Eigenvalues of the Nuclear Pairing Hamiltonian*

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A new technique is developed in this paper for solving Hamiltonians of the form

$$H=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})-\sum_{k,l>0}G(k,l)a_k^\dagger a_{-k}^\dagger a_{-l}a_l,$$

where $G(k,l)$ may have the forms: $G(k,l)=G$ (independent of k and l), $G(k,l)=G_kG_l$, or $G(k,l)=G(k,l)$ (nonseparable in k and l). The eigenvalues obtained with this technique are compared with the exact solutions of Kerman, Lawson, and Macfarlane. The agreement with the exact solutions is fairly good.

THE purpose of this work is to develop a technique for obtaining the low-lying eigenvalues of the nuclear pairing Hamiltonian. Our approach differs from the original version of the quasiparticle formulation[1] in that we drop no terms from our Hamiltonian, nor are there any intermediate parameters to be used in the description of the system, such as λ (the chemical potential). Our approach is similar to that of Bayman[2] in that we always deal with a definite number of particles, but we avoid any errors that may arise from a use of the saddle-point method. The assumptions which we make are (1) protons and neutrons may be treated as separate systems[3] and (2) the pairing interaction is constant over some finite energy interval and zero elsewhere.

The Hamiltonian, which we consider, for one type of particle (e.g., neutrons) is of the form,

$$H=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})-G\sum_{k>0,l>0}a_k^\dagger a_{-k}^\dagger a_{-l}a_l, \quad (1)$$

where ϵ_k is a single-particle energy, $a_k^\dagger$ (a_k) are the usual fermion creation (annihilation) operators, $a_{-k}^\dagger$ creates a particle in the state which is the time reversal conjugate to state k, and G is the pairing interaction constant. We note that the Hamiltonian of Eq. (1) is equivalent[4] to that used by Kerman, Lawson, and Macfarlane[5] (KLM) in their exact calculation of pairing eigenvalues. We shall make use of their exact calculations to test the method formulated here.

It is easiest to develop the ideas involved in the present formulation by having in mind a definite number of pairs of particles, P, and some number of levels, L, which can hold a pair of particles. If we have only one pair the problem is too simple, so we choose $P=2$ as the simplest system which we may treat in which all of the complications arise. The solution of Eq. (1) may be written, for $P=2$, as

$$\Psi=\sum_{i,j}C_{i,j}a_i^\dagger a_{-i}^\dagger a_j^\dagger a_{-j}^\dagger, \quad (2)$$

where $C_{i,j}$ is the probability amplitude for having levels i and j occupied and all other levels vacant. Using

$$H\Psi=\lambda\Psi, \quad (3)$$

we may obtain[4] sets of equations of the form

$$C_{i,j}(E_{i,j}-\lambda)=G\sum_{t\neq i}C_{i,t}+G\sum_{t\neq j}C_{j,t}, \quad (4)$$

where

$$E_{i,j}\equiv 2\epsilon_i+2\epsilon_j\equiv E_i+E_j \quad (5)$$

and λ is the eigenvalue of the pairing Hamiltonian.

The amplitude of the most probable configuration is

$$C_{1,2}(E_{1,2}-\lambda)=G\sum_{t\neq 1}C_{1,t}+G\sum_{t\neq 2}C_{2,t}, \quad (6)$$

and the equation for some configuration $C_{1,m}$ is

$$C_{1,m}(E_{1,m}-\lambda)=G\sum_{t\neq 1}C_{1,t}+G\sum_{t\neq m}C_{m,t}. \quad (7)$$

We next subtract Eq. (6) from Eq. (7) to obtain

$$C_{1,m}(E_{1,m}-\lambda)=C_{1,2}(E_{1,2}-\lambda)-G[\sum_{t\neq 2}C_{2,t}-\sum_{t\neq m}C_{m,t}]. \quad (8)$$

