"Seniority-Zero" Excited States of the Pairing Hamiltonian*

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(Received 10 November 1964)

The seniority-zero excited-state spectrum of the Hamiltonian

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

is studied in detail. Approximate excited-state wave functions of the form

$$\psi^\lambda=\sum_\alpha F(\lambda,\alpha)\sum_i D(\alpha,i)a_i^\dagger a_{-i}^\dagger\sum_{j>i}D(\alpha,j)a_j^\dagger a_{-j}^\dagger\cdots|0\rangle$$

are developed. These solutions are compared with exact solutions of a small system and the agreement is quite good. A somewhat larger system is studied in order to see how the excited-state spectrum changes as the number of separable functions is increased. The method is applied to heavy nuclei and is in good agreement with observed 0^+ excited states for nuclei having 144 to 150 neutrons. A theoretical 0^+ spectrum is displayed for each even neutron system from 144 to 152 neutrons.

I. INTRODUCTION

In the past year or two, it has become increasingly clear how to obtain good ground-state wave functions for the pairing Hamiltonian. The two general approaches which have been followed are (1) making improvements[1–6] of the quasiparticle method and (2) developing non-quasiparticle methods[7–10] for handling the problem. The various methods which have been developed for the ground-state wave function can also be applied with considerable success to obtain approximate wave functions of the lowest energy state having a set of specified levels occupied by unpaired particles. Such states, however, constitute only a small fraction of the eigenstates of the pairing Hamiltonian. It is the purpose of this paper to develop methods for obtaining approximate eigenvalues and eigenfunctions of states, other than those mentioned above, with an accuracy approaching that obtained for the lowest energy states.

The reason for quotation marks in the title is that our method is not restricted in applicability to states of seniority zero. In an even-even nucleus, the states which we are attempting to describe correspond to the $I=0$, positive-parity excited states (beta vibrations) which have been observed in many deformed nuclei. Our method is also applicable in even systems to the seniority-two states which appear at roughly the energies of the lowest seniority-four states, etc. In an odd-mass nucleus, the states which we describe correspond to seniority-one excited states having the same spins and parities as the ground state and other low-lying single-particle levels and should have energies roughly comparable to the lowest seniority-three states.

II. FORMULATION OF THE PROBLEM

In the course of this paper, we shall use the notation $S=R$ to mean a state of seniority R, i.e., there are R unpaired particles in the configuration of interest. We shall use the symbol P to indicate the number of pairs of particles in the system of interest and L to indicate the number of levels.

The Hamiltonian which we are investigating is

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

where ϵ_k is a single-particle energy and the sum over k means some specified finite number of levels in the vicinity of the Fermi surface. $a_k^\dagger(a_k)$ is a fermion creation (annihilation) operator; G is a constant pairing interaction energy; $-k$ indicates the time reversal partner of k and

$$b_k^\dagger=a_k^\dagger a_{-k}^\dagger,\qquad b_l=a_{-l}a_l. \qquad (2)$$

The fundamental approximation which is made in most[11] approaches to the ground-state wave function is the separability of the amplitudes of the various configurations; a somewhat less restrictive approximation was made in II. If we examine exact solutions for the Hamiltonian of Eq. (1), which are obtained by diagonalization of a matrix for systems of small P and L, it becomes immediately clear that separability is a totally inadequate approximation for the excited states which we are now studying. If we give up separability, it becomes quite difficult to solve for the eigenstates of Eq. (1) directly as we did in I and II. Furthermore,

* Based on work performed under the auspices of the U. S. Atomic Energy Commission.

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[11] See, however, Refs. 7 and 8.

nonseparable amplitudes are not very useful in computing matrix elements between various states of a system having reasonably large numbers of pairs, and must be computed one by one for each configuration. The compromise that we wish to pursue in this paper is to describe the excited states of the pairing Hamiltonian as sums of separable functions.

The separable ground-state wave function ψ_0 of Eq. (1) for a system having an even number of particles is of the form

$$\psi_0=\sum_i D_i b_i^\dagger \sum_{j>i} D_j b_j^\dagger \sum_{k>j} D_k b_k^\dagger \cdots |0\rangle, \quad (3)$$

where $|0\rangle$ indicates the vacuum state and the number of summations in Eq. (3) is equal to P. The factors D_i are numbers and a method for obtaining them is given in I. A method for obtaining an improved set of factors D_i is given in Appendix A. The form of excited states that we shall consider is

$$\psi_{\rm exc}=\sum_\alpha \sum_i D(\alpha,i) b_i^\dagger \sum_{j>i} D(\alpha,j) b_j^\dagger \times \sum_{k>j} D(\alpha,k) b_k^\dagger \cdots |0\rangle, \quad (4)$$

and our problem is to determine the factors $D(\alpha,i)$ and over how many values the index α is to run. It is clear that our excited-state solutions are in a considerably messier form than the ground-state solution, but this is inherent in the problem because of the inadequacy of a function of the form of Eq. (3) to represent the excited states.

