Eigenfunctions of the Nuclear Pairing Hamiltonian*

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An examination of the approximation of separability is made for the pairing Hamiltonian

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

separability being defined as the decomposition of the amplitude of any configuration in the eigenfunctions of the pairing Hamiltonian as a product of factors, one factor associated with each occupied level. This approximation is found to be inadequate for the single-particle energy-level spacings and values of G typically used in nuclear calculations. A somewhat less restrictive approximation is introduced which leads to considerably improved solutions of the pairing Hamiltonian. The results of the approximate calculations are compared with available exact solutions and the agreement is found to be extraordinarily good.

I. INTRODUCTION

IN a previous paper,[1] we developed an approach to the treatment of pairing forces in nuclei, which has the virtue of *never* giving a "trivial" ($\Delta=0$ in quasiparticle language) solution for a nonzero pairing interaction, no matter how weak the pairing interaction may be. The one approximation made in our treatment is separability. By separability, we mean that the amplitude of any configuration is a product of factors, one factor being associated with each occupied level in the given configuration. This approximation, among others, is also made in the quasiparticle treatment of pairing interactions. The purpose of this paper is to examine in detail some of the implications of separability and to point out a less drastic approximation which leads to considerably improved values for approximate eigenvalues and eigenfunctions of the pairing interaction.

II. EXAMINATION OF SEPARABILITY

We consider a system having two pairs of particles and at least five levels available for occupancy by a pair, in order to investigate separability. The pairing Hamiltonian which we discuss is

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

where ϵ_k is a single-particle energy; $a_k^\dagger(a_k)$ is a fermion creation (annihilation) operator; $-k$ indicates the time reversal partner of k, and G is a constant-pairing interaction matrix element. The arguments that we shall develop concerning the Hamiltonian of Eq. (1) are also pertinent to the more complicated pairing interactions of the forms I-22 and I-23.

For a system with two pairs of particles, we have the exact relations[1]

$$C_{1,m}(E_{1,m}-\lambda)=G\sum_{t\neq1}C_{1,t}+G\sum_{t\neq m}C_{m,t} \quad (2)$$

and

$$C_{2,m}(E_{2,m}-\lambda)=G\sum_{t\neq2}C_{2,t}+G\sum_{t\neq m}C_{m,t}, \quad (3)$$

where $C_{i,j}$ is the probability amplitude of the configuration having levels i and j occupied, λ is the eigenvalue of the Hamiltonian, and

$$E_{i,j}\equiv2\epsilon_i+2\epsilon_j\equiv E_i+E_j. \quad (4)$$

The subscripts 1 and 2 denote the lowest and next to lowest single-particle levels. We specialize our discussion to a system of nondegenerate levels

$$E_i\neq E_j \quad (5)$$

for all i and j. Separability is formulated as

$$C_{i,j}=D_iD_j, \quad (6)$$

where D_i and D_j are numerical factors associated with the levels i and j, respectively. Subtracting Eq. (3) from Eq. (2), making use of Eq. (6), we obtain

$$\left(\frac{D_1-D_2}{D_2}\right)\left(\frac{1}{E_2-E_1}\right)=\frac{D_m}{D_m(E_{1,m}-\lambda)-G\sum_{t\neq1,2}D_t}. \quad (7)$$

As Eq. (7) is valid for all levels m other than 1 or 2, we may consider any two levels m_0 and n_0 and employ Eq. (7) to obtain

$$(D_{m_0}-D_{n_0})G\sum_{t\neq1,2}D_t=D_{m_0}D_{n_0}(E_{n_0}-E_{m_0}). \quad (8)$$

If, in place of Eq. (3), we use the relation

$$C_{3,m}(E_{3,m}-\lambda)=G\sum_{t\neq3}C_{3,t}+G\sum_{t\neq m}C_{m,t}, \quad (3')$$

we obtain, in place of Eq. (8)

$$(D_{m_0}-D_{n_0})G\sum_{t\neq1,3}D_t=D_{m_0}D_{n_0}(E_{n_0}-E_{m_0}). \quad (8')$$

