Linearization of the Pairing Hamiltonian*

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The pairing-Hamiltonian eigenstates are used to test linearization procedures for the equations of motion of pair-creation operators. It is found that standard linearization techniques are inadequate and additional terms are suggested by a detailed examination of pairing wave functions. The new linearization procedure is applied with considerable success to the pairing vibration problem. Possible extension of the results to more general two-body interactions is discussed.

I. INTRODUCTION

LINEARIZATION of the equations of motion is a popular approach to the problem of determining eigenvalues of a Hamiltonian containing residual two-body interactions. The pairing Hamiltonian contains a comparatively simple residual two-body interaction; yet, a linearization of the equations of motion sometimes leads[1] to rather poor results. Although there are very accurate techniques[2–4] for determining eigenvalues of the pairing Hamiltonian, we feel that a detailed study of the linearization technique is of considerable interest for this case. Hopefully, any improvements which we find in the pairing linearization procedure will be applicable to more general nuclear two-body interactions because pairing forces are such an important part of nuclear forces. In this study, we employ good fixed-particle[3] pairing wave functions, so corrections to be made arise from the linearization procedure.

II. ANALYSIS

We consider the Hamiltonian

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

where the symbols have their usual[3] meaning. The operators $a_k^\dagger$ (a_k) obey the fermion anticommutation rules

$$a_k^\dagger a_l+a_l a_k^\dagger=\delta_{k,l};\quad a_k^\dagger a_l^\dagger+a_l^\dagger a_k^\dagger=a_k a_l+a_l a_k=0. \quad (2)$$

We set

$$A_k^\dagger=a_k^\dagger a_{-k}^\dagger, \quad (3)$$

and evaluate the commutator with the Hamiltonian of Eq. (1) to obtain the result[1]

$$[H,A_k^\dagger]=2\epsilon_k A_k^\dagger-G\sum_l A_l^\dagger(1-N_k-N_{-k}), \quad (4)$$

where

$$N_k=a_k^\dagger a_k, \quad (5)$$

and, in the case of the pairing Hamiltonian, we note that

$$\langle 0'|N_k|0'\rangle=\langle 0'|N_{-k}|0'\rangle. \quad (6)$$

Equation (4) is to be evaluated between a system containing $N-2$ particles and a system containing N particles; we specialize here to the ground state of the $(N-2)$-particle system which we denote by $|0'\rangle$. We obtain the result

$$(2\epsilon_k-\lambda)\langle\alpha|A_k^\dagger|0'\rangle=G\sum_l\langle\alpha|A_l^\dagger(1-2N_k)|0'\rangle, \quad (7)$$

where we have made the substitution

$$\lambda=E_\alpha-E_0'. \quad (8)$$

Equation (7) is exact and leads directly to a set of eigenvalues in the N-particle system; the only difficulty is the evaluation of the quantity $\sum_l\langle\alpha|A_l^\dagger N_k|0'\rangle$. We note that when the $(N-2)$-particle system is completely empty or full, there are no problems in the evaluation of $\sum_l\langle\alpha|A_l^\dagger N_k|0'\rangle$. Similarly, Eq. (7) is simply solved when all single-particle energies ϵ_k are degenerate. In this case, we can sum over k to obtain the result

$$(2\epsilon-\lambda)\sum_k\langle\alpha|A_k^\dagger|0'\rangle=G(L-2P)\sum_l\langle\alpha|A_l^\dagger|0'\rangle \quad (9)$$

or more simply,

$$(2\epsilon-\lambda)=G[L-2P], \quad (9')$$

where we have set

$$L=\sum_l 1,$$

and

$$P\equiv\sum_{k>0}\langle 0'|N_k|0'\rangle\equiv(N-2)/2. \quad (10)$$

When the single-particle energies are not degenerate, we have

$$\sum_k(2\epsilon_k-\lambda)\langle\alpha|A_k^\dagger|0'\rangle=G(L-2P)\sum_l\langle\alpha|A_l^\dagger|0'\rangle, \quad (11)$$

