BCS}|\hat{H}|\text{BCS}\rangle \\ &= \sum_{k=1}^{\Omega} 2\epsilon_k v_k^2 - G\sum_{k=1}^{\Omega} v_k^4 - G\sum_{k,l=1}^{\Omega} u_k v_k u_l v_l \\ &= \Omega\epsilon(v_U^2 - v_L^2) \\ &\quad -\frac{\Omega G}{2}\left[v_U^4 + v_L^4 + \frac{\Omega}{2}(u_L v_L + u_U v_U)^2\right]. \end{aligned} \tag{12}$$

In the special case of $N=\Omega$, it is easy to show that the BCS energy has only a trivial minimum if $G < G_c \equiv 2\epsilon/(\Omega-1)$. In this case, the BCS energy reaches its lowest value (not an extremum) when $v_L^2=1$, and is identical to the HF energy (and to the IPA energy). One can also show that in the strong pairing limit, i.e., $G \gg G_c = 2\epsilon/(\Omega-1)$, the limit of the BCS pairing energy ($E_{\text{BCS}} - E_{\text{HF}}$) is $(\Omega-1)/\Omega$ of the exact result (10).

However, these observations are no longer true if we go beyond $N=\Omega$ to a more general case for which $N \neq \Omega$. In the latter case, the BCS energy has a nontrivial minimum for all values of (G/ϵ). And, in the small G/ϵ limit, the BCS energy is *higher* than the IPA energy while it is obviously lower than the HF energy. In fact, one can write down for $G \to 0$

$$E_{\text{BCS}} - E_{\text{IPA}} = \begin{cases} \frac{GN(\Omega-N)}{2\Omega} \ge 0 & (\text{for } N \le \Omega), \\ \frac{G(N-\Omega)(2\Omega-N)}{2\Omega} \ge 0 & (\text{for } N \ge \Omega); \end{cases} \tag{13}$$

and

$$E_{\text{BCS}} - E_{\text{HF}} = \begin{cases} \frac{GN(\Omega-N)(2-\Omega)}{4\Omega} \le 0 & (\text{for } N \le \Omega), \\ \frac{G(N-\Omega)[2(2\Omega-N)-N\Omega]}{4\Omega} \le 0 & (\text{for } N \ge \Omega). \end{cases} \tag{14}$$

The equalities hold only when $N=\Omega$. In this case, the HF, BCS, and IPA wave functions are equal.

The inequalities (13) and (14) can be understood by noting that in the $N \neq \Omega$ case, even in the small G/ϵ limit, there are several degenerate Slater determinants available to form the ground state. The exact wave function, which, when $G=0$, is also the IPA wave function, is a proper mixing of all these degenerate Slater determinants. The HF state is only one of them. The BCS state contains a configuration mixing of all the components but it also includes components with a wrong particle number. We can thus say that for $N \neq \Omega$ and in the small G/ϵ limit, the BCS energy is lower than the HF energy because of configuration mixing in the BCS state; it is higher than the IPA energy because of the particle number fluctuation in the BCS wave function.

IV. BCS WITH PARTICLE NUMBER PROJECTION

A state with a definite number of particles can be obtained by applying the particle number projection operator $\hat{P}_N$ to the BCS state. Closely following Ring and Schuck [8], we write the projection operator as (for N even)

$$\hat{P}_N = \frac{1}{\pi}\int_0^{\pi} d\phi \exp[i\phi(\hat{N} - N)]. \tag{15}$$

In a system of a finite number of particles, the above integral can be replaced by a sum [13]. Replacing the integral by a K-point trapezoid sum leads to the following operator:

$$\hat{P}_N^{(K)} = \frac{1}{K}[1 + e^{i(\hat{N}-N)\pi/K} + e^{i(\hat{N}-N)2\pi/K} + \cdots + e^{i(\hat{N}-N)(K-1)\pi/K}] = \frac{1}{K}\left[\frac{1-e^{i(\hat{N}-N)\pi}}{1-e^{i(\hat{N}-N)\pi/K}}\right]. \quad (16)$$

When applied to the BCS state, this operator removes all except the $N \pm 2K$, $N \pm 4K$, ..., spurious components. It is therefore an exact projection operator for a model space which can hold less than $2K$ particles. In the case of the two-level model that we consider here, we need $K > \max\{\frac{N}{2}, \frac{2\Omega-N}{2}\}$ for an exact projection.