A comparison of Eq. (8) and Eq. (8′) leads us to the result

$$D_2=D_3, \quad (9)$$

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

[1] R. R. Chasman, Phys. Rev. **132**, 343 (1963). This paper will be referred to as I, and equations from it will be given as I-15, e.g., for Ref. 1, Eq. (15).

since, if we take $D_{m_0}=D_{n_0}$, Eq. (8) leads us to

$$E_{n_0}=E_{m_0}, \tag{10}$$

which is in conflict with Eq. (5). However, if we interchange the roles of m_0 and n_0 with 2 and 3 in the derivations through Eq. (8′), we conclude

$$D_{m_0}=D_{n_0}, \tag{11}$$

which again implies Eq. (10). We see that separability leads to contradictions for systems of nondegenerate levels. We rewrite Eq. (8) in the form

$$(D_{m_0}-D_{n_0})=D_{m_0}D_{n_0}(E_{n_0}-E_{m_0})/G\sum_{t\neq 1,2}D_t, \tag{8″}$$

which suggests that separability becomes a better approximation as the energy levels approach each other in value for constant G, or as G is increased and the energy spacing held constant. Equation (8″) also implies that separability will become a better approximation as we increase the number of levels since $\sum_{t\neq 1,2}D_t$ increases. Generally, the single-particle spacings and values of G used in nuclear calculations are such as to suggest that separability is not a particularly good approximation.

It is interesting to note that the failure of separability, as seen in the disagreement between Eq. (5) and Eq. (10) is a direct consequence of the exclusion principle. The restrictions on the summations on the right-hand sides of Eqs. (2), (3), and (3′) are just the expression of the exclusion principle. If we do away with these restrictions, we are not able to obtain the result of Eq. (10). We know that separability is exact for a system of degenerate energy levels and also for a system having only one pair of particles. It is for just these systems that the effects of the exclusion principle are mitigated; i.e., if we have only one pair, all levels are accessible and for the degenerate system all levels are equivalent. In general, separability is inconsistent with the exclusion principle.

III. MODIFIED APPROXIMATION

It was pointed out[2] that the errors introduced into the approximate eigenfunctions of Eq. (1) through the use of Eq. (6) are manifested in the higher order amplitudes of the approximate wave function; separability gives higher order amplitudes which are smaller than the corresponding amplitudes in the exact wave function. By an nth order configuration, we mean one in which n of the levels, which are occupied in the most probable configuration, are unoccupied. In order to obtain improved approximations for the eigenfunction and eigenvalue, we introduce P new variational parameters into the treatment; P is the number of pairs in the system. In I, we considered a system having two pairs of particles, and we shall re-examine such a system with our modified treatment. For a system of two pairs, we replace Eq. (6) by

$$C_{i,j}=F_nD_iD_j, \tag{12}$$

where F_n is a variational parameter depending only on the order n of the configuration i, j. We set

$$\begin{aligned} F_0&=1,\\ F_1&=1, \end{aligned} \tag{13}$$

and F_2 will be the only variational parameter to be determined for a $P=2$ system.

In I, based on Eq. (6), we set

$$C_{m,n}=\frac{C_{1,m}C_{2,n}}{C_{1,2}}=\frac{C_{1,n}C_{2,m}}{C_{1,2}} \tag{14}$$

for all second-order configurations m, n. The approximation of Eq. (12) leads us to

$$C_{m,n}=F_2\frac{C_{1,m}C_{2,n}}{C_{1,2}}=F_2\frac{C_{1,n}C_{2,m}}{C_{1,2}} \tag{15}$$

for the second-order configurations. For our derivation, it is convenient to set

$$F_2=1+\beta, \tag{16}$$

but β is not necessarily small and is not treated as a small quantity. For the zeroth-order amplitude, we have[1]

$$C_{1,2}(E_{1,2}-\lambda)=G\sum_{t\neq 1}C_{1,t}+G\sum_{t\neq 2}C_{2,t}, \tag{17}$$

and we combine this with the relation for the first-order amplitude $C_{1,m}$ given in Eq. (2) to obtain

$$C_{1,m}(E_{1,m}-\lambda)=C_{1,2}(E_{1,2}-\lambda)-G\left[\sum_{t\neq 2}C_{2,t}-\sum_{t\neq m}C_{m,t}\right]. \tag{18}$$

