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PHYSICAL REVIEW C VOLUME 5, NUMBER 1 JANUARY 1972

Two-Body Interactions: The Method of Correlated Quasiparticles. I.

R. R. Chasman
Chemistry Division, Argonne National Laboratory, Argonne, Illinois 60439
(Received 27 September 1971)

A method is proposed for determining the ground state of the Hamiltonian

$$H=\sum_k \epsilon_k N_k - \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

when the residual interaction is such that

$$\langle a_i^\dagger a_j^\dagger a_k a_l\rangle = \langle N_i N_j (1-N_k)(1-N_l)\rangle^{1/2} \langle N_k N_l (1-N_i)(1-N_j)\rangle^{1/2}$$

is a good approximation. The method is applied to pairing interactions involving one type of nucleon as well as to the generalized pairing problem containing neutron-neutron, neutron-proton, and proton-proton interactions.

I. INTRODUCTION

In this work, we study the ground state of the Hamiltonian

$$H=\sum_k \epsilon_k N_k - \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \tag{1}$$

when the following approximation is valid for the ground-state wave function:

$$\langle a_i^\dagger a_j^\dagger a_k a_l\rangle = \langle N_i N_j (1-N_k)(1-N_l)\rangle^{1/2} \times \langle N_k N_l (1-N_i)(1-N_j)\rangle^{1/2}. \tag{2}$$

The symbol $a_i^\dagger$ (a_i) denotes a fermion creation (annihilation) operator; N_i denotes a number operator; and the angular brackets enclose ground-state expectation values. In Sec. II, we discuss the conditions under which Eq. (2) is a reasonable approximation and consider the implications of Eq. (2) with respect to particle correlations. In Sec. III, we make a detailed study of particle correlations in the case of the pairing-force model, and use this approach to construct ground-state solutions of the simple pairing model. These solutions are compared with exact solutions of the pairing Hamiltonian. The same approach is applied to the generalized pairing problem which includes proton-proton, proton-neutron, and neutron-neutron pairing interactions. The correlations in the ground-state wave function of this problem are analyzed in detail. Our hope is to apply this approach to other two-body interactions in future publications.

II. GENERAL CONSIDERATIONS

The ground-state (or any other state) wave function is of the form:

$$|\Psi\rangle = \sum_{i>j>k>l\cdots} C_{ijkl\ldots} a_i^\dagger a_j^\dagger a_k^\dagger a_l^\dagger \cdots |0\rangle, \tag{3}$$

where $|0\rangle$ denotes the true vacuum state, and $C_{ijkl\ldots}$ denotes the amplitudes of the various configurations in the ground-state wave function. In terms of the coefficients $C_{ijkl\ldots}$, the approximation of Eq. (2) is just

$$\left\langle \sum_{ijkl\neq\alpha\beta\gamma\delta} C^2_{\alpha\beta ijkl\ldots}\right\rangle^{1/2}\left\langle \sum_{ijkl\neq\alpha\beta\gamma\delta} C^2_{\gamma\delta ijkl\ldots}\right\rangle^{1/2} = \left\langle \sum_{ijkl\neq\alpha\beta\gamma\delta} C_{\alpha\beta ijkl\ldots}C_{\gamma\delta ijkl\ldots}\right\rangle. \tag{4}$$

This relation can readily be seen to be exact whenever the amplitudes $C_{ijkl\ldots}$ are separable; i.e.,

$$C_{ijkl\ldots} = D_i D_j D_k D_l \cdots, \tag{5}$$

where D_i is a numerical factor. We have found[1] in the case of the pairing interaction, where Eq. (5) is not a particularly good approximation, that the approximation of Eq. (2) is nevertheless extremely good. In general, we expect that Eq. (2) is a reasonable approximation when the interaction matrix elements are in proper phase with one another. When the matrix elements are in phase, the sum on the right-hand side of Eq. (4) is coherent. If this sum is incoherent, clearly the approximation is bad; but in this instance, the correlations would be unimportant.