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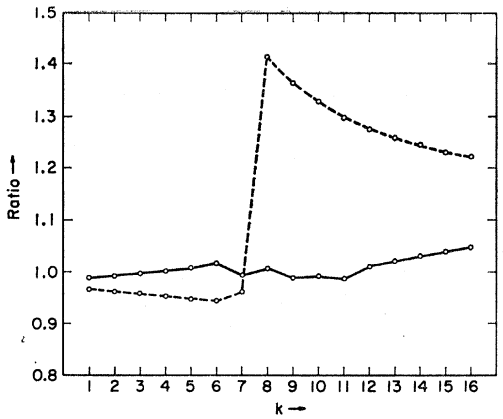

FIG. 1. Ratio of $\sum_l \langle\alpha|A_l^\dagger N_k|0'\rangle$ to various approximations. The dashed curve gives the ratio with respect to the right-hand side of Eq. (12). The solid curve gives the ratio with respect to Eq. (15) of the text.

which suggests the obvious approximation

$$\sum_l \langle\alpha|A_l^\dagger N_k|0'\rangle=\langle N_k\rangle \sum_l \langle\alpha|A_l^\dagger|0'\rangle, \quad (12)$$

where we have adopted the notation

$$\langle 0'|N_k|0'\rangle\equiv\langle N_k\rangle. \quad (13)$$

By combining Eq. (12) with Eq. (7), we obtain the elegant relation

$$1=G\sum_k \frac{1-2\langle N_k\rangle}{2\epsilon_k-\lambda}. \quad (14)$$

Unfortunately, Eq. (14) is not adequate[1] for computing eigenvalues in many cases. The question which we have studied is: What can be used in place of Eq. (12)? The restriction which we place on possible replacements for Eq. (12) is that the replacement must reduce to Eq. (12) when we consider an empty, a full, or a degenerate system. We impose the additional limitation that all terms must be linear in the matrix elements $\langle\alpha|A_l^\dagger|0'\rangle$. We have constructed approximate, fixed-particle-number, pairing wave functions using previously described[3] methods. We have determined the ground-state wave function for systems of seven and eight pairs of particles in sixteen equally spaced levels and chosen $G/\Delta\epsilon=\frac{1}{2}$. With these wave functions, we have computed the quantities $\langle 0|A_l^\dagger N_k|0'\rangle$, $\langle 0|A_l^\dagger|0'\rangle$, and $\langle N_k\rangle$. In Fig. 1, we have plotted the ratio

$$\frac{\sum_l \langle\alpha|A_l^\dagger N_k|0'\rangle}{\langle N_k\rangle\sum_l \langle\alpha|A_l^\dagger|0'\rangle}$$

as a function of k. These points are connected by the dashed line. Figure 1 indicates that there is considerable room for improvement on the approximation of Eq. (12).

Using trial and error methods, we hit upon the approximation

$$\sum_l \langle 0|A_l^\dagger N_k|0'\rangle=\langle N_k\rangle\sum_l \langle 0|A_l^\dagger|0'\rangle + B\langle N_k\rangle(1-\langle N_k\rangle)\{[\sum_l \langle N_l\rangle^2(1-\langle N_l\rangle)]\langle 0|A_k^\dagger|0'\rangle - \langle N_k\rangle[\sum_l \langle N_l\rangle(1-\langle N_l\rangle)\langle 0|A_l^\dagger|0'\rangle]\}, \quad (15)$$

where the coefficient B is given by the relation

$$B=\frac{P}{2}\frac{[1+\sum_l \langle N_l\rangle(1-\langle N_l\rangle)]}{[\sum_l \langle N_l\rangle(1-\langle N_l\rangle)][\sum_m \langle N_m\rangle^2(1-\langle N_m\rangle)]}. \quad (16)$$