By algebraic manipulation of Eqs. (15)–(18), we obtain

$$\frac{C_{1,m}}{C_{1,2}}\left[E_m-E_2+G\sum_{t\neq 1}\frac{C_{1,t}}{C_{1,2}}+G\frac{C_{2,m}}{C_{1,2}}-\beta G\sum_{t\neq 1,2,m}\frac{C_{2,t}}{C_{1,2}}\right]=G\sum_{t\neq 1}C_{1,t}+G\frac{C_{2,m}}{C_{1,2}}, \tag{19}$$

and

$$\sum_{m\neq 1,2}\frac{C_{1,m}}{C_{1,2}}=G\sum_{m\neq 1,2}\frac{\sum_{t\neq 1}(C_{1,t}/C_{1,2})+(C_{2,m}/C_{1,2})}{E_m-E_2+G\sum_{t\neq 1}(C_{1,t}/C_{1,2})+G(C_{2,m}/C_{1,2})-\beta G\sum_{t\neq 1,2,m}(C_{2,t}/C_{1,2})}. \tag{20}$$

[2] J. O. Rasmussen (private communication).

Equations (19) and (20) reduce to I-15 and I-16 for $\beta=0$. We obtain similar equations for $C_{2,m}$ by interchanging all subscripts 1 and 2 in Eqs. (19) and (20). Equations (19), (20) and their analogs for $C_{2,m}$ are solved iteratively for a given value of β. The development from Eq. (17) to Eq. (20) for the case $\beta=0$ is discussed in more detail in I. If there is degeneracy at the Fermi surface and the levels at the Fermi surface are only partially occupied, e.g., levels 2 and 3 are degenerate in the $P=2$ case, the equations are slightly different but the problem can still be treated without any difficulty. After the iteration process is completed, we have all of the first-order amplitudes and now we compute the factors D_i to associate with each level. Normalizing

$$D_1=1, \tag{21}$$

we set

$$D_2=\sum_{t\neq 2,1} C_{2,t}\Big/\sum_{t\neq 2,1} C_{1,t} \tag{22}$$

and

$$D_m=\left[\frac{(C_{1,m}/C_{1,2}+C_{2,m}/C_{1,2})}{(1/D_1+1/D_2)}\right] \tag{23}$$

for all levels m other than 1 or 2. In terms of the D's, the zeroth-order amplitude is D_1D_2; the first-order amplitudes are D_1D_m or D_2D_m and the second-order amplitudes are $(1+\beta)D_mD_n$. Our sole motivation for defining the amplitudes in this way is to make a computation of the eigenvalue feasible. Defining amplitudes in this way, it is possible to compute the eigenvalue λ for a given value of β as

$$\lambda=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{24}$$

with some minor modifications of the summation techniques of Mang and Dietrich.[3] We repeat the calculation for several values of β in order to minimize λ with respect to β. This completes the calculation for a system of two pairs.

For a general system containing more than two pairs, we have

$$C_{i,j,k}\ldots=F_nD_iD_jD_k\cdots, \tag{25}$$

where the number of subscripts on $C_{i,j,k}\ldots$ is equal to the number of pairs in the system. Equation (13) still defines F_0 and F_1. The derivation of the P equations equivalent to Eq. (19) and Eq. (20) is carried through in much the same way as for the $P=2$ system. The important thing to note is that F_2 (or β) is the only one of our variational parameters that enters the computation of the first-order amplitudes, no matter how many pairs we may have in the system. The higher order parameters $F_n(n>2)$ do enter the calculation, however, when we compute λ using Eq. (24). The procedure that we have adopted is to make some guess of the parameters F_n in terms of F_2 when we minimize λ with respect to F_2. After minimizing λ with respect to F_2, we keep F_2 and all of the D's fixed and vary F_3 until λ is minimized with respect to F_3. After fixing F_3, we continue by varying F_4, etc. The first guess that we used for F_n in our calculations was