The projected BCS state with N particles is

$$|\mathrm{BCS}\rangle_N = \hat{P}_N|\mathrm{BCS}\rangle = \frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{e^{iN\phi/2}}\prod_{k>0}(u_k + v_k e^{i\phi}a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle, \quad (17)$$

where we have used the relation

$$e^{i\hat{N}\phi}|\mathrm{BCS}\rangle = \prod_{k>0}(u_k + v_k e^{2i\phi}a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle. \quad (18)$$

The wave function (17) is not normalized to unity. The normalization is given by the integral

$$\langle\mathrm{BCS}|\mathrm{BCS}\rangle_N = \frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{e^{iN\phi/2}}\prod_{k>0}(u_k^2 + v_k^2 e^{i\phi}) \equiv R_0^0. \quad (19)$$

Note that the quantity v_k^2 cannot be identified as the occupation probability of states $|k\rangle$ and $|\bar{k}\rangle$, which is instead determined by

$$n_k = \frac{\langle\mathrm{BCS}|a_k^\dagger a_k|\mathrm{BCS}\rangle_N}{\langle\mathrm{BCS}|\mathrm{BCS}\rangle_N} = \frac{v_k^2 R_1^1(k)}{R_0^0}. \quad (20)$$

In the above equations, we have defined for convenience [8]

$$R_n^m(k_1, k_2, \ldots, k_m) = \frac{1}{2\pi}\int_0^{2\pi}\frac{d\phi}{e^{i(N/2-n)\phi}}\prod_{k>0, k\neq k_1,k_2,\ldots,k_m}(u_k^2 + e^{i\phi}v_k^2). \quad (21)$$

The pairing energy for the projected BCS state is then given by

$$E_p^{\mathrm{proj}} = \frac{\langle\mathrm{BCS}|\hat{H}|\mathrm{BCS}\rangle_N}{\langle\mathrm{BCS}|\mathrm{BCS}\rangle_N} - E_{\mathrm{HF}}, \quad (22)$$

where

$$\langle\mathrm{BCS}|\hat{H}|\mathrm{BCS}\rangle_N = \sum_{k=1}^{N}\left[2\epsilon_k v_k^2 R_1^1(k) - G v_k^4 R_2^2(k,k)\right] - G\sum_{k,l=1}^{N} u_k v_k u_l v_l R_1^2(k,l). \quad (23)$$

For the case of N=Ω, one has the simplification v_L=u_U, v_U=u_L. It is relatively easy to work out the pairing energy for the exactly projected BCS state, which is

$$E_p^{\mathrm{Proj}} = \frac{N\epsilon\int_0^\pi d\phi\,\mathcal{A}^{N/2-2}\left[\mathcal{A}^2 - \mathcal{B}\right]}{\int_0^\pi d\phi\,\mathcal{A}^{N/2}}, \quad (24)$$

where the functions $\mathcal{A}(\phi)$ and $\mathcal{B}(\phi)$ are given by

$$\mathcal{A}(\phi) = \cos^2\phi + c^2\sin^2\phi, \quad (25)$$

$$\mathcal{B}(\phi) = \mathcal{A}c + \frac{xs^2}{2}\left[(N-2)\cos^2\phi + \mathcal{A}\right] \quad (26)$$

with

$$c = v_L^2 - u_L^2 = u_U^2 - v_U^2, \qquad s = 2v_L u_L = 2v_U u_U. \quad (27)$$

