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Some Formulas for the Bounds on the Energy and Wave Functions and Their Applications to ^{20}Ne

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The variational principle in quantum mechanics gives an upper bound on the energy eigenvalue E_k of the kth state if its trial wave function is orthogonal to the eigenfunctions of all the lower states. A lower bound on E_k has been derived assuming that: (i) its upper bound be less than E_{k+1}, and (ii) the energy fluctuation $(\langle H^2\rangle - \langle H\rangle^2)^{1/2}$ be less than $\frac{1}{2}(E_{k+1}-E_k)$. An upper bound on the error in the wave function of the kth state has also been derived. The formulas for the bounds have been applied to calculate the accuracy of the energies and wave functions of the various J states of the ground and excited $K=0$ bands in ^{20}Ne. The intrinsic wave functions of the $K=0$ bands were taken from the earlier calculations performed by using the deformed Hartree-Fock and Tamm-Dancoff approximations. Techniques for calculating $\langle H^2\rangle$ have also been discussed. Our results show that the energies and wave functions calculated by these approximations are fairly accurate for a number of states. The wave functions of the ground and first excited $J=0$ states are accurate at least to the order of 92.5 and 87.3%, respectively.

I. INTRODUCTION

The exact solution of the Schrödinger equation, which determines the energy of the stationary states of a physical system, is possible only for some very simple or idealized potential fields. In the investigation of real atomic and nuclear systems, it becomes imperative to resort to approximate methods of calculating the eigenvalues and eigenfunctions of the Hamiltonian operator. Perturbation theory provides an analytical method for calculating the approximate eigenvalues and eigenfunctions of the real physical systems. However, the practical application of perturbation theory is limited to only those real systems which do not differ very much from the idealized systems which can be solved exactly. In fact, in many atomic and nuclear systems the perturbation theory cannot be applied conveniently, because the first approximation is not accurate enough, while the labor of calculating higher-order perturbation terms is extremely great. For many such systems the method based on the variational principle provides a good approximate scheme for calculating, especially, the ground-state energy and wave function.[1] The method can also be used to calculate the excited-state energy and wave function, but it becomes quite inconvenient in practice.[1]

It is interesting and important to test the accuracy of the variational wave function and energy. A convenient method of testing the accuracy consists in calculating the bounds on the errors in the approximate wave function and energy. The purpose of this paper is to discuss some formulas for the bounds and consider their application to examine the accuracy of the wave functions and the energies obtained by the Hartree-Fock (HF) and Tamm-Dancoff (TD) approximations for the nucleus ^{20}Ne.[2,3]

The nuclear shell model provides the basic framework for calculating the spectroscopic properties of the nuclei. The shell model reduces the problem of the calculation to solving the Schrödinger equation or, equivalently, diagonalizing the matrix of the effective Hamiltonian operator in an appropriately chosen finite basis. The choice of the appropriate effective Hamiltonian and the appropriate basis is a complicated and difficult problem and is far from being settled. However, even if one has the right effective Hamiltonian and the right basis, the shell-model calculation can, in general, turn out to be a prohibitive task because the number of configurations can be very large even for only a few particles outside the closed shell.

In recent years the variational approach of the HF theory together with the angular momentum projection technique has been successfully used as a substitute for the complete shell-model diagonalization program for the deformed nuclei in the lower half of the $2s, 1d$ shell.[4] A number of calculations have also been performed to estimate how accurate the projected HF wave functions are compared to the wave functions that can be obtained by the complete shell-model calculation.[3,5,6] The results of these calculations provide only some semiquantitative estimates on the accuracy of the projected wave functions. In the opinion of this author the formulas for the bounds are very useful in providing some definite quantitative estimate on the accuracy within definite limits. Formulas for the upper and lower bounds on the energy will be discussed in Sec. II. Section III will contain the discussion of the formula for the upper bound on the error in the wave function. In Sec. IV we will present the method for calculating the bounds for the projected wave functions. Results and conclusions on ^{20}Ne will be presented in Sec. V.

II. UPPER AND LOWER BOUNDS ON THE ENERGY

Let H denote the Hamiltonian operator and $\Psi_0, \Psi_1, \ldots, \Psi_n, \ldots$ its complete set of eigenfunctions so that we have

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \quad \text{for } n=0,1,\ldots,n,\ldots, \tag{1}$$

where E_n is the eigenvalue belonging to the eigenfunction Ψ_n. According to the variational principle in quantum mechanics the expectation value

$$W = \langle\Phi|H|\Phi\rangle \tag{2}$$

for an arbitrary wave function Φ gives an upper bound to the lowest eigenvalue E_0,[1] i.e.,

$$W \geqslant E_0 . \tag{3}$$

To use this principle to determine the ground state of the system we use a trial function Φ that depends on a number of parameters which are varied until W is a minimum. If good judgement has been exercised in choosing the trial function Φ, it is hoped that the minimum of W may be very close to E_0, and the Φ which gives the minimum will have good overlap with Ψ_0. For a number of physical systems the trial function Φ can be chosen in the form of a determinant. The minimization of W with a determinantal form of Φ leads to the well-known HF equation.[4] The variational principle can also be used to obtain an upper bound for one of the higher eigenvalues if the trial function is orthogonal to the eigenfunctions of all the lower states.