The value of B was fixed by examining several other pairing systems. In Fig. 1, we have also plotted the ratio of the left to right side of Eq. (15). These points are connected by the uninterrupted line. It is clear that Eq. (15) is an extremely good approximation. We note that Eq. (15) obeys the sum rule

$$\sum_{l,k} \langle\alpha|A_l^\dagger N_k|0'\rangle=\sum_k \langle N_k\rangle\sum_l \langle\alpha|A_l^\dagger|0'\rangle. \quad (17)$$

However, it is not at all clear that it obeys the sum rule

$$\sum_k \langle\alpha|A_l^\dagger N_k|0'\rangle=(\sum_k \langle N_k\rangle)\langle\alpha|A_l^\dagger|0'\rangle. \quad (18)$$

We note that the relation

$$\langle 0|A_l^\dagger N_k|0'\rangle=\langle N_k\rangle\langle 0|A_l^\dagger|0'\rangle+\frac{\langle N_k\rangle}{L-1}\langle 0|A_k^\dagger|0'\rangle + B\langle N_k\rangle(1-\langle N_k\rangle)\langle N_l\rangle(1-\langle N_l\rangle)[\langle N_l\rangle\langle 0|A_k^\dagger|0'\rangle-\langle N_k\rangle\langle 0|A_l^\dagger|0'\rangle] \quad (19)$$

appears to be quite good, so our approximation does not violate the sum rule of Eq. (18) very seriously.

When the state $\langle\alpha|$ is the first excited seniority-zero state we find that Eq. (15) is considerably better than Eq. (12) as an approximation, but even Eq. (15) is unsatisfactory. Besides keeping any more terms which we may add to Eq. (15) linear in the matrix elements $\langle\alpha|A_k^\dagger|0'\rangle$, we must be careful not to ruin the approximation of Eq. (15) for the matrix elements $\langle 0|A_l^\dagger N_k|0'\rangle$. This consideration leaves very few choices of additional terms. We find that a term of the form

$$D[\langle N_k\rangle(1-\langle N_k\rangle)]\left[\langle\alpha|A_k^\dagger|0'\rangle-\langle 0|A_k^\dagger|0'\rangle\frac{\sum_l \langle N_l\rangle(1-\langle N_l\rangle)\langle\alpha|A_l^\dagger|0'\rangle}{\sum_l \langle N_l\rangle(1-\langle N_l\rangle)\langle 0|A_l^\dagger|0'\rangle}\right] \quad (20)$$

leads to a fairly good approximation for the first excited state $\langle 1|$ when this term (20) is added to Eq. (15). The coefficient D is given by the relation

$$D=L+\tfrac{1}{2}P, \tag{21}$$

but we emphasize that the approximation for the excited state is considerably worse than that for the ground state.

Substitution of our approximation into Eq. (6) leads to the working equations

$$(2\epsilon_k-\lambda)\langle\alpha|A_k^\dagger|0'\rangle=G(1-2\langle N_k\rangle)\sum_l\langle\alpha|A_l^\dagger|0'\rangle$$

$$-2GB\langle N_k\rangle(1-\langle N_k\rangle)[\sum_l\langle N_l\rangle^2(1-\langle N_l\rangle)\langle\alpha|A_k^\dagger|0'\rangle-\langle N_k\rangle\sum_l\langle N_l\rangle(1-\langle N_l\rangle)\langle\alpha|A_l^\dagger|0'\rangle]$$

$$-2GD\langle N_k\rangle(1-\langle N_k\rangle)\left[\langle\alpha|A_k^\dagger|0'\rangle-\frac{\langle 0|A_k^\dagger|0'\rangle\sum_l[\langle N_l\rangle(1-\langle N_l\rangle)\langle\alpha|A_l^\dagger|0'\rangle]}{\sum_l[\langle N_l\rangle(1-\langle N_l\rangle)\langle 0|A_l^\dagger|0'\rangle]}\right]. \tag{22}$$