Our approach to the solution of this problem is based on the quasiparticle method,[2] and we shall use Lagrangian multipliers to insure that the desired number of particles are present in the ground-state solution. The working equation for the ground-state wave function is

$$\begin{aligned} H = &\sum_{k=\text{neutrons}} (\epsilon_k-\lambda_n)\langle N_k\rangle + \sum_{k=\text{protons}}(\epsilon_k-\lambda_p)\langle N_k\rangle \\ &- \sum_{ijkl} V_{ijkl}\langle N_i N_j(1-N_k)(1-N_l)\rangle^{1/2} \\ &\times\langle N_k N_l(1-N_i)(1-N_j)\rangle^{1/2}, \end{aligned}\tag{6}$$

and the problem is to be solved by solving the set of algebraic equations

$$\frac{\partial\langle H\rangle}{\partial\langle N_k\rangle}=0, \tag{7}$$

while adjusting λ_n and λ_p appropriately, in complete analogy with the quasiparticle method. Without the multipliers λ_n and λ_p, the minimum energy usually corresponds to a system with zero or fewer particles. Before we can carry out the differentiations in Eq. (7), we must first decompose the expressions involving products of number operators in terms of the fundamental variables $\langle N_k\rangle$. In the quasiparticle method, one ignores correlations other than those between N_k and N_{-k} and sets

$$\langle N_i N_j N_k\rangle = \langle N_i\rangle\langle N_j\rangle\langle N_k\rangle,$$

and this is our point of departure from the quasiparticle method. We plan to take the other correlations into account.

The basic point in our approach is that in the ground-state wave function all possible correlations and anticorrelations are such as to minimize the energy. We can, therefore, get a good approximation to the ground-state wave function by apportioning correlations and anticorrelations in a reasonable way. Before apportioning correlations and anticorrelations, we must first consider constraints on the total amounts of correlation and anticorrelation available. For this purpose, it is convenient to make the following definitions:

$$\alpha(i,j) \equiv \langle N_i N_j\rangle[1-\tfrac{1}{2}(\langle N_i\rangle+\langle N_j\rangle)], \tag{8}$$

and

$$\beta(i) \equiv \langle N_i\rangle\langle 1-N_i\rangle. \tag{9}$$

First, we consider the question of constraints on the anticorrelation. These constraints follow directly from exact sum-rule considerations, i.e.,

$$\sum_{s\neq i,j}\langle N_i N_j N_s\rangle = \langle N_i N_j\rangle \sum_{s\neq i,j}\langle N_s\rangle - 2\alpha(i,j) \tag{10}$$

and the complementary sum rule

$$\sum_{\substack{j\neq s\\ i\neq j,s}}\langle N_i N_j N_s\rangle = \langle N_s\rangle \sum_{\substack{j\neq s\\ i\neq j,s}}\langle N_i N_j\rangle - 2(P-1)\beta(s), \tag{11}$$

where P denotes the number of particles in the system.

The constraints on the correlation do not follow quite so directly or exactly. If the residual interaction does not correlate levels i and j, we have the relation

$$\langle N_i N_j\rangle = \langle N_i\rangle\langle N_j\rangle, \tag{12}$$

whereas if the two levels are totally correlated by the interaction, we have

$$\langle N_i N_j\rangle = \langle N_i\rangle = \langle N_j\rangle, \tag{13}$$

which may be rewritten as

$$\langle N_i N_j\rangle = \langle N_i\rangle\langle N_j\rangle + \beta(i). \tag{14}$$

The two-body interaction correlates two levels at a time and both i and j may correlate with other levels, so the correlation enhancement must be shared. We convert Eq. (14) to a sum-rule constraint by setting

$$\sum_j{}'\langle N_i N_j\rangle = \langle N_i\rangle\sum_j{}'\langle N_j\rangle + \beta(i), \tag{15}$$

where the prime in Eq. (15) indicates that the sum is just over the levels j with which i is correlated.

Next, we consider a typical ground-state expectation value in Eq. (6), $\langle N_{i0}N_{j0}(1-N_{k0})(1-N_{l0})\rangle$. In order that the energy of the system be minimized, the pair of operators $\langle N_{i0}N_{j0}\rangle$ should be correlated, the two triples $\langle N_{i0}N_{j0}N_{k0}\rangle$ and $\langle N_{i0}N_{j0}N_{l0}\rangle$ should be anticorrelated, and the quadruple $\langle N_{i0}N_{j0}N_{k0}N_{l0}\rangle$ should be correlated. Similar conclusions result from an inspection of the expression $\langle N_{k0}N_{l0}(1-N_{i0})(1-N_{j0})\rangle$. Making use of Eq. (15), we set

$$\langle N_{i0}N_{j0}\rangle = \langle N_{i0}\rangle\langle N_{j0}\rangle + f(i0, j0)\beta(i0)\beta(j0)\,, \tag{16}$$

where $f(i0, j0)$ contains any additional correlation enhancements and obeys the sum rules

$$\begin{aligned}&\sum_j{}' f(i0, j)\beta(j) = 1\,,\\ &\sum_i{}' f(i, j0)\beta(i) = 1\,.\end{aligned} \tag{17}$$