To prove the inequality in Eq. (3) for an arbitrary eigenvalue E_k, let us denote the approximate eigenvalue and eigenfunction of the kth state by W_k and Φ_k, respectively. First, consider the case of the ground state. Since Φ_0 is not equal to Ψ_0, one can expand Φ_0 in terms of the complete set $\Psi_0, \Psi_1, \ldots,$ obtaining

$$\Phi_0 = \sum_{n=0} a_n \Psi_n \tag{4a}$$

with

$$\sum_{n=0} a_n^2 = 1 . \tag{4b}$$

For simplicity we have assumed the expansion coefficients a_n to be real. The approximate ground-state energy W_0 is given by

$$W_0 = \sum_{n=0} a_n^2 E_n . \tag{5a}$$

Subtracting E_0 from both sides gives

$$W_0 - E_0 = \sum_{n=0} a_n^2 (E_n - E_0) . \tag{5b}$$

From Eq. (5b) it is clear that

$$W_0 \geqslant E_0 . \tag{6}$$

In the case of the kth state, the approximate wave function Φ_k is chosen in the following form:

$$\Phi_k = \sum_{n=k} a_n \Psi_n \tag{7}$$

with

$$a_0 = a_1 = \cdots = a_{k-1} = 0 .$$

Clearly then,

$$W_k = \sum_{n=k} a_n^2 E_n \tag{8a}$$

and

$$W_k - E_k = \sum_{n=k} a_n^2 (E_n - E_k) . \tag{8b}$$

It follows immediately from Eq. (8b) that

$$W_k \geqslant E_k . \tag{9}$$

It is also possible to obtain a lower bound for E_k if the following conditions are satisfied:

$$W_k < E_{k+1} \tag{10a}$$

and

$$A_k < \tfrac{1}{2}(E_{k+1} - E_k) , \tag{10b}$$

where A_k is given by

$$A_k^2 = B_k^2 - W_k^2 . \tag{11}$$

The quantity B_k^2 in Eq. (11) is the expectation value of H^2, i.e.,

$$B_k^2 = \langle\Phi_k|H^2|\Phi_k\rangle . \tag{12}$$

Using the definition of Φ_k in Eq. (7) we can write

$$B_k^2 = \sum_{n=k} a_n^2 E_n^2 . \tag{13}$$

Subtracting W_k^2 from both sides of Eq. (13) gives

$$\begin{aligned} A_k^2 = B_k^2 - W_k^2 &= \sum_{n=k} a_n^2 E_n^2 - W_k^2 \\ &= \sum_{n=k} a_n^2 E_n^2 - 2W_k \sum_{n=k} a_n^2 E_n + W_k^2 \sum_{n=k} a_n^2 \\ &= \sum_{n=k} a_n^2 (W_k - E_n)^2 . \end{aligned} \tag{14}$$

In view of the conditions (9) and (10a), $(W_k - E_n)^2$

will have its smallest value when either

$$E_n = E_{k+1} \tag{15a}$$

or

$$E_n = E_k \, , \tag{15b}$$

provided that the other eigenvalues are not degenerate with E_k or E_{k+1}.

In the first case, Eq. (15a), we get

$$A_k^2 \geqslant (E_{k+1} - W_k)^2 \sum_{n=k} a_n^2$$

or

$$A_k \geqslant (E_{k+1} - W_k) \, , \tag{16}$$

which gives

$$W_k + A_k \geqslant E_{k+1} \, . \tag{17}$$

Now it will be shown that the above inequality violates condition (10b).

In order that $(W_k - E_n)^2$ be smallest for $E_n = E_{k+1}$ we must have

$$W_k \geqslant E_k + \tfrac{1}{2}(E_{k+1} - E_k) \, . \tag{18}$$

Using this in relation (17) we get

$$A_k \geqslant \tfrac{1}{2}(E_{k+1} - E_k) \, , \tag{19}$$

which is in violation with condition (10b).