As mentioned before, all the integrals which appeared in the foregoing equations can be replaced by sums using the trapezoid rule. For Ω=10, a sum over K=6 points [see Eq. (16)] is already sufficient for an exact projection. The numerical result for E_p^{Proj} for a given set of parameters (N, ϵ, G) can then be obtained. For small Nx (i.e., $NG \ll 2\epsilon$), we find

$$E_p^{\mathrm{Proj}} \simeq -N\epsilon\left(\frac{Nx^2}{4}\right)\left(1 + \frac{(N-2)x}{2}\right) \quad (N=\Omega). \quad (28)$$

For large Nx,

$$E_p^{\mathrm{Proj}} \simeq -N\epsilon\left(\frac{Nx}{2} - 1 + \frac{1}{2(N-1)x}\right) \quad (N=\Omega). \quad (29)$$

The above two expressions are identical to the exact results (9), (10). Therefore the projected BCS result, although it is not exact, is very accurate in both the small and the large (Nx) limits. It will be of interest to see whether this is also true for the intermediate range of (Nx).

In Fig. 1 we show for the case of N=Ω the ratio R of E_p^{Proj} to E_p^{exact}; the latter is the exact pairing energy from matrix diagonalization (K=6 solid line). The results of replacing the integral in (24) by a two-point sum (K=2) or a four-point sum (K=4) are also shown. One sees that BCS with exact number projection is accurate in both the small x and large x limits. It introduces a relative error of less than 3.5% to the pairing energy when x is close to the critical value of $x_c = G_c/(2\epsilon) = 1/(\Omega-1) = \frac{1}{9}$.

The two-point (K=2) approximation (which removes the N=8 and 12 spurious components from the BCS wave function) is not good for all values of x. In the small x limit, with K=2, one obtains about 50% of the exact pairing energy. The four-point (K=4) approximation (which removes most spurious components from the BCS wave function but retains N=2, 18 components) is accurate for small x but not for large x. The superiority of the K=4 approximation may be connected with the fact that in this order one takes account of the fact that the parameters v may be complex. The order parameter for the pairing transition has dimension two, involving a gap parameter Δ and a gauge angle ϕ. The K=2 order projection uses only real values of v, see Eq. (18).

Also shown in the figure are the results for the Kamlah and the Lipkin-Nogami approximate projection methods which we will discuss next.

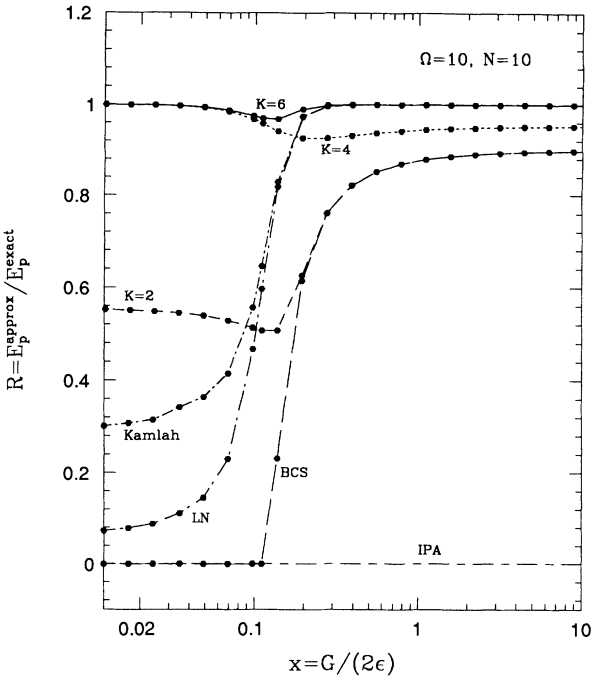

FIG. 1. The ratios of the pairing energy in various approximations to the exact result as a function of x=$G/(2\epsilon)$ in the case of N=Ω=10. The black dots signify points at which calculations were performed. Note that the K=6 curve is equivalent to BCS with exact particle number projection. See text for more details.