From Eqs. (10) and (11), we infer the anticorrelation relation

$$\begin{aligned}\langle N_{i0}N_{j0}N_{k0}\rangle = {}&\langle N_{i0}N_{j0}\rangle\langle N_{k0}\rangle\\ &- g(i0, j0\!: k0)\alpha(i0, j0)\beta(k0)\,,\end{aligned} \tag{18}$$

where the term $g(i0, j0\!: k0)$ includes special anticorrelation enhancements and obeys the sum-rule condition

$$\sum_k g(i0, j0\!: k)\beta(k) = 2\,. \tag{19}$$

The constraint of Eq. (11) will not usually cause any problems and we shall ignore it. Finally, $\langle N_{i0}N_{j0}N_{k0}N_{l0}\rangle$ should be as large as possible, consistent with the previously discussed correlations and anticorrelations. A reasonable expression for this term is

$$\begin{aligned}&\langle N_{i0}N_{j0}N_{k0}N_{l0}\rangle\\ &= \tfrac{1}{4}\left(\langle N_{i0}N_{j0}N_{k0}\rangle\frac{\langle N_{k0}N_{l0}\rangle}{\langle N_{k0}\rangle} + \langle N_{i0}N_{j0}N_{l0}\rangle\frac{\langle N_{k0}N_{l0}\rangle}{\langle N_{l0}\rangle}\right.\\ &\left.\quad + \langle N_{i0}N_{k0}N_{l0}\rangle\frac{\langle N_{i0}N_{j0}\rangle}{\langle N_{i0}\rangle} + \langle N_{j0}N_{k0}N_{l0}\rangle\frac{\langle N_{i0}N_{j0}\rangle}{\langle N_{j0}\rangle}\right).\end{aligned} \tag{20}$$

Equations (16), (18), and (20) contain all the effects of correlations in a formal sense. The objective is to see how these relations apply and to determine factors $f(i, j)$ and $g(i, j\!: k)$.

III. CORRELATION EFFECTS IN THE PAIRING HAMILTONIAN

Our motivation for starting with the pairing Hamiltonian is the fact that we have extremely accurate[3] wave functions available to guide us in the analysis. A pairing interaction, for one type of nucleon leads to a simplified version of Eq. (6). In a j_z representation (or Nilsson representation in deformed nuclei), we have

$$\begin{aligned}\langle H\rangle = {}&\sum_{k>0}(2\epsilon_k - \lambda - G)\langle N_k\rangle\\ &- 2G\sum_{\substack{k>0\\ l>k}}\langle N_k N_{-k}(1-N_l)(1-N_{-l})\rangle^{1/2}\\ &\times\langle N_l N_{-l}(1-N_k)(1-N_{-k})\rangle^{1/2}\,.\end{aligned} \tag{21}$$

Because each level has a single correlation partner, we have the additional simplification

$$\begin{aligned}&\langle N_k N_{-k}\rangle = \langle N_k\rangle = \langle N_{-k}\rangle\\ &\langle N_l N_{-l}\rangle = \langle N_l\rangle = \langle N_{-l}\rangle\,,\end{aligned} \tag{22}$$

and there are no problems of determining correlation enhancements. The problem that remains to be solved for this pairing Hamiltonian is the determination of the anticorrelation function $g(k, -k\!: l)$. Making use of Eq. (22) we set

$$\langle N_k N_{-k}(1-N_l)(1-N_{-l})\rangle = \langle N_k(1-N_l)\rangle\,, \tag{23}$$

and we may simply set

$$\langle N_k N_l\rangle = \langle N_k\rangle\langle N_l\rangle - g(k, l)\beta(k)\beta(l)\,, \tag{24}$$

where we have used the fact that

$$\alpha(k, -k) = \beta(k) \tag{25}$$

in this pairing problem. The sum-rule condition is

$$\sum_{l>0} g(k, l)\beta(l) = 1\,, \tag{26}$$

and if there were no special anticorrelation enhancements we would have

$$\langle N_k N_l\rangle = \langle N_k\rangle\langle N_l\rangle - \frac{\beta(k)\beta(l)}{\sum_r \beta(r)}\,. \tag{27}$$