To be consistent with conditions (10a) and (10b) we can consider only the second possibility, Eq. (15b), which, when used in Eq. (14), gives the lower bound for E_k:

$$E_k \geqslant W_k - A_k \, . \tag{20}$$

It may be noted that conditions (10a) and (10b) for the validity of the lower bound (20) can be lumped into one condition,

$$W_k - E_k < \tfrac{1}{2}(E_{k+1} - E_k) \, . \tag{21}$$

However, in this form the condition is very difficult to test for the Hamiltonians used in the nuclear shell-model calculations, because it requires the knowledge of the eigenvalues E_k and E_{k+1}. One cannot use the experimental values of E_k and E_{k+1} because, in general, the shell-model Hamiltonians can, at the most, only reproduce the low-lying experimental energy spectrum and not the actual experimental energies. Conditions (10a) and (10b) are more suitable for such calculations. It is quite often possible to test condition (10a) by approximately calculating E_{k+1}. Condition (10b) depends only on the energy difference $E_{k+1} - E_k$, which can, to a very good approximation, be taken from the experiment.

These remarks will be more clearly understood in Sec. V, which discusses the application of formula (20) to the results of HF and TD calculations in ^{20}Ne.

III. UPPER BOUND ON THE ERROR IN THE WAVE FUNCTION

The calculations of the upper and lower bounds on the energy eigenvalue provide important information regarding the accuracy of the approximate methods. If the two bounds are close, one can claim to have a good estimate of the energy eigenvalue. However, one can say nothing about the discrepancy between the approximate wave function and the exact eigenfunction. Eckart has derived a formula for calculating the upper bound on the error in the ground-state wave function by using W_0 and the experimental values of E_0 and E_1.[7] This formula can be generalized to the excited states also if the approximate wave function of the excited state is orthogonal to the eigenfunctions of all the lower states.[8] Eckart's formula, though useful in atomic physics, has some distinct disadvantages in applying it to nuclear-structure calculations, as pointed out by this author in a recent publication.[8] In the same publication a new formula has been derived for the upper bound which can be conveniently applied to the HF wave functions of atoms as well as nuclei. This formula will be briefly discussed here.

Let us first consider the case of the approximate wave function Φ_k of the kth state. We have

$$\begin{aligned} W_k = \langle \Phi_k | H | \Phi_k \rangle &= a_k^2 E_k + \sum_{n=k+1} a_n^2 E_n \\ &= a_k^2 E_k + b^2 X \\ &= E_k + b^2 \Delta \, , \end{aligned} \tag{22}$$

where

$$b^2 = \sum_{n=k+1} a_n^2 \, , \tag{23a}$$

$$X = \sum_{n=k+1} \frac{a_n^2 E_n}{b^2} \, , \tag{23b}$$

and

$$\Delta = X - E_k = E_{k+1} - E_k + \sum_{n=k+2} \frac{a_n^2 (E_n - E_{k+1})}{b^2} \tag{23c}$$

$$= E_{k+2} - E_k + \sum_{n=k+3} \frac{a_n^2 (E_n - E_{k+2})}{b^2} - \frac{a_{k+1}^2 (E_{k+2} - E_{k+1})}{b^2} \, . \tag{23d}$$

Squaring Eq. (22) gives

$$W_k^2 = \langle \Phi_k | H | \Phi_k \rangle^2 = E_k^2 + b^4 \Delta^2 + 2 E_k \Delta b^2 \, . \tag{24}$$

Further,

$$B_k{}^2 = \langle\Phi_k|H^2|\Phi_k\rangle = a_k{}^2E_k{}^2 + \sum_{n=k+1} a_n{}^2E_n{}^2$$
$$= a_k{}^2E_k{}^2 + b^2Y^2$$
$$= E_k{}^2 + b^2(Y^2 - E_k{}^2), \qquad (25)$$

where

$$Y^2 = \sum_{n=k+1} \frac{a_n{}^2E_n{}^2}{b^2}. \qquad (26)$$

It can be shown[8] that $Y^2 > X^2$, so that we can write

$$Y^2 = X^2 + \delta, \qquad (27)$$

where δ is some positive quantity.

Now subtracting Eq. (24) from Eq. (25) gives

$$A_k{}^2 = B_k{}^2 - W_k{}^2 = b^2\delta + b^2(X^2 - E_k{}^2) - b^4\Delta^2 - 2E_k\Delta b^2$$
$$= b^2\delta + \Delta^2(b^2 - b^4). \qquad (28)$$

Since $b^2\delta/\Delta^2$ is a positive quantity, it follows from Eq. (28) that

$$b^2 - b^4 \leqslant A_k{}^2/\Delta^2. \qquad (29)$$

If b^4 is negligible compared to b^2, we can write

$$b^2 \leqslant A_k{}^2/\Delta^2. \qquad (30)$$

With the aid of Eq. (23c) the above inequality can be further simplified to give

$$b^2 \leqslant A_k{}^2/(E_{k+1} - E_k)^2. \qquad (31)$$

If the amplitude a_{k+1} is of the same order of magnitude as a_n with $n > k+1$, or not much larger than them, and also if the energy level density does not rapidly increase above E_{k+2}, then the third term is greater than the fourth term on the right side in Eq. (23d). Under this condition one can further improve the upper bound given by inequality (31), obtaining

$$b^2 \leqslant A_k{}^2/(E_{k+2} - E_k)^2. \qquad (32)$$

The equality sign in relations (29) to (32) is applicable only when $A_k{}^2 = 0$, i.e., when Φ_k is an eigenstate.