A. Kamlah method

In the Kamlah approximation [4], the pairing energy as a function of $\{v_k\}$ is given by

$$E_p^K(v_L) = E_{\rm BCS} - h_2\langle(\Delta\hat{N})^2\rangle \tag{30}$$

with $\Delta\hat{N} \equiv \hat{N} - N$ and "$\langle\hat{O}\rangle$" means the expectation value of the operator $\hat{O}$ in the *unprojected* BCS wave function (11). The parameter h_2 in the above equation is also a function of v_L and is given by

$$h_2 = h_2(v_L) = \frac{\langle\hat{H}[(\Delta\hat{N})^2 - \langle(\Delta\hat{N})^2\rangle]\rangle - \langle\hat{H}\Delta\hat{N}\rangle\langle(\Delta\hat{N})^3\rangle/\langle(\Delta\hat{N})^2\rangle}{\langle(\Delta\hat{N})^4\rangle - \langle(\Delta\hat{N})^2\rangle^2 - \langle(\Delta\hat{N})^3\rangle^2/\langle(\Delta\hat{N})^2\rangle}. \tag{31}$$

To evaluate h_2, we make use of the following identity [cf. Eq. (18)]:

$$\langle{\rm BCS}|e^{i\phi\hat{N}}|{\rm BCS}\rangle = \prod_{k>0}(u_k^2 + v_k^2 e^{2i\phi}) \tag{32}$$

and differentiate with respect to ϕ. In this way we obtain

$$\langle(\Delta\hat{N})^2\rangle = 4\sum_{k>0} u_k^2 v_k^2, \tag{33}$$

$$\langle(\Delta\hat{N})^3\rangle = 8\sum_{k>0} u_k^2 v_k^2 (u_k^2 - v_k^2), \tag{34}$$

$$\langle(\Delta\hat{N})^4\rangle = 3\langle(\Delta\hat{N})^2\rangle^2 + 4\langle(\Delta\hat{N})^2\rangle - 6\sum_{k>0}(2u_k v_k)^4. \tag{35}$$

Furthermore we have

$$\langle a_k^\dagger a_k(\Delta\hat{N})\rangle = \langle a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{k}} a_k(\Delta\hat{N})\rangle = 2u_k^2 v_k^2, \tag{36}$$

$$\langle a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{l}} a_l(\Delta\hat{N})\rangle = 2u_k v_k u_l v_l(1 - v_k^2 - v_l^2) \quad (k \neq l), \tag{37}$$

$$\left\langle a_k^\dagger a_k\left[(\Delta\hat{N})^2 - \langle(\Delta\hat{N})^2\rangle\right]\right\rangle = \left\langle a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{k}} a_k\left[(\Delta\hat{N})^2 - \langle(\Delta\hat{N})^2\rangle\right]\right\rangle = 4u_k^2 v_k^2(u_k^2 - v_k^2), \tag{38}$$

$$\left\langle a_k^\dagger a_{\bar{k}}^\dagger a_{\bar{l}} a_l\left[(\Delta\hat{N})^2 - \langle(\Delta\hat{N})^2\rangle\right]\right\rangle = 4u_k v_k u_l v_l\left[1 - 3(v_k^2 + v_l^2) + 2(v_k^4 + v_l^4) + 2v_k^2 v_l^2\right], \tag{39}$$

where the last equation holds for $k \neq l$. Therefore

$$\langle \hat{H}(\Delta\hat{N})\rangle = \sum_{k>0}\epsilon_k(2u_kv_k)^2 - G\sum_{k>0}(2u_kv_k^2)^2 + 2G\left(\sum_{k>0}u_kv_k\right)\sum_{k>0}u_kv_k(v_k^2-u_k^2), \tag{40}$$

$$\left\langle \hat{H}\left[(\Delta\hat{N})^2 - \langle(\Delta\hat{N})^2\rangle\right]\right\rangle = -8\sum_{k>0}\epsilon_k(u_kv_k)^2(v_k^2-u_k^2) + 8G\sum_{k>0}u_k^2v_k^4(v_k^2-2u_k^2)$$
$$+2G\left(\sum_{k>0}u_kv_k\right)\sum_{k>0}u_kv_k(8v_k^2u_k^2-1) - 2G\left(\sum_{k>0}u_kv_k(v_k^2-u_k^2)\right)^2. \tag{41}$$