We have compared this estimate with values of $\langle N_k N_l\rangle - \langle N_k\rangle\langle N_l\rangle$ obtained from our[3] wave functions. We find that Eq. (27) over corrects when levels k and l are on the same side of the Fermi level and underestimates the anticorrelation when the levels are on opposite sides of the Fermi level. Because of the particle-hole symmetry in the pairing-force problem, we should include this enhancement with a factor $s(k, l)$,

$$s(k, l) = \langle N_k\rangle\langle 1 - N_l\rangle + \langle N_l\rangle\langle 1 - N_k\rangle \tag{28}$$

or $s(k, l)$ raised to some power. We interpret this enhancement in the anticorrelation as a reflection of the dominant role of the zeroth-order configuration in the total wave function. The zeroth-order configuration is the one in which all levels up to the Fermi level have an occupation probability of 1. Because this is the most important configuration, the residual interaction populates particle states by removing pairs of particles from hole states rather than from other particle states. This accounts for the enhancement expressed by $s(k, l)$ raised to some power. Note also that as the occupation probabilities get smeared out, the weighting role of $s(k, l)$ is reduced in importance. We find that the simplest dependence,

$$\langle N_k N_l \rangle = \langle N_k \rangle \langle N_l \rangle - \eta\beta(k)\beta(l)s(k, l)\,, \tag{29}$$

does give a good approximation. The value of η is determined by the sum rule of Eq. (26), and we set

$$\eta = [\bar{N}\sum_r \beta(r)\langle 1 - N_r \rangle + (1 - \bar{N})\sum_r \beta(r)\langle N_r \rangle]^{-1}\,, \tag{30}$$

where $\bar{N}$ is the average occupation probability of levels in the system being studied. This choice of η satisfies all the sum rules of the form of Eq. (26) in an average way. It is also possible to satisfy the sum rules somewhat more precisely by introducing a set of quantities $\eta_{k,l}$; but we have not pursued this point. It should also be noted that we are satisfying the sum rules only to the order $[\beta^2(k)/\sum\beta(r)]$ with this choice of η; a given level k is not anticorrelated with itself. In the case $\bar{N} = 0.5$, commonly used in pairing calculations, Eq. (30) reduces to the simple form

$$\eta = [0.5\sum_r \beta(r)]^{-1}\,. \tag{31}$$

TABLE I. Comparison of ΔE as a function of G and P.

Pairs	G/ϵ	$\Delta E/\epsilon$[a] Exact	$\Delta E/\epsilon$[a] Quasiparticle	$\Delta E/\epsilon$ Present work
4	0.7	5.309	3.939	5.221
4	0.8	6.610	5.028	6.502
4	0.9	8.018	6.229	7.886
4	1.0	9.513	7.520	9.357
4	1.1	11.081	8.885	10.897
8	0.42	5.468	3.978	5.433
8	0.48	6.954	5.167	6.938
8	0.54	8.704	6.636	8.705
8	0.60	10.710	8.374	10.718
8	0.66	12.954	10.357	12.961
12	0.38	7.487	5.532	7.465
12	0.42	9.083	6.819	9.099
12	0.46	10.950	8.390	11.004
12	0.50	13.096	10.251	13.180
12	0.54	15.518	12.398	15.622
16	0.345	8.829	6.572	8.793
16	0.375	10.402	7.826	10.415
16	0.405	12.231	9.346	12.296
16	0.435	14.337	11.152	14.448
16	0.465	16.726	13.249	16.878

[a] Taken from Ref. 4.

Putting everything together, we obtain

$$\langle H \rangle = \sum_{k>0}(2\epsilon_k - \lambda - G)\langle N_k \rangle - 2G\sum_{\substack{k>0\\ l>k}}[\beta(k)\beta(l)T_{k,l}]^{1/2}\,, \tag{32}$$

with

$$T_{k,l} = 1 + \eta S^2(k, l)[1 + \eta\beta(k)\beta(l)]\,; \tag{33}$$

and the problem is now solved by setting $\partial\langle H \rangle/\partial\langle N_k \rangle = 0$ and solving the resulting equations for different choices of λ. We have found that it is straightforward to construct a program for solving this set of equations iteratively and have carried out a few calculations. The results of these calculations are spectacularly good – and in Tables I and II, we have compared these results with some exact solutions[4] of the pairing problem. We have also included quasiparticle estimates of the tabulated quantities. In Table I, we compare energy shifts; the energy shift is the change in ground-state energy due to the pairing interaction. From Table I, we see that the errors in the energy shift using the quasiparticle method are ~20%. By taking cor-

TABLE II. Comparison of occupation probabilities.