The ground state is, generally, the most interesting case for testing various approximate methods. Formulas (30) to (32) are, clearly, valid in this case also and are written as

$$b^2 \leqslant A_0{}^2/\boldsymbol{\Delta}^2, \qquad (33)$$

$$b^2 \leqslant A_0{}^2/(E_1 - E_0)^2, \qquad (34)$$

$$b^2 \leqslant A_0{}^2/(E_2 - E_0)^2, \qquad (35)$$

where

$$b^2 = \sum_{n=1} a_n{}^2, \quad \Phi_0 = \sum_{n=0} a_n{}^2\Psi_n, \qquad (36)$$

and

$$\Delta = E_1 - E_0 + \sum_{n=2} \frac{a_n{}^2(E_n - E_1)}{b^2}, \qquad (37a)$$

$$= E_2 - E_0 + \sum_{n=3} \frac{a_n{}^2(E_n - E_2)}{b^2} - \frac{a_1{}^2(E_2 - E_1)}{b^2}. \qquad (37b)$$

IV. CALCULATION OF ENERGY FLUCTUATION FOR PROJECTED STATES

The HF and TD approximations have been used by several authors to calculate the intrinsic states of the ground and the excited $K=0$ bands in ^{20}Ne.[2,9] The energy levels calculated with the angular momentum states projected out of these intrinsic states reproduce fairly well the low-lying experimental energy spectrum in ^{20}Ne.[2,3]

In order to apply the formulas in Secs. II and III to estimate the accuracy of the projected angular momentum states and the energies calculated with them, one first needs to calculate the difference $\langle H^2\rangle - \langle H\rangle^2$ for the projected states. Because of the projection operator the calculation of $\langle H^2\rangle$ can turn out to be a difficult task. However, in the case of the HF ground states of the closed-shell nuclei the calculation of $\langle H^2\rangle$ is quite straightforward and simple because the HF wave functions, in such cases, are the eigenfunctions of J^2 with eigenvalue $J=0$. Let us first consider this case. Let Φ^J be the HF wave function which describes the ground state of a closed-shell nucleus. Operating on Φ^J by H we get

$$H|\Phi^J\rangle = \langle\Phi^J|H|\Phi^J\rangle|\Phi^J\rangle + \sum_n a_n\phi_n, \qquad (38)$$

where $\phi_1, \phi_2, \ldots, \phi_n, \ldots$ define a complete set of two-particle–two-hole (2p-2h) states. The 1p-1h states do not contribute, because $\langle 1\mathrm{p}1\mathrm{h}|H|\Phi^J\rangle = 0$. Further, particle-hole configurations of higher order than two also do not contribute, because H is a sum of only one-body and two-body operators. The quantities $a_1, a_2, \ldots, a_n, \ldots$, etc., are the matrix elements defined as

$$a_n = \langle\phi_n|H|\Phi^J\rangle = \langle\mu_1\mu_2|\vartheta|\lambda_1\lambda_2\rangle \qquad (39a)$$

with

$$\phi_n = b^\dagger_{\mu_1}b^\dagger_{\mu_2}b_{\lambda_1}b_{\lambda_2}|\Phi^J\rangle. \qquad (39b)$$

Here μ_1 and μ_2 are empty one-particle (1p) HF orbits belonging to the same space as the filled 1p HF orbits λ_1 and λ_2. ϑ is the two-body part of H.

Squaring Eq. (38) and then subtracting the HF energy of Φ^J we get

$$A_0{}^2 = \langle \Phi^J | H^2 | \Phi^J \rangle - \langle \Phi^J | H | \Phi^J \rangle^2 = \sum_n a_n{}^2 \,, \tag{40}$$

which can be easily computed using Eq. (39a).

The number n of the 2p-2h states contributing to the summation in Eq. (40) can be greatly reduced by using symmetry properties of H and Φ^J. This point will be discussed in some detail in connection with the calculation of $\langle H^2 \rangle$ for the deformed HF states of the even-even $N=Z$ nuclei.

To extend the discussion of the calculation of $\langle H^2 \rangle$ to a deformed nucleus, it is necessary for us to introduce the projection operator which extracts out the observed angular momentum states of the nucleus from its intrinsic states. Let M and K be the projection of J along the laboratory (lab) and the body-fixed z axis, respectively; then the angular momentum projection operator P^J_{MK} is defined by

$$P^J_{MK} = \tfrac{1}{2}(2J+1) \int_0^\pi d^J_{MK}(\theta) e^{-i\theta J_y} \sin\theta \, d\theta \,, \tag{41}$$

where $d^J_{MK}(\theta)$ is the reduced rotation matrix.