The approach that we shall take in this paper is to make a very detailed study of $S=0$ excited states in two limiting cases, namely $G\to 0$ and $G\to\infty$. From our analysis of these two limits, we can generalize to more physically plausible values of G and we shall find that wave functions of the form of Eq. (4) give good descriptions of $S=0$ excited states over the entire range of values of G.

III. $S=0$ EXCITED STATES AS $G\to\infty$

In the limit $G/\Delta\epsilon\to\infty$, where $\Delta\epsilon$ is the single-particle energy level spacing, the BCS method[12] gives good ground-state wave functions and is a useful guide to the low-lying $S=0$ excited states. We shall use $\psi^{\rm BCS}$ to indicate the BCS wave function and $\psi^{\rm PBCS}$ to indicate that part of the BCS wave function which contains the correct number of pairs of particles.

As $G\to\infty$,

$$\psi_0{}^{\rm BCS}=(1/\sqrt{N_0})\prod^k (1+b_k^\dagger)|0\rangle, \quad (5)$$

where $\psi_0{}^{\rm BCS}$ is the ground-state wave function and N_0 is the normalization. The BCS method then goes on to obtain the low-lying excited $S=0$ states by constructing functions

$$\psi_{k_0}{}^{\rm BCS}=(1/\sqrt{N_{k_0}})(1-b_{k_0}^\dagger)\prod^{k\neq k_0}(1+b_k^\dagger)|0\rangle, \quad (6)$$

and identifying these states as the $S=0$ excited states. In fact, the BCS method does give the energies of the $S=0$ excited states correctly in this limit. However, there are difficulties. In general

$$\langle\psi_0{}^{\rm PBCS}|\psi_{k_0}{}^{\rm PBCS}\rangle\neq 0. \quad (7)$$

In the special case that $L=2P$, $\psi_{k_0}{}^{\rm PBCS}$ will be orthogonal to $\psi_0{}^{\rm PBCS}$; but even in this special case we still have the difficulty that

$$\langle\psi_{k_0}{}^{\rm PBCS}|\psi_{m_0}{}^{\rm PBCS}\rangle\neq 0. \quad (8)$$

The nonorthogonality problems of Eq. (7) and (8) are intimately related[13] to the fact that there are L functions of the form of Eq. (6) but only $(L-1)$ $S=0$ excited states at the energy of the lowest $S=2$ states.

The changes that must be made in the BCS point of view are comparatively slight in this limit. We define the set of functions

$$\varphi_{k_0}=b_{k_0}^\dagger \sum_{l\neq k_0} b_l^\dagger \sum_{\substack{m>l\\ m\neq k_0}} b_m^\dagger \cdots |0\rangle, \quad (9)$$

where the number of summations in Eq. (9) is $P-1$. We must then diagonalize the Hamiltonian using this set of L functions as our basis. If we carry through this procedure, we obtain the ground-state wave function and the $(L-1)$ $S=0$ lowest excited states. If the single-particle energy levels are degenerate, our results are exact.

Because the functions φ_{k_0} are not mutually orthogonal the problem that we must solve is of the form

$$H_{k_0,l_0}-\lambda(OV)_{k_0,l_0}=0, \quad (10)$$

where H_{k_0,l_0} is a matrix whose elements are $\langle\varphi_{k_0}|H|\varphi_{l_0}\rangle$ and the elements of OV (the overlap matrix) are $\langle\varphi_{k_0}|\varphi_{l_0}\rangle$; the main point here is

$$(OV)_{k_0,l_0}\neq\delta_{k_0,l_0}. \quad (11)$$

Fortunately, a computer subroutine[14] has recently become available for just this problem and extensive use has been made of it in the course of this work. The necessary matrix elements for diagonalizing the Hamiltonian are given in Appendix B.

It is interesting to note that this approach can be immediately extended to higher $S=0$ excited states by considering the set of functions

$$\phi_{k_0,l_0}=b_{k_0}^\dagger b_{l_0}^\dagger \sum_{m\neq k_0,l_0} b_m^\dagger \sum_{\substack{n>m\\ n\neq k_0,l_0}} b_n^\dagger \cdots |0\rangle \quad (12)$$

in place of the functions φ_{k_0} of Eq. (9). There are $P-2$

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summations in Eq. (11). If we diagonalize this set of functions, we obtain the ground-state wave function, the $(L-1)$ lowest $S=0$ excited states and the R_2 $S=0$ excited states at the next highest energy where

$$R_2=\frac{L!}{(L-2)!2!}-\frac{L!}{(L-1)!1!}. \tag{13}$$

This approach can be extended to the R_P highest $S=0$ excited states where

$$R_P=\frac{L!}{(L-P)!P!}-\frac{L!}{(L-P+1)!(P-1)!}, \tag{14}$$

although the size of the matrix will probably be prohibitively large long before we get to the R_P highest states.