$$F_n=(F_2)^{n-1} \tag{26}$$

for $n>2$; but in all cases that we used it we found that this guess consistently underestimated the magnitudes of the higher order variational parameters. At the end of the complete variational procedure, we had values of F_n larger than the estimates of Eq. (26). In place of Eq. (26), we have adopted a power law with a second difference of 1/2 in the exponent, i.e.,

$$\begin{aligned} F_3&=(F_2)^{2.5}\\ F_4&=(F_2)^{4.5}\\ F_5&=(F_2)^{7.0}, \end{aligned} \tag{27}$$

etc. We find that Eq. (27) gives a fairly good first guess of the higher order variational parameters. Whether we use Eq. (26) or Eq. (27) when minimizing λ with respect to F_2, we find the values of F_n to be pretty much the

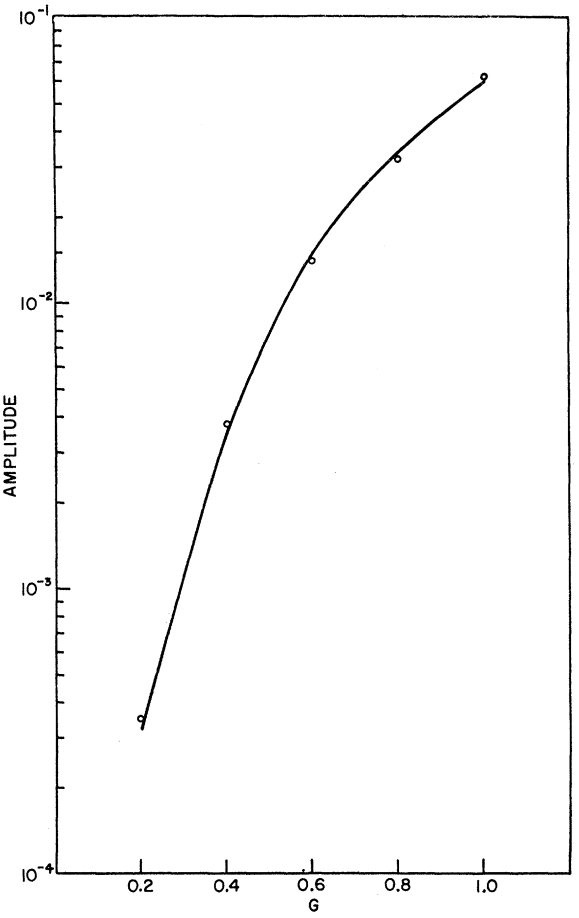

FIG. 1. Comparison of exact and approximate third-order amplitudes. The curve connects the exact values of $C_{4,5,6}/C_{1,2,3}$ computed in Ref. 2 and the open circles give the values of $F_3(D_4D_5D_6/D_1D_2D_3)$ computed with the techniques of this paper.

[3] H. J. Mang and K. Dietrich (unpublished).

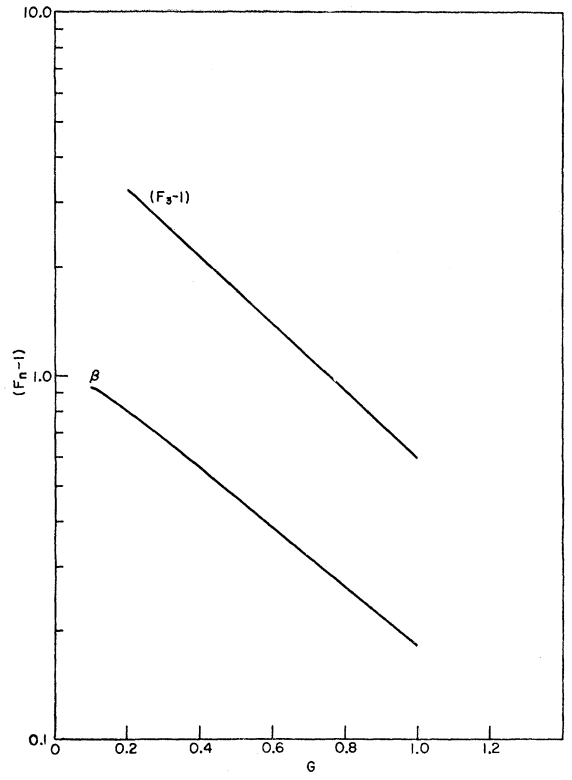

FIG. 2. The variational parameters β and F_3-1 as a function of G.