P	G/ϵ	Level No.	$\langle N \rangle$[a] Exact	$\langle N \rangle$[a] Quasiparticle	$\langle N \rangle$ Present work
4	0.8	+3	0.122	0.117	0.120
		+2	0.197	0.203	0.190
		+1	0.347	0.377	0.344
4	1.0	+3	0.175	0.173	0.170
		+2	0.258	0.265	0.251
		+1	0.397	0.411	0.394
8	0.48	+3	0.093	0.090	0.094
		+2	0.157	0.169	0.155
		+1	0.306	0.355	0.307
8	0.60	+3	0.160	0.165	0.157
		+2	0.243	0.259	0.237
		+1	0.387	0.409	0.387
12	0.42	+3	0.106	0.108	0.107
		+2	0.175	0.194	0.173
		+1	0.326	0.373	0.329
12	0.46[b]	+3	0.138	0.143	0.137
		+2	0.216	0.237	0.213
		+1	0.367	0.398	0.369
16	0.375	+3	0.105	0.109	0.108
		+2	0.174	0.196	0.173
		+1	0.325	0.374	0.328
16	0.435	+3	0.166	0.176	0.164
		+2	0.249	0.271	0.245
		+1	0.392	0.415	0.393

[a] Taken from Ref. 4.

[b] Our approximation indicates that some numbers were transposed and the exact occupation probabilities listed for $G/\epsilon = 0.50$ in Ref. 4 are actually for $G/\epsilon = 0.46$. We have recomputed the quasiparticle occupation probabilities for this case.

relations into account properly, the errors are reduced to ~1.5% for the systems containing four pairs of particles and to ≤1% for the larger systems. In Table II, we list occupation probabilities $\langle N_k\rangle$ for the first three levels just above the Fermi level. Because of the symmetry of the systems considered here, the occupation probabilities of the levels just below the Fermi level are just $\langle 1-N_k\rangle$, where k is the equivalent level above the Fermi level. Again our results are in extremely good agreement with the exact results. The occupation probabilities given by the quasiparticle method are also quite good once we get away from the Fermi level.

Let us next consider the somewhat more complicated pairing interaction with G replaced by $G_{k,l}$ in Eq. (21). Consider two levels l_1 and l_2 having the same single-particle energies and the same occupation probabilities ($\langle N_{l_1}\rangle=\langle N_{l_2}\rangle$), and the matrix element $G_{k,l_1}>G_{k,l_2}$. In this instance, the residual interaction scatters pairs into l_1 preferentially, as compared to l_2, from level k; hence the anticorrelation between k and l_1 is enhanced. We can incorporate this feature into our formalism by setting

$$\langle N_k N_l\rangle=\langle N_k\rangle\langle N_l\rangle-\eta\tilde{G}_{k,l}\beta(k)\beta(l)S(k,l)\,, \qquad (34a)$$

where η is fixed by the sum-rule constraints and

$$\tilde{G}_{k,l}=G_{k,l}(O_kO_l)^{-1}\,, \qquad (34b)$$

with the quantities O_k defined by the relations

$$O_k\sum_{l\neq k}O_l\equiv\sum_{l\neq k}G_{k,l}\,. \qquad (35)$$

The solution is then essentially the same as in the case of the constant G interaction.

We next consider the generalized pairing problem[5] including proton-proton, proton-neutron, and neutron-neutron pairing interactions. Again, we are working in a j_z (or Nilsson) representation, and allow the matrix elements to vary. For convenience we assume the relation

$$\langle N_\alpha P_{-\alpha}|V|N_\beta P_{-\beta}\rangle=\langle N_{-\alpha}P_\alpha|V|N_\beta P_{-\beta}\rangle\,, \qquad (36)$$

although this assumption is not necessary. In Eq. (36), N_α denotes a neutron state and P_α denotes a proton state.