Equations (33)–(41) are all we need to evaluate $h_2(v_L)$ and $E_p^K(v_L)$. The (VAP) Kamlah pairing energy is then obtained by minimizing $E_p^K(v_L)$ with respect to v_L, i.e.,

$$E_p^K = E_p^K(v_L^K) \tag{42}$$

with v_L^K determined by

$$\left[\frac{dE_p^K(v_L)}{dv_L}\right]_{v_L=v_L^K} = 0. \tag{43}$$

For $N=\Omega$, it is easy to show that

$$\frac{h_2}{\epsilon} = \frac{c-(N/2-1)x+(N-3/2)xs^2}{2+(N-3)s^2}, \tag{44}$$

where c and s have been defined in Eq. (27). When (Nx) is small ($Nx \ll 1$) the Kamlah pairing energy is approximately

$$E_p^K \simeq -N\epsilon\left(\frac{N^2x^2}{8(2N-3)}\right)\left(1+\frac{N(3N-4)(N-2)x}{(2N-3)^2}\right) \quad (N=\Omega). \tag{45}$$

Note that when N is large (but $Nx \ll 1$), the Kamlah pairing energy is about $\frac{1}{4}$ of the exact result (9) .

For $Nx \gg 1$, we find

$$E_p^K \simeq -N\epsilon\left(\frac{Nx}{2}-1+\frac{1}{2(N-1)x}\right) \quad (N=\Omega). \tag{46}$$

This agrees with the exact result (10).

It should be mentioned that, in the Kamlah method, it is only an approximation to identify $(v_L^K)^2$ which minimizes the energy (30) as the occupation probability of the lower level. A more consistent expression for this probability is given by

$$n_L^K = (v_L^K)^2 - \lambda_2\langle(\Delta\hat{N})^2\rangle, \tag{47}$$

where the parameter $\lambda_2(v_L^K)$ is given by the right-hand side of Eq. (31) with $\hat{H}$ replaced by the operator $(a_L^\dagger a_L)$ and evaluated at $v_L=v_L^K$.

B. Lipkin-Nogami method

At first glance, the Lipkin-Nogami (LN) projection method [5–7] is formally quite similar to the Kamlah method. The expression for the pairing energy is also (30). But to obtain the LN pairing energy, one performs a variation of the energy $E_p^K(v_L)$ with respect to v_L *while keeping* h_2 *constant*, i.e.,

$$E_p^{\rm LN} = E_p^K(v_L^{\rm LN}) \tag{48}$$

with $v_L^{\rm LN}$ determined by

$$\left[\frac{\partial E_p^K(v_L,h_2(v_L^{\rm LN}))}{\partial v_L}\right]_{v_L=v_L^{\rm LN}} = 0. \tag{49}$$

The LN pairing energy is therefore always higher than the Kamlah pairing energy.

In the case of $N=\Omega$, Eq. (49) leads to

$$\frac{h_2}{\epsilon} = \frac{1}{2c} - \frac{(N-1)x}{2}. \tag{50}$$

With this Eq. (44) can be simplified to yield:

$$\frac{h_2}{\epsilon} = \frac{(N-s^2)x}{2(N-1)s^2}. \tag{51}$$

Note that Eqs. (50) and (51), when combined, determine the value of c, s, or $v_L^{\rm LN}$ to be used to evaluate the LN pairing energy (48) for the case of $N=\Omega$.

For $Nx \ll 1$, the LN pairing energy is

$$E_p^{\rm LN} \simeq -N\epsilon\left(\frac{N^2x^2}{8(N-1)^2}\right)\left(1+\frac{2N(N-2)x}{N-1}\right) \quad (N=\Omega). \tag{52}$$

When $N \gg 1$ (but $Nx \ll 1$), this is only about $1/(2N)$ of the exact pairing energy (9). For large (Nx), we have

$$E_p^{\rm LN} \simeq -N\epsilon\left(\frac{Nx}{2}-1+\frac{1}{2(N-1)x}\right) \quad (N=\Omega). \tag{53}$$

This agrees with the exact result (10).