same when we complete the entire variational procedure. This agreement leads us to believe that the variational parameters are meaningfully evaluated even though we do not vary all of the parameters simultaneously. For $n \gtrsim P/2+1$, small changes in F_n do not affect the eigenvalue, so these parameters are not given reliably by the calculation.

IV. DISCUSSION OF RESULTS

The treatment developed in this paper gives approximate eigenvalues which are considerably better than those obtained in I. In I, Table I, we compared approximate eigenvalues with the exact calculations of Kerman, Lawson, and Macfarlane.[4] The calculations have been repeated for several cases and the errors quoted in I, Table I, are reduced by roughly a factor of 20. Using Eq. (24), rather than I-19, reduces the errors by roughly a factor of two. The variation of the parameters F_n reduces the eigenvalue again by roughly the same amount as the use of Eq. (24) and reduces the errors by roughly an additional factor of 10. The modified treatment of this paper typically gives eigenvalues which are less than 10 keV above the exact values of Kerman, Lawson, and Macfarlane. As an example, we use the ground state of Ni^{66}. For $G=0$, the ground-state

[4] A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. **124**, 162 (1961).

TABLE I. Comparison of eigenvalues.

G	E_{exact}[a]	$E_{\text{approx}}-E_{\text{exact}}$
0	12.00	0
0.2	11.3118	0.0007
0.4	10.3827	0.0022
0.6	9.1384	0.0032
0.8	7.5904	0.0033
1.0	5.8108	0.0034
1.2	3.871	0.003
2.0	−4.7066	0.0019

[a] See Ref. 2.

energy is 4.68 MeV; an exact solution of the pairing interaction[4] gives a ground-state energy of 1.699 MeV; the treatment of I gave a ground-state energy of 1.84 MeV and the treatment of this paper gives a ground-state energy of 1.706 MeV.

In order to obtain some feeling of the magnitudes of the parameters introduced here and their variations, we examine numerically systems of equally spaced levels varying such things as $G/\Delta\epsilon$, P, and L. $\Delta\epsilon$ is the single-particle energy-level spacing; P, the number of pairs and L is the number of levels. We first consider a system of six equally spaced levels, $\epsilon_1=1$ and $\Delta\epsilon=1$, $P=3$ as exact calculations have been done[2] for that system. In Table I, we give the exact eigenvalue[2] and the difference of the approximate and exact eigenvalue for several values of G. From Table I, we see that the

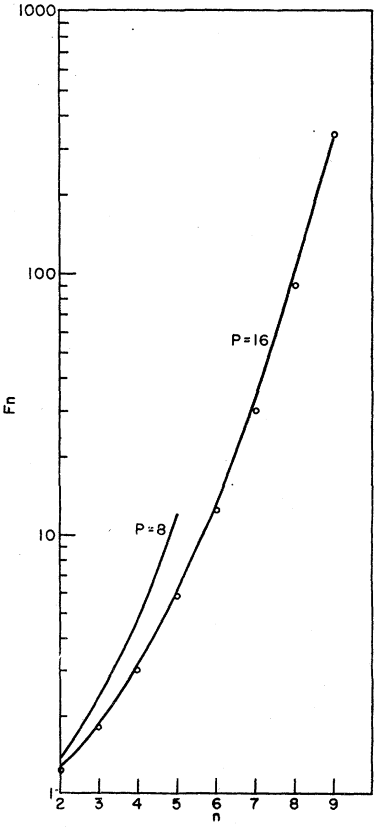

FIG. 3. The variational parameters F_n. The curves connect the points computed for $P=8$ and $P=16$ using Eq. (27) as a starting point and the open circles give the values of F_n for $P=16$ using Eq. (26) as the starting point.