One can always choose the lab z axis to coincide with the body-fixed z axis; then Eq. (41) becomes

$$P^J_K = \tfrac{1}{2}(2J+1) \int_0^\pi d^J_{KK}(\theta) e^{-i\theta J_y} \sin\theta \, d\theta \,. \tag{42}$$

The projection operator defined in Eqs. (41) and (42) is applicable only when the deformed intrinsic states are axially symmetric and have, therefore, K as a good quantum number. The quantum number K is commonly known as the band quantum number. If Φ^K is the intrinsic wave function of a band with band quantum number K, then the energy E^J of the angular momentum state Ψ^J belonging to the band is given by

$$E^J = \langle \Phi^K | P^J_K H | \Phi^K \rangle / N^K_J \,, \tag{43}$$

where

$$\Psi^J = P^J_K \Phi^K \,, \tag{44a}$$

$$P^J_K P^J_K = P^J_K \,, \tag{44b}$$

and

$$N^K_J = \langle \Phi^K | P^J_K | \Phi^K \rangle \,. \tag{44c}$$

In its most general form, Φ^K may be very complicated in structure, which can make the calculation of E^J a prohibitive task. In the HF approximation Φ^K is simply a Slater determinant, and consequently the calculation becomes quite simple. If Φ^K_{HF} denotes Φ^K in the HF approximation, we have

$$H\Psi^J = HP^J_K \Phi^K_{\mathrm{HF}} = E^K_{\mathrm{HF}} P^J_K \Phi^K_{\mathrm{HF}} + P^J_K \sum_n a_n \phi_n \,, \tag{45}$$

where a_n and ϕ_n are defined in a similar way as in Eqs. (39a) and (39b) and E^K_{HF} is the HF energy defined by

$$E^K_{\mathrm{HF}} = \langle \Phi^K_{\mathrm{HF}} | H | \Phi^K_{\mathrm{HF}} \rangle \,. \tag{46}$$

Using Eq. (45) in Eq. (43) we get

$$E^J = E^K_{\mathrm{HF}} + \frac{1}{N^K_J} \sum_n a_n \langle \Phi^K_{\mathrm{HF}} | P^J_K | \phi_n \rangle \,. \tag{47}$$

To obtain the expectation value of H^2 we square both sides of Eq. (45) and then divide by the normalization $\langle \Psi^J | \Psi^J \rangle$.

$$\begin{aligned} \frac{\langle \Psi^J | H^2 | \Psi^J \rangle}{\langle \Psi^J | \Psi^J \rangle} &= \frac{\langle \Phi^K_{\mathrm{HF}} | P^J_K H^2 | \Phi^K_{\mathrm{HF}} \rangle}{N^K_J} \\ &= (E^K_{\mathrm{HF}})^2 + \frac{1}{N^K_J} \Big(\sum_n a_n{}^2 \langle \phi_n | P^J_K | \phi_n \rangle \\ &\qquad + 2E^K_{\mathrm{HF}} \sum_n a_n \langle \Phi^K_{\mathrm{HF}} | P^J_K | \phi_n \rangle \\ &\qquad + 2 \sum_{\substack{n \\ n' > n}} a_n a_{n'} \langle \phi_n | P^J_K | \phi'_n \rangle \Big) \,. \end{aligned} \tag{48}$$

Since P^J_K cannot connect states with different radial quantum numbers and H is rotational- and space-reflection-invariant, only those 2p-2h states ϕ_n contribute in Eqs. (47) and (48) which belong to the same major shell as Φ^K_{HF} and also have the same band and parity quantum numbers as Φ^K_{HF}.

In the case of even-even $N=Z$ nuclei we always have $K=0$ for the HF ground state. Consequently, we have some additional symmetry properties of Φ^0_{HF} and P^J_0 which can simplify the computation in Eqs. (47) and (48). Let G_i denote the following symmetry operators:

(i) G_1 – the time-reversal operator,

(ii) G_2 – the operator which changes a neutron into a proton and vice versa,

(iii) G_3 – the product of G_1 and G_2.