At this point, we introduce the *only* approximation to be used in our work

$$C_{m,t}=C_{2,t}(C_{1,m}/C_{1,2}). \quad (9)$$

It is of considerable interest to consider the approximation of Eq. (9) in terms of the quasiparticle formulation of the problem. In the quasiparticle approximation, the wave function of the system is given as

$$\Psi=\prod_k(U_k+V_ka_k^\dagger a_{-k}^\dagger)|0\rangle, \quad (10)$$

where $|0\rangle$ indicates the vacuum and both U_k and V_k are numbers. In terms of the quasiparticle wave func-

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tion, we have

$$\frac{C_{m,t}}{C_{2,t}}=\frac{V_mU_2}{U_mV_2}=\frac{C_{1,m}}{C_{1,2}}. \tag{11}$$

As Eq. (9) is the *only* approximation in our treatment of the Hamiltonian of Eq. (1), it is clear that our approach should give the best possible solution of the separable type, which includes all quasiparticle-type solutions. By separable we mean

$$C_{i,j}=(C_i)(C_j). \tag{12}$$

Actually our solutions should be a little better than any approximation of the separable type, since we make use of it only to evaluate $\sum_{t\neq m}C_{m,t}$. When $E_m\gg E_2$, $\sum_{t\neq m}C_{m,t}$ will be much less than $\sum_{t\neq 2}C_{2,t}$ and the approximation is unimportant.

Next, we substitute from Eq. (9) to Eq. (8) and obtain

$$C_{1,m}(E_{1,m}-\lambda)=C_{1,2}(E_{1,2}-\lambda)-G[\sum_{t\neq 2,m}C_{2,t}]\left(1-\frac{C_{1,m}}{C_{1,2}}\right), \tag{13}$$

and using Eq. (6), we obtain

$$C_{1,m}(E_{1,m}-\lambda)=C_{1,2}(E_{1,2}-\lambda)-[C_{1,2}(E_{1,2}-\lambda)-G\sum_{t\neq 1}C_{1,t}-GC_{2,m}]\times[1-(C_{1,m}/C_{1,2})], \tag{14}$$

which may be rearranged to give

$$C_{1,m}\left[E_m-E_2+G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}+G\frac{C_{2,m}}{C_{1,2}}\right]=G\sum_{t\neq 1}C_{1,t}+GC_{2,m}. \tag{15}$$

We next divide both sides of Eq. (15) by $C_{1,2}$ and by the coefficient of $C_{1,m}$ and summing over m, we obtain

$$\sum_{m\neq 1,2}\frac{C_{1,m}}{C_{1,2}}=G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}\left(\sum_{m\neq 1,2}\left[E_m-E_2+G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}+G\frac{C_{2,m}}{C_{1,2}}\right]^{-1}\right)+G\sum_{m\neq 1,2}\frac{(C_{2,m}/C_{1,2})}{[E_m-E_2+G\sum_{t\neq 1}(C_{1,t}/C_{1,2})+G(C_{2,m}/C_{1,2})]}. \tag{16}$$

The term $C_{2,m}/C_{1,2}$ is, in general, small, but unfortunately, it is far from negligible. We also note that

$$\sum_{m\neq 1,2}\frac{C_{1,m}}{C_{1,2}}=\sum_{m\neq 1}\frac{C_{1,m}}{C_{1,2}}-1. \tag{17}$$

By using a similar series of steps, we obtain

$$\left(\sum_{m\neq 2}\frac{C_{2,m}}{C_{1,2}}-1\right)=G\sum_{t\neq 2}\frac{C_{2,t}}{C_{1,2}}\left(\sum_{m\neq 1,2}\left[E_m-E_1+G\sum_{t\neq 2}\frac{C_{2,t}}{C_{1,2}}+G\frac{C_{1,m}}{C_{1,2}}\right]^{-1}\right)+G\sum_{m\neq 1,2}\frac{(C_{1,m}/C_{1,2})}{[E_m-E_1+G\sum_{t\neq 2}(C_{2,t}/C_{1,2})+G(C_{1,m}/C_{1,2})]}. \tag{18}$$