IV. $S=0$ EXCITED STATES AS $G\to 0$

Next we consider the limit $G/\Delta\epsilon\to 0$. In this limit the BCS approach is not too useful; in fact it breaks down completely. As $G\to 0$, we make the obvious but useful observation that the excited states should be similar to what they would be in the absence of pairing forces. We again start out by defining a set of L functions

$$\varphi_{k_0}=b_{k_0}^{\dagger}\sum_{l\neq k_0}D(k_0,l)b_l^{\dagger}\sum_{\substack{m>l\\ m\neq k_0}}D(k_0,m)b_m^{\dagger}\cdots|0\rangle, \tag{15}$$

such functions being a natural generalization of the functions defined in Eq. (8). We compute the amplitudes $D(k_0,l)$ by blocking the level k_0 with one pair of particles and determine the ground-state amplitudes of the system having one less pair and one less level than our original system, using the method of Appendix A. We choose the amplitudes $D(k_0,l)$ in this way in order to treat the effects of pairing in the L functions from which the $L-1$ excited states are to be constructed. It is clear that the amplitudes $D(0,l)$, i.e., those appropriate to the ground state of our original system are not quite right for the excited states. In the ground state, all configurations have their amplitudes in phase with each other; whereas in the excited states, which must be orthogonal to the ground state, not all amplitudes can be in phase. This means that the pairing term in the Hamiltonian will be comparatively more effective in mixing in configurations of higher single-particle energy in the ground state than it will be in the excited states. The blocking procedure that we use has just this effect, although we make no claim that this is the best possible way to fix the functions φ_{k_0}. Our choice of functions φ_{k_0} is to be either justified or modified by its utility in describing excited states.

If we construct the functions φ_{k_0} as described above, and diagonalize the appropriate Hamiltonian matrix, we find that some of our eigenvalues are rather poor for the $L-1$ lowest $S=0$ excited states, when we compare with exact results for rather small systems. The reason for this becomes clear if we consider φ_{k_0} for $k_0\leq P$. As $G\to 0$, all P of these functions will approach each other and for $G=0$ they will all be the same. To make this more explicit, we consider a set of six equally spaced levels and three pairs. As $G\to 0$, using our recipe for determining the amplitudes $D(k_0,l)$, we find

$$\begin{aligned}
&\varphi_1\to b_1^{\dagger}b_2^{\dagger}b_3^{\dagger}|0\rangle,\\
&\varphi_2\to b_1^{\dagger}b_2^{\dagger}b_3^{\dagger}|0\rangle,\\
&\varphi_3\to b_1^{\dagger}b_2^{\dagger}b_3^{\dagger}|0\rangle,\\
&\varphi_4\to b_1^{\dagger}b_2^{\dagger}b_4^{\dagger}|0\rangle,\\
&\varphi_5\to b_1^{\dagger}b_2^{\dagger}b_5^{\dagger}|0\rangle,
\end{aligned} \tag{16}$$

and

$$\varphi_6\to b_1^{\dagger}b_2^{\dagger}b_6^{\dagger}|0\rangle,$$

but if we want all of the $(L-1)$ lowest excited states in the limit $G\to 0$, we should have beside these functions, an additional three functions

$$\begin{aligned}
&\varphi_7\to b_1^{\dagger}b_3^{\dagger}b_4^{\dagger}|0\rangle,\\
&\varphi_8\to b_2^{\dagger}b_3^{\dagger}b_4^{\dagger}|0\rangle,
\end{aligned} \tag{17}$$

and

$$\varphi_9\to b_1^{\dagger}b_3^{\dagger}b_5^{\dagger}|0\rangle.$$

From this examination of the $G\to 0$ limit, we can see that it will be necessary to diagonalize a matrix that is somewhat larger than $L\times L$ if we want the $(L-1)$ lowest excited eigenstates to be correct in both limits. Again, it is not entirely clear how to construct functions which are most suitable for φ_7, φ_8, and φ_9. Our approach is to impose asymptotic restrictions on these functions, i.e., as $G\to 0$ these functions should reduce to those of Eq. (17) and as $G\to\infty$ they should become identical with the functions φ_{k_0} of Eq. (9). There are many ways of choosing such functions, so we choose one which is calculationally convenient and gives good numerical results. To construct φ_7, we set

$$\begin{aligned}
&D(7,i)=D(4,i), \quad i\neq 2,3\\
&D(7,3)=D(4,2),\\
&D(7,2)=D(4,3),
\end{aligned} \tag{18}$$

and we construct φ_8 in a similar way by switching $D(4,1)$ with $D(4,3)$ and finally we obtain φ_9 by switching $D(5,2)$ with $D(5,3)$. As we shall see in our discussion of numerical results, the eigenvalues that we obtain by diagonalizing the matrix of Eq. (10) for this expanded set of functions are quite good.