The symmetry properties of Φ^0_{HF} and P^J_0 are then given by

$$\begin{gathered} G_i | \Phi^0_{\mathrm{HF}} \rangle = | \Phi^0_{\mathrm{HF}} \rangle \,, \\ [G_i, P^J_0] = 0 \quad \text{for } i = 1, 2, 3 \,. \end{gathered} \tag{49}$$

It should be noted that H is also invariant under G_i. By carefully using these symmetry properties of H, P^J_0, and Φ^0_{HF}, various summations on the right sides in Eqs. (47) and (48) can be reduced to include contributions from only a number m of 2p-2h states, where m is generally much smaller than n. Incorporating the effect of G in Eqs. (47) and (48) we get

$$E^J = E^0_{\mathrm{HF}} + \frac{1}{N^0_J} \sum_m g_m a_m \langle \Phi^0_{\mathrm{HF}} | P^J_0 | \phi_m \rangle \tag{50a}$$

and

$$\frac{\langle\Psi^J|H^2|\Psi^J\rangle}{\langle\Psi^J|\Psi^J\rangle}=(E^0_{\mathrm{HF}})^2+\frac{1}{N^0_J}\Big\{\sum_m g_m a_m{}^2\langle\phi_m|P^J_0(1+\sum_i G_i)|\phi_m\rangle$$
$$+2E^0_{\mathrm{HF}}\sum_m g_m a_m\langle\Phi^0_{\mathrm{HF}}|P^J_0|\phi_m\rangle+2\sum_{\substack{m\\ m'>m}} g_m a_m a_{m'}\langle\phi_m|P^J_0(1+\sum_i G_i)|\phi_{m'}\rangle\Big\}, \qquad (50b)$$

where g_m is equal to 1, 2, and 4 according to whether ϕ_m is invariant under both G_1 and G_2 or under only one of them or none of them. The summation $\sum_i G_i$ excludes the G_i for which $G_i|\phi_m\rangle = |\phi_m\rangle$.

In the case of the excited $K=0$ bands of the even-even $N=Z$ nuclei calculated by the TD approximation, expressions similar to Eqs. (50a) and (50b) can be also derived for E^J and $\langle H^2\rangle$ because the symmetries used earlier are applicable in this case also. However, the calculations of E^J and $\langle H^2\rangle$ are now more laborious because, in addition to 2p-2h states, 1p-1h states also contribute, as Φ^0_{TD} is composed of more than one Slater determinant.

V. RESULTS AND CONCLUSIONS

The Hamiltonian H and its HF and TD wave functions for the ground and excited $K=0$ bands in ^{20}Ne were taken from the Ref. 2. The expressions of $\langle H\rangle$ and $\langle H^2\rangle$ for the J states projected from the HF and TD wave functions contain terms of the types a_n, $\langle\phi_n|P^J_0|\phi_n\rangle$, and $\langle\phi_{n'}|P^J_0|\phi_n\rangle$. These were calculated by using the techniques discussed by Tewari and Grillot.[10] The upper and lower bounds on the energy eigenvalues calculated by using the J states projected from the HF wave function are presented in Table I. In Table II are listed the corresponding results for the J states from the TD wave function.

It should be noted that formula (20) for the lower bound is applicable only under conditions (10a) and (10b). We will now show that these conditions are satisfied in the case of the $J=0$ states in Tables I and II.

Let us write Eqs. (4a) and (5a) in the following forms appropriate for the present discussion:

$$|\Psi^J_{\mathrm{HF}}\rangle=P^J_0|\Phi^0_{\mathrm{HF}}\rangle/\langle\Phi^0_{\mathrm{HF}}|P^J_0|\Phi^0_{\mathrm{HF}}\rangle^{1/2}$$
$$=\sum_{n=1} a_{J_n}|\psi_{J_n}\rangle, \qquad (51)$$

$$E^J_{\mathrm{HF}}=\langle\Psi^J_{\mathrm{HF}}|H|\Psi^J_{\mathrm{HF}}\rangle=\sum_{n=1} a_{J_n}{}^2E_{J_n}, \qquad (52)$$

and

$$|\Psi^J_{\mathrm{TD}}\rangle=P^J_0|\Phi^0_{\mathrm{TD}}\rangle/\langle\Phi^0_{\mathrm{TD}}|P^J_0|\Phi^0_{\mathrm{TD}}\rangle^{1/2}$$
$$=\sum_{n=2} a_{J_n}|\psi_{J_n}\rangle, \qquad (53)$$

$$E^J_{\mathrm{TD}}=\langle\Psi^J_{\mathrm{TD}}|H|\Psi^J_{\mathrm{TD}}\rangle=\sum_{n=2} a_{J_n}{}^2E_{J_n}, \qquad (54)$$

where

$$H|\psi_{J_n}\rangle=E_{J_n}|\psi_{J_n}\rangle, \quad \langle\psi_{J_n}|\psi_{J_{n'}}\rangle=0, \qquad (55a)$$

and

$$J^2|\psi_{J_n}\rangle=J(J+1)|\psi_{J_n}\rangle. \qquad (55b)$$

Since we are interested only in the states of isospin $T=0$, all the eigenstates ψ_{J_1}, ψ_{J_2}, etc., have $T=0$. The subscript n distinguishes the different eigenstates and eigenvalues of H with the same quantum number J. The ordering of n for a given value of J is according to the increasing value of E_{J_n} starting with $n=1$ for the lowest E_{J_n}.