First, we must determine the wave function $|0'\rangle$ and with it evaluate the quantities $\langle N_k\rangle$. When we are dealing with pairing forces, we can determine $|0'\rangle$ with the methods of Ref. 3. With a wave function of this type, it is straightforward to evaluate $\langle N_k\rangle$. The next step is to solve the L linear equations obtained from Eq. (22) for the lowest eigenvalue λ_0, setting $D=0$. After obtaining λ_0, it is straightforward to evaluate the quantities

$$\frac{\langle 0|A_k^\dagger|0'\rangle}{\sum_l\langle N_l\rangle(1-\langle N_l\rangle)\langle 0|A_l^\dagger|0'\rangle}.$$

We then solve the complete set of L equations given by Eq. (22) for the first two eigenvalues.

As a test of our procedure, we have calculated eigenvalues of the Högaasen-Feldman[1] problem. This problem was the original reason for our study of linearization approximations. In the particular case which we consider, there are two groups of 10 doubly degenerate levels separated by a single-particle spacing of $\frac{1}{2}$ in some arbitrary units. Each level can be occupied by a pair of particles, and there are 10 pairs of particles. We are interested in the energy spacing between the ground state and the first excited 0^+ state, as a function of G, the pairing interaction strength. An exact diagonalization has been done[1] for this system and this result is displayed by the solid curve in Fig. 2. All approximation techniques discussed in Ref. 1 fail badly, for some interval of G values. We note also that Eq. (14) completely fails to reproduce the exact curve. We have used Eq. (22) to compute this energy spacing, and the results of this calculation are indicated by the circles in Fig. 2. These results are extremely good and indicate that our approach has some merit. We note, also, that in spite of the formidable form of Eq. (22), the system of equations is quite easy to solve for the Högaasen-Feldman problem. Once we have the occupation probabilities $\langle N_k\rangle$, Eq. (22) can be solved readily by hand.

Aside from furnishing a severe test of linearization techniques, the Högaasen-Feldman problem displays an interesting phenomenon. For small values of G, the first excited 0^+ state is closer to the ground state in energy than it would be in the absence of pairing forces. This effect can be understood by examination of a much simpler system. We consider a system having one pair of particles. The single-particle levels of the system are one level at energy zero and N levels at single-particle energy $\frac{1}{2}$. For this system, we have the well-known exact eigenvalue equation

$$1=G\left[\frac{1}{-\lambda}+\frac{N}{1-\lambda}\right]. \tag{23}$$

The energy spacing between the two eigenstates, $\Delta\lambda$, is given by the equation

$$\Delta\lambda=[1-2G(N-1)+G^2(N+1)^2]^{1/2}. \tag{24}$$

From Eq. (24), we can see that this system shows the same phenomenon as the Högaasen-Feldman system.

We note, also, that the spacing $\Delta\lambda$ is minimized by choosing the value

$$G=(N-1)/(N+1)^2 \tag{25}$$

and

$$\Delta\lambda_{\min}=\frac{2\sqrt{N}}{N+1}, \tag{26}$$

i.e., $\Delta\lambda_{\min}\to 0$ as $N\to\infty$. The causes of the dip phenomenon are extremely transparent in this system.

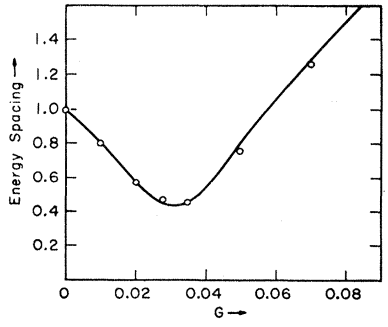

FIG. 2. Energy separation of 0^+ states in the Högaasen-Feldman model. The curve shows the exact value of the splitting. The circles are points calculated with the use of Eq. (22). The unit of energy is arbitrary.