V. $S=0$ EXCITED STATES FOR INTERMEDIATE VALUES OF G

For the values of $G/\Delta\epsilon$ that one expects to find in deformed nuclei, it will be necessary to include the functions introduced in Sec. IV if one wants a good description of the $S=0$ excited-state spectrum. In this case of intermediate values of G, an additional complica-

tion arises. We computed our factors $D(k_0,l)$ by solving for the ground state of a system having one less pair and one less level than our original system. This procedure, while not mixing in as much of the higher energy configurations as we have in the ground state, does still not take into account sufficiently the fact that we have out-of-phase mixtures of functions φ_{k_0} in the excited states. Because of this out-of-phase mixing, the configurations of high single-particle energy may be even less likely than our functions φ_{k_0} would lead us to believe. For explicitness, we consider again six equally spaced levels and three pairs. The lowest $S=0$ excited state is roughly

$$\psi_{\text{exc}}=(1/\sqrt{N})[\varphi_4-\varphi_3], \tag{19}$$

where φ_4 and φ_3 are now normalized functions. The effect that we are discussing shows up most strongly in the first excited state. The second most probable configuration in both φ_4 and φ_3 is $b_1^\dagger b_3^\dagger b_4^\dagger|0\rangle$. Because of cancellation, this configuration becomes much less important in the excited state than it is in either φ_4 or φ_3. This means that we should also have less of the configurations $b_1^\dagger b_4^\dagger b_5^\dagger|0\rangle$ and $b_1^\dagger b_3^\dagger b_5^\dagger|0\rangle$ than we computed in the functions φ_4 and φ_3. We can alleviate this difficulty to a large extent by computing the factors $D(k_0,l)$ in the same way as we do in Sec. IV, but using some G_{eff} rather than the correct value of G. Our calculations indicate roughly that

$$G_{\text{eff}}\simeq(0.8-0.9)G \tag{20}$$

takes care of this problem, by reducing the amplitudes of the higher energy configurations in the functions φ_k. The same value of G_{eff} will not be the optimum one for all of the excited states, but the values of G_{eff} are sufficiently close to each other that one choice gives a good excited-state spectrum.

VI. $S\neq0$ EXCITED STATES

As was mentioned in the introduction, the methods we have developed are not confined in applicability to even systems or to $S=0$. In a system having an odd number of particles, the ground state and the lowest lying $S=1$ excited states are computed by blocking some one level in the vicinity of the Fermi surface with the odd particle and treating the remaining pairs and levels as an even system. Beside these $S=1$ states, there are other $S=1$ states at roughly the energy of the lowest $S=3$ states having the same spins and parities as the lowest $S=1$ states. We compute these higher $S=1$ states by blocking a level with the odd particle and treating the remaining pairs and levels in exactly the same way as we do for the $S=0$ excited states. The same approach is also valid for $S=2, 4, 6\cdots$ states in even systems and $S=3, 5, 7\cdots$ states in odd systems.

VII. DISCUSSION OF NUMERICAL CALCULATIONS

In order to test our ideas about $S=0$ excited states, we have done detailed calculations for a system of six equally spaced levels and three pairs of particles. The single-particle spacing is 0.5 in some arbitrary set of units and we vary G from 0.1 to 2.0. The exact solutions for such a system may be obtained by diagonalizing a 20×20 matrix and we compare the results of our approximate treatment with the exact eigenvalues. In Table I, we compare the exact results with approximate eigenvalues obtained from the diagonalization of a 6×6 matrix of the functions φ_{k_0} defined in Eq. (13). We also compare with the approximate eigenvalues obtained by diagonalizing a 9×9 matrix. The three additional functions in the 9×9 matrix are those that we discuss at the end of Sec. IV. In Table I, we list the ground-state energy as well as the first five excited states. Although the ground state energy is not always as good as that which we obtain using the methods of

TABLE I. $S=0$ excited-state spectra for 3 pairs and 6 levels.

		$G=0.1$			$G=0.3$			$G=0.5$	
	Exact	6×6	9×9	Exact	6×6	9×9	Exact	6×6	9×9
E_0	2.656	2.656	2.656	1.569	1.572	1.571	−0.094	−0.087	−0.088
E_1	3.671	3.671	3.671	2.924	2.926	2.926	2.184	2.190	2.191
E_2	4.678	4.678	4.678	3.915	3.918	3.917	3.035	3.041	3.037
E_3	4.678	5.099	4.678	3.915	4.123	3.919	3.035	3.147	3.043
E_4	5.686	5.686	5.686	4.922	4.924	4.924	3.968	3.975	3.971
E_5	5.686	6.078	5.688	4.922	5.070	4.933	3.968	4.030	3.978
		$G=0.7$			$G=1$			$G=2$	
	Exact	6×6	9×9	Exact	6×6	9×9	Exact	6×6	9×9
E_0	−2.089	−2.080	−2.083	−5.353	−5.347	−5.347	−16.935	−16.933	−16.934
E_1	1.398	1.404	1.408	0.065	0.073	0.076	−5.236	−5.232	−5.228
E_2	2.073	2.079	2.076	0.528	0.531	0.530	−5.053	−5.051	−5.051
E_3	2.073	2.141	2.082	0.528	0.557	0.534	−5.053	−5.049	−5.049
E_4	2.905	2.912	2.908	1.218	1.221	1.219	−4.643	−4.643	−4.643
E_5	2.905	2.933	2.912	1.218	1.227	1.220	−4.643	−4.642	−4.642