For this full-blown pairing problem, we have the lengthy equation:

$$\begin{aligned}\langle H\rangle=&\sum_{k>0}(2\epsilon_k-\lambda_n)\langle N_k\rangle+\sum_{k>0}(2\epsilon_k-\lambda_p)\langle P_k\rangle-\sum_{k>0}(G_{nn}^{kk}\langle N_kN_{-k}\rangle+G_{pp}^{kk}\langle P_kP_{-k}\rangle+2G_{np}^{kk}\langle N_kP_{-k}\rangle)\\&-2\sum_{\substack{k>0\\l>k}}G_{nn}^{k,l}\langle N_kN_{-k}(1-N_l)(1-N_{-l})\rangle^{1/2}\langle N_lN_{-l}(1-N_k)(1-N_{-k})\rangle^{1/2}\\&-2\sum_{\substack{k>0\\l>k}}G_{pp}^{k,l}\langle P_kP_{-k}(1-P_l)(1-P_{-l})\rangle^{1/2}\langle P_lP_{-l}(1-P_k)(1-P_{-k})\rangle^{1/2}\\&-8\sum_{\substack{k>0\\l>k}}G_{np}^{k,l}\langle N_kP_{-k}(1-N_l)(1-P_{-l})\rangle^{1/2}\langle N_lP_{-l}(1-N_k)(1-P_{-k})\rangle^{1/2}\\&-2\sum_{k>0}G_{np}^{k,l}\langle N_kP_{-k}(1-N_{-k})(1-P_k)\rangle^{1/2}\langle N_{-k}P_k(1-N_k)(1-P_{-k})\rangle^{1/2}\,,\end{aligned} \qquad (37)$$

with the letter N used to denote a neutron number operator and the letter P used to denote a proton number operator.

In this problem the following identities hold:

$$\begin{aligned}&\langle N_k\rangle=\langle N_{-k}\rangle\,,\quad \langle P_k\rangle=\langle P_{-k}\rangle\,,\\&\langle N_kP_{-k}\rangle=\langle P_kN_{-k}\rangle\,,\quad \langle N_kP_k\rangle=\langle N_{-k}P_{-k}\rangle\,.\end{aligned} \qquad (38)$$

As we have seen, correlation effects are quite important in solving the problem of like-particle pairing. In the case of the generalized pairing problems the correlations are crucial. A solution that consists of just occupation probabilities is meaningless. In order to gain some insight into the ground-state correlations of the generalized pairing problem, we have solved the problem exactly for some rather small systems and examined the ground-state wave functions in detail. Our examination indicates three types of ground-state correlation pattern (although there may be more). The type-one correlation pattern is that of like-particle pairing. The type-two correlation pattern is that of unlike-particle pairing. The type-three correlation pattern corresponds to a mixture of like- and unlike-particle pairing. If we keep the like-particle pairing strengths fixed and increase the unlike-particle pairing strengths, the ground-state correlations go from type one to type three and finally to type two. We shall consider these three solutions in detail.

In the type-one solution, the correlations are

$$\langle N_kN_{-k}\rangle=\langle N_k\rangle\,,\quad \langle P_kP_{-k}\rangle=\langle P_k\rangle\,. \qquad (39)$$

Neutrons and protons are uncorrelated, and we have two independent pairing problems of the type that we have already considered.

The type-two solution is determined by the matrix elements $G_{np}^{k,l}$. For this solution, the correlation relations are

$$\langle N_k P_{-k}\rangle = \langle N_k\rangle = \langle P_{-k}\rangle, \quad \langle N_{-k} P_k\rangle = \langle N_{-k}\rangle = \langle P_k\rangle, \tag{40}$$

and the anticorrelation constraints come from the sum-rule relations

$$\sum_{l\neq k}\langle N_k P_{-k} N_l\rangle = \langle N_k P_{-k}\rangle \sum_{l\neq k}\langle N_l\rangle - (1-\langle N_k\rangle)\langle N_k P_{-k}\rangle, \tag{41}$$

$$\sum_{l\neq k}\langle N_k P_{-k} P_l\rangle = \langle N_k P_{-k}\rangle \sum_{l\neq k}\langle P_l\rangle - (1-\langle P_{-k}\rangle)\langle N_k P_{-k}\rangle, \tag{42}$$

which by virtue of Eq. (40) can be written as

$$\sum_{l\neq k}\langle N_k N_l\rangle = \langle N_k\rangle \sum_{l\neq k}\langle N_l\rangle - \langle N_k\rangle\langle 1-N_k\rangle \tag{41'}$$

or

$$\sum_{l\neq k}\langle P_{-k} N_l\rangle = \langle P_{-k}\rangle \sum_{l\neq k}\langle N_l\rangle - (1-\langle P_{-k}\rangle)\langle P_{-k}\rangle. \tag{41''}$$