It should be noted that in writing Eq. (53) we have assumed Ψ^J_{TD} to be orthogonal to ψ_{J_1}. This is a justified assumption because, as shown later in this chapter, ψ_{J_1} can be represented by Ψ^J_{HF} to a very good approximation. The overlap $\langle\Psi^J_{\mathrm{HF}}|\Psi^J_{\mathrm{TD}}\rangle$ is likely to be small because Φ^0_{HF} is orthogonal to Φ^0_{TD}.

From the discussions in Refs. 2 and 9 it is clear that the TD method is a good approximation for calculating the energy of the 0_2 state and there-

TABLE I. Upper and lower bounds on the energy eigenvalues of the $J=0_1$, 2_1, 4_1, 6_1 states calculated by using the projected HF wave functions of the ground $K=0$ band. The projected HF wave function Ψ^J_{HF} is defined by Eq. (51).

J	Upper bound E^J_{HF} $=\langle\Psi^J_{\mathrm{HF}}\|H\|\Psi^J_{\mathrm{HF}}\rangle$ (MeV)	$(E^J_{\mathrm{HF}})^2$ (MeV^2)	$\langle H^2\rangle_J$ $=\langle\Psi^J_{\mathrm{HF}}\|H^2\|\Psi^J_{\mathrm{HF}}\rangle$ (MeV^2)	A^2 $=\langle H^2\rangle_J-(E^J_{\mathrm{HF}})^2$ (MeV^2)	Lower bound $=E^J_{\mathrm{HF}}-A$ (MeV)
0_1	−42.2925	1788.656	1793.456	4.800	−44.4835
2_1	−41.0385	1684.158	1687.397	3.239	−42.8383
4_1	−38.2822	1465.527	1469.102	3.575	−40.1730
6_1	−34.4845	1189.181	1190.634	1.453	−35.6899

fore we are justified to assume $E^0_{\mathrm{TD}} < E_{0_3}$. Further, a complete shell-model calculation by Halbert *et al.*[11] for ^{20}Ne in the basis of the $2s, 1d$ shell predicts $E_{0_2} - E_{0_1}$ to be 6.5 MeV, and $E_{0_3} - E_{0_2} > 3.5$ MeV. We can use the same values in our calculations of the bounds without any significant error, because their effective Hamiltonian is very similar to the Hamiltonian used by us in the present calculations as discussed in Ref. 8. One can see from Table II that the value of A for the Ψ^0_{TD} state is less than $\frac{1}{2}(3.5)$ MeV. Therefore both conditions (10a) and (10b) are satisfied and hence the value of -38.0 MeV is truly the value of the lower bound of E_{0_2}. The same statement is true also for the lower bound of E_{0_1} in Table I because both conditions (10a) and (10b) are satisfied in this case. One can see from Table I that E^0_{HF} is less than the lower bound of E_{0_2} and hence $E^0_{\mathrm{HF}} < E_{0_2}$, which is the requirement in condition (10a). One can further see from Table I that A is less than $\frac{1}{2}(E_{0_2} - E_{0_1})$, i.e., $<6.5/2$, which is the requirement in condition (10b).

The values of the lower bounds on the energies of the $J = 2$, 4, 6 states of the HF and TD bands should be taken with some reservation because all the required values of E_{J_n} are not known from a complete shell-model calculation to test conditions (10a) and (10b) in these cases.

We will now estimate the errors in the wave functions Ψ^0_{HF} and Ψ^0_{TD} by using formula (31). Using the value of 4.8 MeV^2 for A^2 from Table I and taking $E_{0_2} - E_{0_1}$ to be 6 MeV, we predict the upper bound on the error in Ψ^0_{HF} to be 4.8/36, i.e., 13.3%. In the case of Ψ^0_{TD} the upper bound is predicted to be 16.5%, where we have taken the value of A^2 as 2.05 MeV^2 from Table II and $E_{0_3} - E_{0_2}$ has been taken to be 3.5 MeV. If $E_{0_3} - E_{0_2}$ be taken to be 4 MeV, the upper bound turns out to be 12.7%. In the case of Ψ^0_{HF} the estimate of the upper bound can be further improved by using formula (32).

We note from our results that ψ_{0_2} can be, to a good approximation, represented by Ψ^0_{TD}. As pointed out earlier in this chapter, the overlap between Ψ^0_{TD} and Ψ^0_{HF} is likely to be very small and therefore we may be justified to assume that in Eq. (52) the amplitude a_{0_2} is not larger or more important than the amplitudes a_{0_3}, a_{0_4}, etc.

We further note that the energy density of the $J = 0$ state does not increase rapidly after the 0_2 state. It is clear, therefore, that the conditions required by formula (32) are satisfied to a good approximation in the case of Ψ^0_{HF}. However, to compensate for the errors arising from the approximate validity of the conditions, we will take $E_{0_3} - E_{0_1}$ to be 8 MeV, which is smaller than the value predicted by Halbert *et al.* Now, using formula (32) the upper bound on the error in Ψ^0_{HF} is predicted to be 4.8/64, i.e., 7.5%.