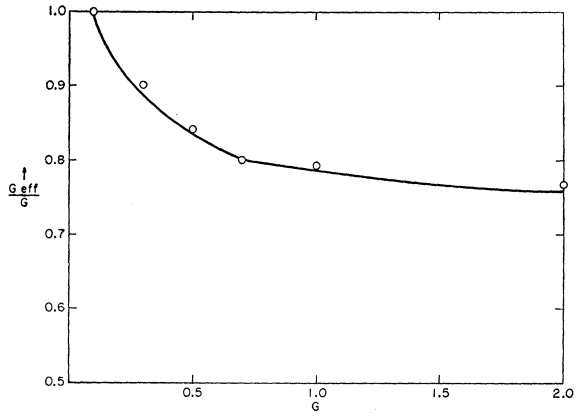

FIG. 1. Ratio of G_{eff} to G as a function of G.

II, it appears sufficiently good that one does not have to orthogonalize the excited states to some better ground-state wave function. Looking at Table I, for $G=0.1$, under the heading 6×6, we see that E_3 and E_5 will not be given correctly as $G\rightarrow 0$. As we increase the value of G, E_3 and E_5 approach the exact values. The 9×9 treatment seems to give satisfactory results over the entire range of values of G. It appears that we get equally good values for the first excited state no matter which treatment we use (6×6 or 9×9) and this should be true in general since the 6×6 treatment gives the first excited state in both limits (as $G\rightarrow 0$, φ_4 is the first excited state). If we want a more detailed picture of the $S=0$ excited-state spectrum, it becomes necessary to use the larger matrices. In Fig. 1, we display the ratio (G_{eff}/G), as a function of G, which we found to give the best results for the excited-state spectrum. A useful observation that we can make from Table I, is that the difference in energies E_3-E_2 that we obtain from the 9×9 treatment is a fair measurement of the differences between the exact and approximate eigenvalues, with the exception of E_1. It seems fairly clear that E_1 can be improved by including two more functions φ_3' and φ_4' which are computed in the same way as φ_3 and φ_4 but with an even smaller value of G_{eff} than the value which gives optimum results for the other excited states. This is not worthwhile in the small system that we are studying, but may be so in larger systems.

TABLE II. $S=0$ excited-state spectrum for 8 pairs and 16 levels.

	16×16	23×23	29×29
E_0	19.456	19.451	19.453
E_1	20.916	20.914	20.915
E_2	21.607	21.593	21.590
E_3	21.976	21.617	21.611
E_4	22.338	22.324	22.322
E_5	22.643	22.369	22.348
E_6	23.093	22.755	22.747
E_7	23.358	23.084	23.084
E_8	23.863	23.162	23.123
E_9	24.088	23.570	23.505
E_{10}	24.643	23.591	23.560
E_{11}	24.822	23.605	23.571
E_{12}	25.431	23.854	23.861
E_{13}	25.564	24.096	23.927
E_{14}	26.229	24.631	24.348
E_{15}	26.332	24.809	24.373

Although we are using roughly $\frac{1}{2}$ as large a matrix in our approximate treatment of the $L=6$ problem as we would use in the exact treatment, we emphasize that this will not be true for larger systems. In general, the size of the matrices we use in the approximate treatment will be roughly $1.5L\times1.5L$; whereas in an exact treatment, the matrices are

$$\frac{L!}{P!(L-P)!}\times\frac{L!}{(L-P)!P!}.$$

We have also done an approximate treatment of a system of 16 equally spaced levels ($\Delta\epsilon=0.4$ MeV) and $P=8$. We use a value of 0.2 MeV for G. In this case, we do not have exact solutions for purposes of comparison. In Table II, we examine the 16 lowest eigenvalues as a function of the size of the matrix that we diagonalize. The 16×16 matrix is made up of the functions φ_{k_0}, given in Eq. (13); the 23×23 matrix includes an additional 7 functions, which would be among the lowest energy states as $G\rightarrow 0$ and the 29×29 matrix includes 6 more such states. We first note that the ground-state eigenvalue is negligibly better than that which one obtains from an optimal[2] separable treatment, and poorer than the ground-state energy that one obtains with the methods of II (which give 19.418 as the ground-state energy). The first excited $S=0$ state is some 40 keV above the lowest $S=2$ state (which we compute with the methods of II). As $G\rightarrow 0$, the $S=2$ state clearly lies lower, and as $G\rightarrow\infty$ the two states become degenerate in energy, so this result looks quite reasonable. The spacing of roughly 20 keV between E_2 and E_3 also suggests that our eigenvalues are quite good. We note again that the 16×16 treatment gives the energy of the first excited state quite well, and fails badly for the first time at E_3. The 23×23 matrix gives fairly good eigenvalues through E_8, relative to the 29×29 treatment.