This solution gives anticorrelations between all pairs of number operators (other than $\langle N_k P_{-k}\rangle$ or $\langle N_{-k} P_k\rangle$), be they proton or neutron number operators. It should be noted that N_k and N_{-k} are anticorrelated in this solution. The anticorrelation equation is again of the form of Eq. (34a). In the Hamiltonian there occur products of number operators that are not fixed by the relations already considered, in the terms of the form

$$\langle N_k N_{-k}(1-N_l)(1-N_{-l})\rangle.$$

As N_k and N_{-k} are anticorrelated, such terms are quite small relative to the neutron-proton interaction terms. We can ignore the anticorrelations in the products $\langle N_k N_{-k} N_l\rangle$, but the energy of the system is computed somewhat more accurately by anticorrelating N_l with $N_k N_{-k}$, again using the sum-rule constraint of Eq. (10); where now the product $N_k N_{-k}$ is itself anticorrelated. If there is a neutron (or proton) excess in the system being considered, the levels occupied by neutrons and not by protons in the zeroth-order configuration are blocked in solutions of type two. The correlations and anticorrelations we have discussed apply to the other levels.

The type-three correlation is a cooperative effect with both like-particle and unlike-particle correlations. This correlation pattern can be seen in the ground-state solution when

$$4\overline{G}_{np} \approx \overline{G}_{nn} + \overline{G}_{pp}. \tag{43}$$

For this class of solutions, we have from Eq. (15) the correlation relation

$$\langle N_k N_{-k}\rangle + \langle N_k P_{-k}\rangle = \langle N_k\rangle\langle N_{-k}\rangle + \langle N_k\rangle\langle P_{-k}\rangle + \langle N_k\rangle\langle 1-N_k\rangle. \tag{44}$$

The numerical examples that we have examined indicate that this relation is good to 10% or better. The total correlation enhancement is a bit less than $\langle N_k\rangle\langle 1-N_k\rangle$. In the case of generalized pairing interactions, we also have the exact relation

$$\langle N_k\rangle = \langle N_k N_{-k}\rangle + \langle N_k P_{-k}\rangle - \langle N_k N_{-k} P_{-k}\rangle, \tag{45}$$

and combining Eqs. (44) and (45) we get the useful relation

$$\langle N_k N_{-k} P_{-k}\rangle = \langle N_{-k}\rangle\langle P_{-k}\rangle, \tag{46}$$

which we use in determining the sum-rule constraints on the anticorrelation. Similar relations hold for the proton operators

$$\langle P_k P_{-k}\rangle + \langle P_k N_{-k}\rangle = \langle P_k\rangle\langle P_{-k}\rangle + \langle P_k\rangle\langle N_{-k}\rangle + \langle P_k\rangle\langle 1-P_k\rangle; \tag{47}$$

and note also

$$\langle N_k N_{-k} P_{-k}\rangle \equiv \langle P_k P_{-k} N_{-k}\rangle \equiv \langle P_k P_{-k} N_k\rangle \equiv \langle N_k N_{-k} P_k\rangle \equiv \langle N_k N_{-k} P_k P_{-k}\rangle. \tag{48}$$

For this solution, the sum-rule constraints on the anticorrelations are given by the equations

$$\sum_{l\neq k,-k}\langle N_k N_{-k} N_l\rangle = \langle N_k N_{-k}\rangle \sum_{l\neq k,-k}\langle N_l\rangle - 2\langle N_k N_{-k}\rangle(1-\langle N_k\rangle), \tag{49}$$

$$\sum_{l\neq k,-k}\langle N_k P_{-k} N_l\rangle = \langle N_k P_{-k}\rangle \sum_{l\neq k,-k}\langle N_l\rangle - (1-2\langle N_k\rangle)\langle N_k P_{-k}\rangle - \langle N_k\rangle\langle P_{-k}\rangle, \tag{50}$$