Also in the LN method, a consistent expression for the occupation probability of the lower level $n_L^{\rm LN}$ is given by Eq. (47) with v_L^K replaced by $v_L^{\rm LN}$ and λ_2 evaluated at $v_L=v_L^{\rm LN}$.

Therefore for the special $N=\Omega$ case, in the small x, large N limit (with $Nx \ll 1$), the Kamlah pairing energy is about $\frac{1}{4}$ of the exact result while the LN pairing energy is only about $1/(2N)$ of the exact one. In the large Nx limit, both methods give very accurate energies. One therefore may conclude that the Kamlah method is better

than the LN method in the $N=\Omega$ case. However, as we will show in the next section, numerical calculations for the $N \neq \Omega$ case indicate the opposite is true, i.e., the LN method is generally better than the Kamlah method for $N \neq \Omega$. We will also show that in the $N \neq \Omega$ case, the Kamlah and LN energies are even larger than the exact energy in the small x region.

V. RESULTS AND DISCUSSION

The results for the BCS approximation, the Kamlah VAP method, and the Lipkin-Nogami prescription (not quite VAP) are shown in Figs. 2–4 for N=4, 6, and 8, respectively. We again show the ratio of the pairing energy for each approximation to the exact result ($R=E_p^{\text{approx}}/E_p^{\text{exact}}$). A ratio of $R=1$ would mean that the approximate pairing energy is exact. As noted in the figures, the curves for a given $N > \Omega$ case are the same as those for the 2Ω–N case. The results for selected values of $x=G/(2\epsilon)$ are also given in Table I. In our calculations, we fix G at 1 MeV and vary ϵ to give a range of x from 0.01 to 10.

Our first observation is that, as pointed out by Bishari *et al.* [11], the BCS wave function does yield a nontrivial minimum for all values of x in the case of $N \neq \Omega$. In the small x limit, this minimum is higher than the IPA energy but it is lower than the HF energy. One sees in the figures that the BCS curve and the IPA curve intersect at a certain value of x below which the IPA energy is a better approximation to the exact energy than the BCS. In the large x limit, the BCS pairing energy is about 10% (independent of N) smaller than the exact pairing energy. Note that for $N=\Omega$ as well as $N \neq \Omega$, the deviation of the BCS pairing energy from the exact result is always about one part in Ω. We also see both the Kamlah and LN pairing energies are very accurate in the large x region.

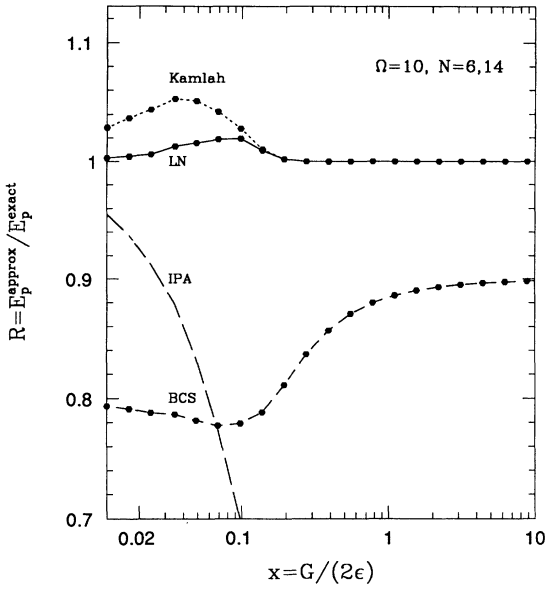

FIG. 3. Same as Fig. 1 but for the case of N=6 or 14 and Ω=10.

We then find that in the small x region the Kamlah pairing energy is too great in magnitude ($R > 1$). Although the overestimation is small for N=4 (Fig. 2), it reaches 30% for N=8 (Fig. 4) in the region of $x < 0.013$. This is somewhat surprising if one recalls (see Sec. IV A) that in the small x limit, the Kamlah pairing energy is only one-fourth the exact result when $N = \Omega$ (see also Fig. 1).