Another interesting feature of this case is that the lowest $S=0$ excited state is, to a good approximation,

$$\psi_1^{\text{exc}}=(1/\sqrt{N_1})[\varphi_9-\varphi_8], \tag{21}$$

where φ_9 and φ_8 are normalized versions of the functions defined in Eq. (15). This suggests a rough selection rule for transition probabilities to the ground state and other members of the ground-state rotational band in deformed nuclei from the first excited $S=0$ state. We designate the one-body operator for the particular

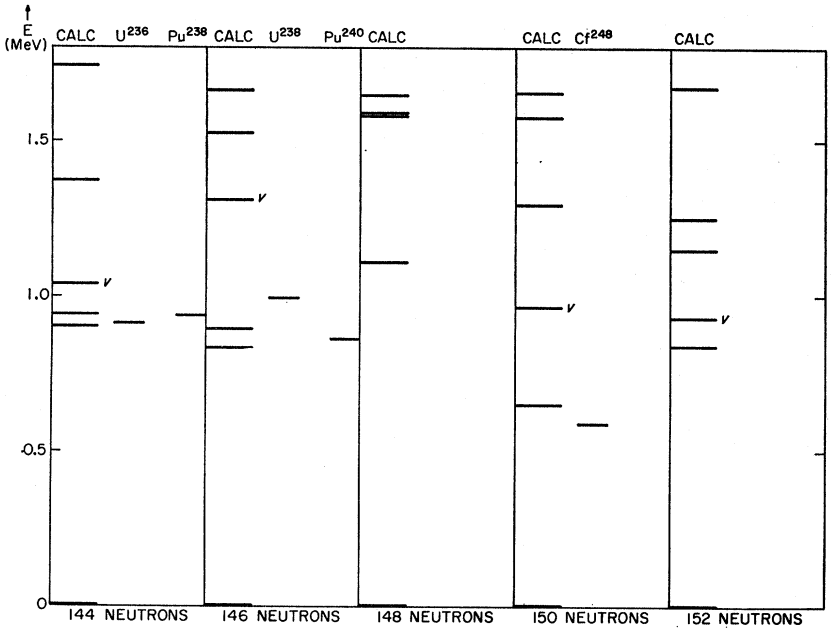

FIG. 2. 0^+ spectra for even neutron numbers. The check beside a calculated level indicates that the state is $S=2$.

transition of interest as M, and

$$A=\langle 0|b_{P+1}Mb_{P+1}^{\dagger}|0\rangle-\langle 0|b_{P}Mb_{P}^{\dagger}|0\rangle. \quad (22)$$

If A is considerably smaller than either of the two matrix elements in Eq. (22), we may expect the transition to be retarded.

VIII. APPLICATION TO THE HEAVY ELEMENTS

In this section, we apply our approach to neutron excitations in the heavy-element region. The assumptions that we make are that neutrons and protons may be treated as noninteracting systems and that the Hamiltonian of Eq. (1) is adequate to describe the 0^+ excited-state spectra of the heavy deformed nuclei. The input quantities for this calculation are a set of single-particle neutron energies and a value for G_N, the neutron pairing interaction constant. For the single-particle neutron energies, we use the values of Mang, Poggenburg, and Rasmussen[15] (removing the five lowest and four highest single-particle states). We determine a pairing force constant for neutrons G_N, by fitting the observed 0^+ excited state for 144 neutrons (U^{236} and Pu^{238}) to experiment. The value of G_N which we obtain in this way is

$$G_N=(21.2/A)\ \text{MeV}, \quad (23)$$

and this is in agreement with other values of G_N.

In Table III, we compare the lowest observed and calculated energies of 0^+ excited states for even neutron numbers between 140 and 152 neutrons. The agreement with experiment appears to be good for 144, 146, and 150 neutrons (144, of course, was fitted). 0^+ excited states have not been observed for 148 and 152 neutrons. For 140 and 142 neutrons, the agreement between the calculation and experiment is not particularly good. There are several possible reasons for these discrepancies. Residual two-body quadrupole interactions are expected to be more important[13,16] for these nuclei than for those having larger numbers of neutrons. Also the energy of the lowest 0^+ excited state is quite sensitive to small changes in G_N. We find that 1 keV changes in G_N can lead to changes of 20–30 keV in the energy of the first 0^+ excited state relative to the ground state; e.g., for 140 neutrons, reducing G_N from 91 to 85 keV gives a lowest 0^+ excited state at 810 instead of 940 keV. In spite of these difficulties, the results of

TABLE III. Energy of lowest 0^+ excited state (keV).

Neutron number	Calculated	Observed
140	940	634,[a] 693[b]
142	1030	730,[b] 810[a]
144	900	910,[a] 935[a]
146	835	863,[a] 997[b]
148	1100	...
150	650	590[c]
152	840	...

[a] See C. M. Lederer, University of California Radiation Laboratory Report UCRL-11028, 1963 (unpublished) for references to experimental measurements.
[b] See E. R. Marshalek, University of California Radiation Laboratory Report UCRL-10046, 1963 (unpublished) for references to experimental measurements.
[c] A. Friedman, K. Flynn, L. Glendenin, H. Griffin, and J. Milstead (to be published).