We have one configuration at $E=0$ and many at $E=1$. As $G\rightarrow 0$, the ground-state wave function approaches $A_0^\dagger|0'\rangle$ because the energy lowering to be obtained from the pairing interaction is more than offset by the single-particle energies of the other configurations. For the excited state, however, the situation is entirely different. There are N configurations at the single-particle energy $E=1$, and the wave function for the first excited state can fully exploit the energy lowering from pairing interactions among these configurations at no cost in increased single-particle energy. As G becomes larger than $(N-1)/(N+1)^2$, the ground-state wave function can exploit the configurations at $E=1$ to a large enough extent to make the spacing $\Delta\lambda$ start to increase. At the minimum, it is interesting to note that the ground-state wave function (in the limit $N\rightarrow\infty$) is of the form

$$\Psi=\frac{1}{\sqrt{2}}\left[A_0^\dagger|0'\rangle+\frac{1}{\sqrt{N}}\left[\sum_{L=1}^{N}A_L^\dagger|0'\rangle\right]\right], \tag{27}$$

i.e., there is already a 50% mixture of excited-state configurations in the ground-state wave function.

It is also interesting to note that this dip phenomenon will not be restricted to seniority-zero excited states. Under similar circumstances, one may find that a seniority-two (one broken pair) state is closer in energy to the ground state when the pairing constant is nonzero than the same state would be in the absence of pairing forces. In the Högaasen-Feldman system which we have studied, this effect would occur when one pair is broken and both of the blocked levels are in either the upper or lower ten levels of the system.

III. CONCLUSIONS

From the results of this study, it is clear how to use linearization techniques to obtain some eigenvalues of the pairing Hamiltonian. It is also clear that a straightforward linearization of the type of Eq. (12) is not adequate. Another note of caution should be raised concerning linearization methods. Although we might be able to determine eigenvalues quite accurately by solving the linear equations given by Eq. (22), we have no guarantee that the state $|\alpha\rangle$ is well represented by the relation

$$|\alpha\rangle\propto\sum_k C_k A_k^\dagger|0'\rangle \tag{28}$$

in general.

We do, however, have some evidence that Eq. (28) is a fairly good approximation when $|\alpha\rangle$ is either the ground state or first excited seniority-zero state of the pairing Hamiltonian. In Ref. 4, the pairing Hamiltonian was diagonalized, using essentially the set of basis states suggested by Eq. (28). This procedure gave fairly good eigenvalues for the two lowest states. The energies of some of the higher states, however, were lowered considerably by the addition of other configurations to the set of basis states.

The general problem which remains to be examined concerns the Hamiltonian

$$H=\sum_k \epsilon_k a_k^\dagger a_k-\sum_{ijkl} V_{ijkl}a_i^\dagger a_j^\dagger a_k a_l. \tag{29}$$

For this case, the analog of Eq. (7) is of the form

$$\begin{aligned}(\epsilon_m+\epsilon_n-\lambda)&\langle\alpha|a_m^\dagger a_n^\dagger|0'\rangle\\ =&\sum_{ij}T_{ijmn}\langle\alpha|a_i^\dagger a_j^\dagger(1-N_m-N_n)|0'\rangle\\ &+\sum_{ij}T_{ijmj}\langle\alpha|a_i^\dagger a_n^\dagger N_j|0'\rangle+\sum_{ij}T_{ijim}\langle\alpha|a_j^\dagger a_n^\dagger N_i|0'\rangle\\ &+\sum_{ij}T_{ijjn}\langle\alpha|a_i^\dagger a_m^\dagger N_j|0'\rangle+\sum_{ij}T_{ijni}\langle\alpha|a_j^\dagger a_m^\dagger N_i|0'\rangle,\end{aligned} \tag{30}$$

where

$$T_{abcd}\equiv V_{abcd}-V_{abdc} \tag{31}$$

and we have not included in Eq. (30) the terms in which the fermion destruction operator differs from all of the creation operators. The problems which face us are: (1) What is the proper way to generalize Eqs. (15) and (20), and (2) how do we determine the eigenfunction $|0'\rangle$? Since pairing forces are a large part of residual nuclear forces, we have some reason to believe that these problems will be solved and we are investigating them at present.

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