Also surprising is that the LN prescription works fairly well for small x in the $N \neq \Omega$ case, unlike the $N=\Omega$ case for which the LN pairing energy is only about $1/(2N)$ of the exact result when $x \to 0$ (Fig. 1). In the $N \neq \Omega$

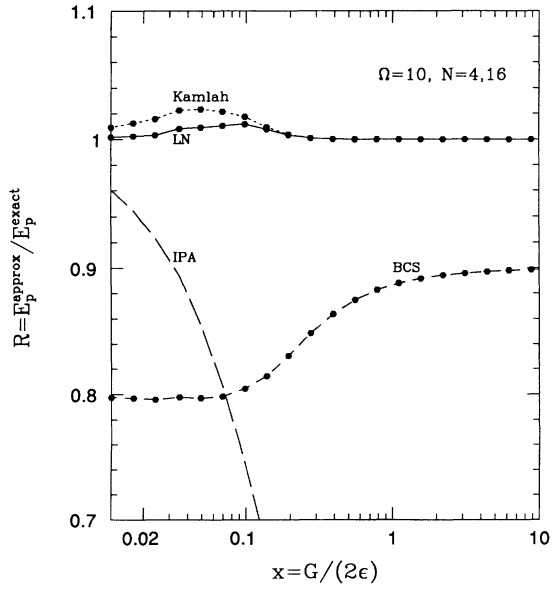

FIG. 2. Same as Fig. 1 but for the case of N=4 or 16 and Ω=10.

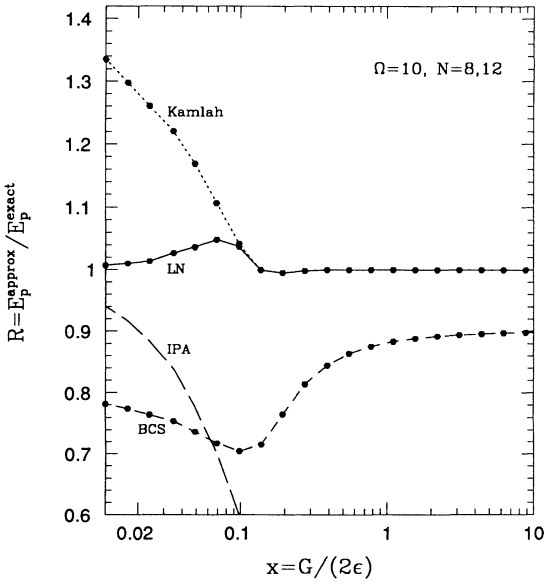

FIG. 4. Same as Fig. 1 but for the case of N=8 or 12 and Ω=10.

TABLE I. The ratios ($R = E_p^{\text{approx}}/E_p^{\text{exact}}$) of the pairing energies in various approximations (BCS, Kamlah, LN) to the exact result for selected values of $x=G/(2\epsilon)$ in the cases of Ω=10 and N=4, 6, 8, 10. Here $n_L^{\text{ex}}=(v_L^{\text{ex}})^2$ represents the occupation probability of the lower level from exact matrix diagonalization; $(v_L^{\text{BCS}})^2$, $(v_L^K)^2$, and $(v_L^{\text{LN}})^2$ are the values at which the minimal BCS, Kamlah, and LN energies were found; n_L^K and n_L^{LN} are the occupation probabilities of the lower level in the Kamlah and LN methods as determined by Eq. (47).