[15] H. J. Mang, J. K. Poggenburg, and J. O. Rasmussen, University of California Radiation Laboratory Report UCRL-11213, 1964 (unpublished).

[16] E. R. Marshalek, University of California Radiation Laboratory Report UCRL-10046, 1963 (unpublished).

Table III indicate that residual quadrupole interactions may not be too important in determining 0^+ excited state energies, especially for 144 neutrons or more.

In Fig. 2, we present the calculated $S=0$, 0^+ excited-state spectra for 144–152 neutrons. We include all neutron $S=0$, 0^+ states up to 1.8 MeV and also give a few neutron $S=2$, 0^+ excited states which appeared to be low in energy on examination of the single-particle energies. The $S=2$ excited states are calculated with the methods of II. We note that the ground-state energies calculated with the methods of II are roughly 10–20 keV below the energies calculated for ground states with the methods of this paper. We do not include any 0^+ excited states due to proton excitations, so the actual 0^+ spectra of deformed nuclei should contain more levels than are presented in Fig. 2.

ACKNOWLEDGMENTS

I would like to thank B. Garbow for providing the computer subroutine for diagonalizing nonorthogonal functions, and for gracious aid in many aspects of the programming of this problem. I would also like to thank D. Kurath for a critical reading of this manuscript and many useful comments made in the course of this work.

APPENDIX A

In this appendix, we wish to point out a method for obtaining better ground-state (and lowest excited state) eigenvalues than those obtained in I, subject to the restriction that the amplitudes of configurations are separable. By separable, we mean that the amplitude $C_{i,j,k\cdots}$ of the configuration $b_i^\dagger b_j^\dagger b_k^\dagger \cdots 10\rangle$ is of the form

$$C_{i,j,k\cdots}=D_iD_jD_k\cdots, \tag{A1}$$

as we have in Eq. (3).

In II, we showed that a better approximation than (A1) for the amplitudes is

$$C_{i,j,k\cdots}=F_nD_iD_jD_k\cdots, \tag{A2}$$

where F_n is a numerical factor depending only on the number of levels n which are occupied in the configuration i, j, $k\cdots$ and are unoccupied in the lowest energy configuration. For the purposes of this discussion, the important feature of F_n is

$$F_n\geqslant 1. \tag{A3}$$

This suggests that we can get a better separable wave function than that obtained in I by increasing the magnitudes of the factors D_k for $k>P$ relative to those for $k<P$. We do just this with a one-parameter variational treatment.

In I, we consider a system of two pairs and L levels and obtained the result

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

We introduce a variational parameter γ into this equation and modify it to read

$$C_{1,m}\left[\gamma(E_m-E_2)+G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}+G\frac{C_{2,m}}{C_{1,2}}\right]=G\sum_{t\neq 1}C_{1,t}+GC_{2,m}, \tag{A4}$$

and we modify (I-16) and (I-18) with the substitutions

$$(E_m-E_2)\rightarrow\gamma(E_m-E_2),$$
$$\text{and} \tag{A5}$$
$$(E_m-E_1)\rightarrow\gamma(E_m-E_1).$$

For a given value of γ, we solve for the coefficients $C_{1,m}$ and $C_{2,m}$ as described after (I-18). From these coefficients we determine the factors D_i using (II-21), (II-22), and (II-23). γ is varied to minimize the energy, which is computed using (II-24). We find quite generally

$$\gamma\leqslant 1, \tag{A6}$$

and this is to be expected.

The eigenvalues which we obtain in this way correspond very closely to those obtained for optimized[2] separable amplitudes but are not as good as those obtained with the approximation of Eq. (A2) as developed in II.

The approximation introduced in (A4) could just as well have been written

$$G\rightarrow G/\gamma, \tag{A7}$$

which is the same type of approximation made by Mikhailov[1] in his improved version of the BCS method. There is, however, a difference in spirit between the two approximations and this shows up in the fact that one needs the largest percentage changes in G as $G\rightarrow 0$ in the BCS treatment. This is necessary to keep the BCS method from going trivial. In our case, $\gamma\simeq 1$ as $G\rightarrow 0$, because the first-order terms are the dominant ones here in determining the energy. As the second-order configurations become more important, but F_2 is still appreciably larger than 1, γ takes on values quite a bit below 1.

APPENDIX B

In this section, we give the matrix elements used in the body of the text between functions φ_{k_0} and φ_{l_0}, which are defined in Eq. (12).

First, the normalization N_k. is

$$N_{k_0}\equiv\langle\varphi_{k_0}|\,\varphi_{k_0}\rangle=[\sum_{l\neq k_0}D(k_0,l)^2]^{P-1}, \tag{B1}$$

where

$$[\sum_{l\neq k_0}D(k_0,l)^2]^{P-1}\equiv\sum_{l\neq k_0}D(k_0,l)^2\sum_{\substack{m>l\\ m\neq k_0}}D(k_0,m)^2\cdots, \tag{B2}$$

and there are $P-1$ such summations in the expression.