Our procedure for solving Eq. (16) and Eq. (18) is iterative. We set $C_{2,m}/C_{1,2}=0$ in Eq. (16) and $C_{1,m}/C_{1,2}=0$ in Eq. (18), and solve for the quantities $\sum_{m\neq 1}C_{1,m}/C_{1,2}$ and $\sum_{m\neq 2}C_{2,m}/C_{1,2}$, and using these numbers with equations of the type of Eq. (15), we obtain estimates of $C_{2,m}/C_{1,2}$ and $C_{1,m}/C_{1,2}$ and continue the iteration. After finishing the iteration procedure, we determine the eigenvalue of the ground state using Eq. (6). The result is

$$\lambda=E_{1,2}-G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}-G\sum_{t\neq 2}\frac{C_{2,t}}{C_{1,2}}. \tag{19}$$

To obtain the eigenvalues of the low lying excited states, we break one pair and put, e.g., one particle in level two and one particle in level three and obtain for that particular case

$$\lambda=E_1+\epsilon_2+\epsilon_3-G\sum_{t\neq 2,3}\frac{C_t}{C_1}, \tag{20}$$

using

$$1=G\sum_{m\neq 2,3}\left[(E_m-E_1)+G\sum_{t\neq 2,3}\frac{C_t}{C_1}\right]^{-1}. \tag{21}$$

The treatment is exact[4] when we deal with only one pair; it is also exact[4] if all of the single-particle energies are degenerate. When all single-particle energies are degenerate, the amplitudes C are all equal, which makes the calculation quite simple.

For the more complex cases, we solve the equations given here on an electronic computer. The problem is solved rapidly and conveniently (we obtained $\sim$10 eigenvalues per minute on an IBM 704). The agreement between this method and the exact treatment of KLM is fair and the present method may be used quite easily when the matrices involved in the KLM treatment are too large to be handled on a computer.

In Table I, we compare our results to those of KLM for the Ni isotopes. We also compare our results to those of KLM for the most complex system that they were able to handle, i.e., Pb^{198} which has five pairs and 17 levels to be treated for the ground-state eigenvalue. The discrepancies between the exact eigenvalues and those computed in the present treatment are a measure of the approximate nature of the notion of separability.

TABLE I. Comparison[a,b] of approximate and exact eigenvalues in MeV.

Isotope	Spins of blocked levels	($E_{s.p.}$) Energy of configuration without pairing	λ_{exact}	λ_{approx}	$\frac{\lambda_{approx}-\lambda_{exact}}{E_{s.p.}-\lambda_{exact}}\times 100\%$
Ni^{60}	None	0	−2.10	−2.02	4
Ni^{62}	None	1.56	−1.75	−1.66	3
Ni^{62}	$\frac{5}{2},\frac{5}{2}$	1.56	0.35	0.36	1
Ni^{62}	$\frac{5}{2},\frac{3}{2}$	2.34	0.68	0.70	1
Ni^{64}	None	3.12	−0.50	−0.40	3
Ni^{64}	$\frac{5}{2},\frac{5}{2}$	3.12	1.60	1.62	1.5
Ni^{64}	$\frac{5}{2},\frac{1}{2}$	3.90	1.89	1.92	1.5
Ni^{66}	None	4.68	1.70	1.84	5
Ni^{66}	$\frac{5}{2},\frac{1}{2}$	5.46	3.76	3.77	1
Pb^{198}	None	5.22	3.29	3.49	10
Pb^{198}	$\frac{3}{2},\frac{3}{2}$	5.22	4.33	4.38	5
Pb^{198}	$\frac{5}{2},\frac{3}{2}$	5.55	4.55	4.62	7
Pb^{198}	$\frac{5}{2},\frac{5}{2}$	5.88	4.78	4.85	7

[a] Single particle energies and values of G are given in Ref. 5.
[b] We do not include some of the levels in Ni for which $P=1$.

It is interesting to note that, using the same approximation as in Eq. (9), it is possible to solve the somewhat more complicated Hamiltonian

$$H=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})+\sum_{k>0,l>0}G_k a_k^\dagger a_{-k}^\dagger G_l a_{-l}a_l \quad (22)$$

in essentially the same way that we solve Eq. (1).