$$\sum_{l\neq k,-k}\langle N_k P_{-k} P_l\rangle = \langle N_k P_{-k}\rangle \sum_{l\neq k,-k}\langle P_l\rangle - (1-2\langle P_k\rangle)\langle N_k P_{-k}\rangle - \langle N_k\rangle\langle P_{-k}\rangle, \tag{51}$$

and

$$\sum_{l\neq k,-k}\langle P_k P_{-k} P_l\rangle = \langle P_k P_{-k}\rangle \sum_{l\neq k,-k}\langle P_l\rangle - 2\langle P_k P_{-k}\rangle(1-\langle P_k\rangle), \tag{52}$$

and we construct the individual anticorrelations in the usual way. We generalize $s(k, l)$ slightly here and replace it by $s'(k, -k; l)$ with

$$s'(k, -k; l) = \tfrac{1}{2}(\langle N_k + P_{-k}\rangle)\langle 1 - N_l\rangle + \langle N_l\rangle(1 - \tfrac{1}{2}\langle N_k + P_{-k}\rangle), \tag{53}$$

for the relations based on Eqs. (50) and (51). A typical relation is of the form

$$\langle N_k P_{-k} N_l\rangle = \langle N_k P_{-k}\rangle \langle N_l\rangle - \eta \tilde{G}_{np}^{k,l} s'(k, -k; l)\beta(l) \times [\langle N_k\rangle \langle P_{-k}\rangle + (1 - 2\langle N_k\rangle)\langle N_k P_{-k}\rangle]. \tag{54}$$

For terms involving $\langle N_k N_{-k} P_k\rangle$ or the like, we use Eqs. (46) and (48).

The real difficulty in the type-three solution is in the evaluation of $\langle N_k N_{-k}\rangle$ and $\langle N_k P_{-k}\rangle$. It is not clear, *a priori*, how to allocate the correlation enhancement associated with $\langle N_k\rangle$ between these two expressions. Our approach is to introduce a single variational parameter, δ, as a measure of the relative strengths of like-particle and unlike-particle correlations. We introduce δ in the following way:

$$\langle N_k N_{-k}\rangle = \langle N_k\rangle \langle N_{-k}\rangle + \delta\langle N_k\rangle \langle 1 - N_k\rangle, \tag{55}$$

which gives, using Eq. (44),

$$\langle N_k P_{-k}\rangle = \langle N_k\rangle \langle P_{-k}\rangle + (1 - \delta)\langle N_k\rangle \langle 1 - N_k\rangle, \tag{56}$$

which in turn gives, using Eq. (47),

$$\langle P_k P_{-k}\rangle = \langle P_k\rangle \langle P_{-k}\rangle + \langle P_k\rangle \langle 1 - P_k\rangle - (1 - \delta)\langle N_k\rangle \langle 1 - N_k\rangle. \tag{57}$$

The same δ is used for all levels k, and its value is fixed by the condition

$$\frac{\partial\langle H\rangle}{\partial\delta} = 0. \tag{58}$$

We note that for $\delta = 1$, the solution is just the type-one solution. However, $\delta = 0$ does not quite correspond to the type-two solution. For $\delta = 0$, N_k and N_{-k} are uncorrelated; whereas, in the type-two solution they are anticorrelated. If the type-three solution yields

$$\delta < 0, \tag{59}$$

or

$$(1 - \delta)\langle N_k\rangle \langle 1 - N_k\rangle > \langle P_k\rangle \langle 1 - P_k\rangle \tag{60}$$

for any k, a correlation sum rule is being violated and the solution should be discarded.

The ground-state solution of the generalized pairing problem is finally determined by comparing the values of $\langle H\rangle$ obtained for the type-two and type-three solutions. The lower value of $\langle H\rangle$, of course, determines the ground-state correlations.

IV. SUMMARY

The method of correlated quasiparticles leads to extremely accurate solutions of the pairing Hamiltonian. Perhaps more important, it leads to an understanding of the ground-state wave function by making the various correlations and anticorrelations transparent. Variational calculations based on this method appear to be quite practicable in terms of such things as programming effort and computer usage time. At this point, the method looks sufficiently straightforward so that we feel it can be profitably applied to yet more realistic interactions.

It is a pleasure to acknowledge the advice and most constructive criticism of D. Kurath on many aspects of this work.

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