Next, we have the overlaps

$$(OV)_{k_0,l_0}\equiv\langle\varphi_{k_0}|\,\varphi_{l_0}\rangle=\frac{1}{\sqrt{(N_{k_0}N_{l_0})}}D(k_0,l_0)D(l_0,k_0)\times[\sum_{m\neq k_0,\,l_0}D(k_0,m)D(l_0,m)]^{P-2}. \tag{B3}$$

We break up our Hamiltonian [Eq. (1)] as

$$\begin{aligned}H&=H_1+H_2,\\ H_1&=\sum_{k>0}\epsilon_k(a_k^\dagger a_k+a_{-k}^\dagger a_{-k})-G\sum_{k>0}b_k^\dagger b_k,\\ H_2&=-G\sum_{k>0}b_k^\dagger\sum_{\substack{l>0\\ l\neq k}}b_l,\end{aligned} \tag{B4}$$

and the matrix elements of H are

$$\langle\varphi_{k_0}|H_1|\,\varphi_{k_0}\rangle=(E_{k_0}/N_{k_0})[\sum_{m\neq k_0}D(k_0,m)^2E_m]^{P-1}-PG, \tag{B5}$$

where we are to understand

$$E_{k_0}E_mE_n\cdots\equiv 2(\epsilon_{k_0}+\epsilon_m+\epsilon_n\cdots), \tag{B6}$$

and

$$\langle\varphi_{k_0}|H_1|\,\varphi_{l_0}\rangle=\frac{D(k_0,l_0)D(l_0,k_0)}{\sqrt{(N_{k_0}N_{l_0})}}E_{k_0}E_{l_0}[\sum_{m\neq k_0,\,l_0}D(k_0,m)D(l_0,m)E_m]^{P-2}-PG\times(OV)_{k_0,l_0}. \tag{B7}$$

For the matrix elements of H_2, we have

$$\langle\varphi_{k_0}|H_2|\,\varphi_{k_0}\rangle=\frac{-2G}{N_{k_0}}\sum_{l\neq k_0}D(k_0,l)\sum_{\substack{m>l\\ m\neq k_0}}D(k_0,m)[\sum_{n\neq k_0,\,l,\,m}D(k_0,n)^2]^{P-2}, \tag{B8}$$

and

$$\begin{aligned}\langle\varphi_{k_0}|H_2|\,\varphi_{l_0}\rangle=\frac{-G}{\sqrt{(N_{k_0}N_{l_0})}}\{&[\sum_{m\neq k_0,\,l_0}D(k_0,m)D(l_0,m)]^{P-1}+D(k_0,l_0)D(l_0,k_0)\\ &\times[\sum_{\substack{m,n\neq k_0,l_0\\ n>m}}D(k_0,m)D(l_0,n)+D(l_0,m)D(k_0,n)][\sum_{r\neq k_0,\,l_0,\,m,\,n}D(k_0,r)D(l_0,r)]^{P-3}\\ &+[D(k_0,l_0)\sum_{m\neq k_0,\,l_0}D(l_0,m)+D(l_0,k_0)\sum_{m\neq k_0,\,l_0}D(k_0,m)][\sum_{n\neq k_0,\,l_0,\,m}D(k_0,n)D(l_0,n)]^{P-2}\}.\end{aligned} \tag{B9}$$

Next we consider a state φ_α of the type discussed at the end of Sec. IV. Let us say that φ_α is formed by interchange of some of the amplitudes $D(k_0,i)$. The matrix elements between φ_α and φ_{l_0} will be the same as those between φ_{k_0} and φ_0. with the following substitutions:

$$N_{k_0}\rightarrow N_{\alpha_0},\quad D(k_0,i)\rightarrow D(\alpha,i), \tag{B10}$$

and things such as $D(l_0,k_0)$ and E_{k_0} are not to be changed.

Finally, we consider matrix elements between φ_α and φ_{k_0}.

$$(OV)_{k_0,\alpha}=\frac{1}{\sqrt{(N_{k_0}N_\alpha)}}[\sum_{m\neq k_0}D(k_0,m)D(\alpha,m)]^{P-1}. \tag{B11}$$

$$\langle\varphi_{k_0}|H_1|\,\varphi_\alpha\rangle=\frac{E_{k_0}}{\sqrt{(N_{k_0}N_\alpha)}}[\sum_{m\neq k_0}D(k_0,m)D(\alpha,m)E_m]^{P-1}-PG\times(OV)_{k_0,\alpha} \tag{B12}$$

and

$$\langle\varphi_{k_0}|H_2|\,\varphi_\alpha\rangle=\frac{-G}{\sqrt{(N_\alpha N_{k_0})}}[\sum_{\substack{l,m\neq k_0\\ m>l}}D(k_0,l)D(\alpha,m)+D(k_0,m)D(\alpha,l)][\sum_{n\neq k_0,\,l,\,m}D(k_0,n)D(\alpha,n)]^{P-2}. \tag{B13}$$