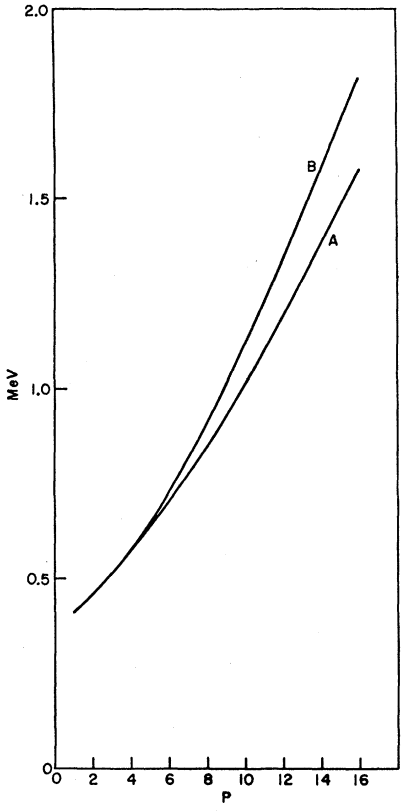

FIG. 4. The energy of the first-excited state above the ground state as a function of the number of pairs. The upper curve connects the points computed with the use of the treatment of this paper and the lower curve connects the points obtained using separability.

approximate methods of this paper give the eigenvalues almost perfectly for these systems. In Fig. 1, we plot $C_{4,5,6}/C_{1,2,3}$ and $F_3(D_4D_5D_6/D_1D_2D_3)$ for several values of G. The excellent agreement between the exact[2] and approximate third-order amplitudes is strong evidence that our procedure leads to meaningful estimates of the higher order amplitudes. In Fig. 2, we plot β and F_3-1 as a function of G. For $G<0.2$, λ becomes insensitive to small variations in F_3. If we regard the size of β as a measure of the validity of separability, we see that the arguments following Eq. (8″) are quite valid; as G becomes large β decreases in magnitude. Figure (2) also suggests $\beta\leq 1 (F_2\leq 2)$ and if we substitute $F_2=2$ in Eq. (27) and remember the definitions of F_0 and F_1, we may hypothesize that

$$F_n\leq n!. \tag{28}$$

For the special case of the first P levels being degenerate at energy ϵ_1 and all other single-particle levels degenerate at some higher energy ϵ_2, it is straightforward to show that $F_n\rightarrow n!$ as $G\rightarrow 0$. In nuclear calculations $G\lesssim 1/2\Delta\epsilon$, so, Fig. 2 also indicates that separability is a poor approximation for nuclear calculations.

The next series of systems that we wish to discuss are those having a constant single-particle spacing ($\Delta\epsilon=0.25$ MeV) and a constant G ($G=0.125$ MeV). We keep the ratio of P/L fixed at 0.5 and vary the number of pairs and levels. In Fig. 3, we plot $F_n(n\leq 5)$ for a system having eight pairs and $F_n(n\leq 9)$ for a system having sixteen pairs. For the $P=16$ system, we display F_n computed using both Eq. (26) and Eq. (27) as starting points; for the $P=8$ system, we display only the results obtained using Eq. (27) as a starting point (the differences are quite small for the $P=8$ system). Although the parameters F_n rise more sharply in the $P=8$ system, the effects on the eigenvalue are considerably larger in the $P=16$ system. There are, of course, many more higher order configurations in the $P=16$ system. We have calculated that the probability of the system being in a zeroth- or first-order configuration is roughly 0.8 for the $P=8$ system, but decreases to about 0.4 for the $P=16$ system.