Finally, we note that using the approximation of Eq. (9), it is possible to obtain a set of cumbersome, but tractable, equations for a nonseparable interaction of the pairing type. We take

$$H=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})+\sum_{k>0,l>0}G(l,k)a_k^\dagger a_{-k}^\dagger a_{-l}a_l \quad (23)$$

considering again, e.g., $P=2$. Again using the same steps as before, we arrive at the analog of Eq. (15), which has the form

$$C_{1,m}\left[E_m-E_2+\sum_{t\neq 1}\frac{G(2,t)C_{1,t}}{C_{1,2}}+G(1,m)\frac{C_{2,m}}{C_{1,2}}\right]=\sum_{t\neq 1}G(m,t)C_{1,t}+G(1,m)C_{2,m}. \quad (24)$$

We divide both sides of Eq. (24) by $C_{1,2}$ and multiply both sides by $G(A,m)$. We divide by the coefficient of $G(A,m)C_{1,m}/C_{1,2}$ and sum over m, which gives

$$X_A'=\sum_m\frac{G(A,m)[X_m'+G(1,m)C_{2,m}/C_{1,2}]}{[E_m-E_2+X_2'+G(1,m)C_{2,m}/C_{1,2}]}, \quad (25)$$

where

$$X_A'=\sum_{t\neq 1}G(A,t)\frac{C_{1,t}}{C_{1,2}}. \quad (26)$$

We handle the problem of the term $C_{2,m}/C_{1,2}$, using the same iteration procedure as before.

To solve the set of equations given by Eq. (25), we may also use an iteration procedure, i.e., guess at X_2', solve Eq. (25) by diagonalizing a matrix, and obtain a new value for X_2'. The advantage of the present method is that we have to diagonalize P matrices which are $(L-P)\times(L-P)$ rather than one matrix which is $L!/(L-P)!P!\times L!/(L-P)!P!$ for an exact solution.

In order to make clear how the present techniques are to be used for any number of pairs, we consider the case of $P=3$ for the Hamiltonian of Eq. (1).

For the most probable configuration, for $P=3$, we have

$$C_{1,2,3}(E_{1,2,3}-\lambda)=G\sum_{t\neq 1,2}C_{1,2,t}+G\sum_{t\neq 2,3}C_{2,3,t}+G\sum_{t\neq 1,3}C_{1,3,t}, \quad (27)$$

and for some other amplitude $C_{1,2,m}$, we have the relation

$$C_{1,2,m}(E_{1,2,m}-\lambda)=G\sum_{t\neq 1,2}C_{1,2,t}+G\sum_{t\neq 2,m}C_{2,m,t}+G\sum_{t\neq 1,m}C_{1,m,t}. \quad (28)$$

We use the approximation of separability to obtain

$$C_{2,m,t}=C_{2,3,t}(C_{1,2,m})/(C_{1,2,3}) \quad (29)$$

and

$$C_{1,m,t}=C_{1,3,t}(C_{1,2,m})/(C_{1,2,3}). \quad (30)$$

We may then carry through the operations equivalent to Eq. (13) through Eq. (15) and obtain

$$C_{1,2,m}\left[E_m-E_3+G\sum_{t\neq 1,2}\frac{C_{1,2,t}}{C_{1,2,3}}+G\frac{(C_{2,3,m}+C_{1,3,m})}{C_{1,2,3}}\right]=G\sum_{t\neq 1,2}C_{1,2,t}+G(C_{2,3,m}+C_{1,3,m}), \quad (31)$$

and by the series of steps that we used to go from Eq. (15) to Eq. (16), we obtain an equation for $\sum_{t\neq 1,2}C_{1,2,t}/C_{1,2,3}$ of the same type as Eq. (16). In exactly the same way, we obtain equations for $\sum_{t\neq 2,3}C_{2,3,t}/C_{1,2,3}$ and $\sum_{t\neq 1,3}C_{1,3,t}/C_{1,2,3}$.

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