N	x	n_L^{ex}	$(v_L^{\text{BCS}})^2$	R_{BCS}	$(v_L^K)^2$	n_L^K	R_K	$(v_L^{\text{LN}})^2$	n_L^{LN}	R_{LN}
4	6.250	0.2057	0.2055	0.898	0.2051	0.2057	1.000	0.2051	0.2057	1.000
	1.105	0.2319	0.2307	0.888	0.2288	0.2319	1.000	0.2288	0.2319	1.000
	0.138	0.3640	0.3658	0.814	0.3568	0.3660	1.010	0.3620	0.3708	1.008
	0.024	0.3988	0.3991	0.796	0.3977	0.3986	1.016	0.3991	0.3994	1.004
6	6.250	0.3075	0.3074	0.898	0.3067	0.3075	1.000	0.3067	0.3075	1.000
	1.105	0.3421	0.3414	0.886	0.3379	0.3421	1.000	0.3379	0.3421	1.000
	0.138	0.5450	0.5499	0.788	0.5331	0.5492	1.011	0.5386	0.5547	1.009
	0.024	0.5985	0.5990	0.788	0.5957	0.5982	1.044	0.5990	0.5996	1.006
8	6.250	0.4085	0.4085	0.897	0.4077	0.4085	1.000	0.4077	0.4085	1.000
	1.105	0.4483	0.4480	0.883	0.4434	0.4482	1.000	0.4434	0.4482	1.000
	0.138	0.7254	0.7353	0.715	0.7062	0.7320	1.000	0.7038	0.7293	0.999
	0.024	0.7986	0.7993	0.765	0.7908	0.7989	1.260	0.7993	0.8002	1.014
10	6.250	0.5089	0.5089	0.897	0.5080	0.5089	1.000	0.5080	0.5089	1.000
	1.105	0.5503	0.5503	0.879	0.5453	0.5503	1.000	0.5452	0.5502	1.000
	0.138	0.9053	0.9023	0.231	0.8511	0.8864	0.829	0.8327	0.8641	0.818
	0.111[a]	0.9515	1.0000	0.000	0.9146	0.9545	0.646	0.8864	0.9186	0.597
	0.024	0.9991	1.0000	0.000	0.9956	1.0034	0.315	0.9916	0.9989	0.088

[a] $x = 0.111 = 1/(N-1)$ is the critical value below which the BCS wave function has only a trivial minimum in energy, the HF energy. Note that for $N \neq \Omega$, no such critical value exists.

case, the LN pairing energy agrees with the exact energy within 5% for all values of x and N considered (N=4, 6, 8, 12, 14, 16). The agreement is unexpectedly good, considering that we are comparing a small portion of the total energy, i.e., the correction to the HF energy due to the pairing correlations.

As we mentioned in the previous sections, the values $(v_L^K)^2$ and $(v_L^{\text{LN}})^2$ listed in Table I should not be directly compared with the exact occupation probability $n_L^{\text{ex}}=(v_L^{\text{ex}})^2$ which is also given in the table. More consistent values for the probability in the Kamlah and LN methods are determined by Eq. (47). These are also listed in Table I under the entries n_L^K and n_L^{LN}. We see that n_L^K and n_L^{LN} are in general closer to the exact result n_L^{ex} than $(v_L^K)^2$ and $(v_L^{\text{LN}})^2$ especially in the large x region.

Why should the LN energy be closer to the exact energy than the Kamlah energy in the $N \neq \Omega$ case but not in the N=Ω case for small x? Recall that the expressions for the Kamlah and LN energies as a function of v_L are exactly the same; both are given by Eq. (30). In seeking the minimum of the right-hand side of Eq. (30), one should vary v_L in all its occurrences, as one does in the Kamlah method. In the LN method, however, one treats $h_2(v_L)$ as a constant in computing the slope and therefore one does not reach the true minimum of the Kamlah energy function. Now in the N=Ω case, we have shown analytically that the Kamlah energy is higher than the exact energy and is therefore closer to the exact energy. In the $N \neq \Omega$ case, however, the Kamlah energy turns out to be *lower* than the exact energy, giving rise to a possibility of finding the LN energy closer to the exact energy (either above or below it). What the calculation shows is that the LN energy lies only very slightly below the exact energy (ratio $R > 1$) and so becomes an excellent approximation.

It would be of interest to make a more detailed study of the unexpected behavior we found in this work. It is also worthwhile to study a more realistic case in which an arbitrary number of particles occupy a multilevel model space. Work along this line is in progress.

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