In Fig. 4, we examine the changes in an estimate of an observable property due to switching from separability [using Eq. (24)] to the variational procedure of this paper. We examine the energy difference of the ground state and the excited state obtained by breaking one pair and blocking levels P and $P+1$. G is again 0.125 MeV; $\Delta\epsilon$ is 0.25 MeV; $L=2P$ and P is varied. The disagreement between the two curves is mostly due to the fact that separability does not lead to a ground state which is sufficiently depressed in energy. In Fig. 5, we plot β for the ground and excited states considered in Fig. 4. We see that β decreases as we increase the number of levels, again in accord with the implications of Eq. (8″). The large values of β for the excited states are to be generally expected when levels near the Fermi surface are blocked.

V. CONCLUSIONS

From the calculations discussed in the previous section, it becomes clear that separability leads to eigenfunctions and eigenvalues of rather limited reliability. We feel that calculations which make use of separability, such as quasiparticle calculations, have semiquantitative meaning at best and are not reliable for details of the pairing eigenfunction. We also feel

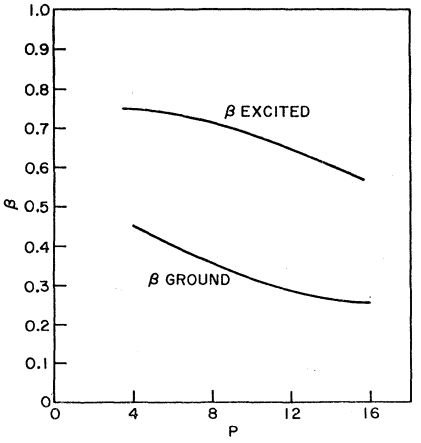

FIG. 5. The dependence of β on the number of pairs and levels. The lower curve pertains to the ground states and the upper curve pertains to the excited states.

that the methods developed in this paper lead to sufficiently accurate wave functions to make meaningful comparisons of theory and experiment possible.

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Dynamic Theory of the Nuclear Collective Model*

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The rotation-vibration model and the hydrodynamic dipole-oscillation model are unified. A coupling between the dipole oscillations and the quadrupole vibrations is introduced in the adiabatic approximation. The dipole oscillations act as a "driving force" for the quadrupole vibrations and stabilize the intrinsic nucleus in a nonaxially symmetric equilibrium shape. The higher dipole resonance splits into two peaks separated by about 1.5–2 MeV. On top of the several giant resonances occur bands due to rotations and vibrations of the intrinsic nucleus. The dipole operator is established in terms of the collective coordinates and the γ-absorption cross section is derived. For the most important 1^- levels the relative dipole excitation is estimated. It is found that some of the dipole strength of the higher giant resonance states is shared with those states in which one surface vibration quantum is excited in addition to the giant resonance.

I. INTRODUCTION

IT has been emphasized by Faessler and Greiner[1] that the anharmonicity of the nuclear surface vibrations implies in a certain sense a triaxiality of the nucleus. In this paper we show that this triaxiality manifests itself in the photonuclear giant resonance. The degeneracy of the upper peak, which in the static model[2,3] is due to the equality of the two minor axes, disappears. Thus, in a dynamic treatment, there appear three dipole peaks which, however, overlap due to the damping of the giant resonance. In the remainder of the Introduction we first give some background material, and then we describe the contents of this paper.

The collective model of surface vibrations and rotations has been spectacularly successful in explaining the nuclear low-energy spectrum.[4–6] Similarly, the collective model predictions of the most important electric dipole transitions have been quite well confirmed by the experiments within the region of applicability, and significantly, the agreement has improved with the increase of details of the theory and with the improvement of the experimental accuracy.[7,8] In the present paper we intend to unify these two aspects of the collective model of the nucleus, namely the unified model and the dipole giant resonance model. In other words, we would like to develop the complete quantum-mechanical collective model of the nucleus, treating all collective degrees of freedom as quantum-mechanical variables. However, we consider in this paper only even-even nuclei. We should emphasize that our treatment is phenomenological in that we do not attempt to derive the collective Hamiltonian from the nuclear many-body problem. Instead, we assume the model and determine its consequences in as consistent a way as possible. By comparing our results with experiment one can then decide the limits of the validity of the model.

We just note for completeness that a considerable amount of work on a "fundamental" level has been

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