It may be asked how useful the estimates of the various bounds for the different J states of the excited $K = 0$ band are, since the formulas used for calculating them are seriously tied to the assumption that Ψ^J_{TD} is orthogonal to ψ_{J_1}. This question led us to find a reliable estimate of the overlap $\langle \Psi^J_{\mathrm{TD}} | \psi_{J_1} \rangle$ and determine if it is small enough to not affect the validity of the formulas for the bounds.

It is clear that if Ψ^J_{TD} is not orthogonal to ψ_{J_1} and Ψ^J_{HF} is a reasonably good approximation of ψ_{J_1}, a reliable estimate of the contribution of Ψ^J_{TD} to ψ_{J_1} can be found by diagonalizing H in the 2×2 basis spanned by Ψ^J_{HF} and Ψ^J_{TD}. Such a calculation has been performed. The nonorthogonality of Ψ^J_{HF} and Ψ^J_{TD} was duly taken into account. The calculation shows that the contribution of Ψ^J_{TD} to ψ_{J_1} for $J = 0$, 2, 4, 6 states is, respectively, 1.7, 0.07, 7.8, and 40.5%. The large contribution in the case of the $J = 6$ state is due to a large overlap between Ψ^J_{TD} and Ψ^J_{HF}. The diagonalization of H in an extended basis including other high-lying states will certainly yield an improved approximation for ψ_{J_1}, but it is highly unlikely that it will significantly change the contribution of Ψ^J_{TD} to ψ_{J_1} in the case of $J = 0$, 2 states and possibly the $J = 4$ state also. The effect of the overlap of 1 to 8% on the formulas for the upper and lower bounds has been examined in the Appendix. We have demonstrated in the Appendix that our estimates for the various bounds are sufficiently accurate in the case of $J = 0$ and 2 states of the excited $K = 0$ band and quite likely in

TABLE II. Upper and lower bound on the energy eigenvalues of the $J = 0_2$, 2_2, 4_2, 6_2 states calculated by using the projected TD wave functions of the first excited $K = 0$ band. The projected TD wave function Ψ^J_{TD} is defined by Eq. (53).

J	Upper bound E^J_{TD} $= \langle \Psi^J_{\mathrm{TD}} \| H \| \Psi^J_{\mathrm{TD}} \rangle$ (MeV)	$(E^J_{\mathrm{TD}})^2$ (MeV^2)	$\langle H^2 \rangle_J$ $= \langle \Psi^J_{\mathrm{TD}} \| H^2 \| \Psi^J_{\mathrm{TD}} \rangle$ (MeV^2)	A^2 $= \langle H^2 \rangle_J - (E^J_{\mathrm{TD}})^2$ (MeV^2)	Lower bound $= E^J_{\mathrm{TD}} - A$ (MeV)
0_2	-36.5686	1337.262	1339.310	2.048	-37.9996
2_2	-33.7953	1142.122	1146.147	4.025	-35.8013
4_2	-32.0852	1029.460	1042.699	13.239	-35.7238
6_2	-32.3244	1044.867	1060.184	15.317	-36.2382

the case of its $J=4$ state also. The estimates for its $J=6$ state are perhaps not very useful, because the formulas for the bounds cannot be used in this case with sufficient justification owing to the large overlap between $\Psi^J_{\rm TD}$ and ψ_{J_1}.

Some comments may be necessary on the behavior of A^2 in column 5 of Tables I and II. The energy spread between the upper and lower bounds measured by A decreases more or less with increasing J in Table I, but in Table II it increases with increasing J. The contrasting behavior of A in Tables I and II appears quite puzzling. However, this gives rise to no contradictions, because the exact amount of error in the wave function is not related to A in a straightforward way. A large or small A does not imply a large or small error in the wave function.

Finally, we would like to conclude our discussion with the remark that the HF and TD methods together with the angular momentum projection technqiue provide a very good approximation for calculating the energy eigenvalues and eigenfunctions of the ground and first excited $J=0$ states of ^{20}Ne in the basis of the $2s, 1d$ shell. Results for the upper and lower bounds in Tables I and II suggest that these methods may be fairly accurate in the case of other J states also.

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APPENDIX

By including ψ_{J_1} in the expansion of $\Psi^J_{\rm TD}$ given by Eq. (53) and following the arguments of Sec. II we get

$$\begin{aligned} E^J_{\rm TD} - E_{J_2} &= \sum_{n=1} a_{J_n}{}^2 (E_{J_n} - E_{J_2}) \\ &= a_{J_1}{}^2 (E_{J_1} - E_{J_2}) + \sum_{n=3} a_{J_n}{}^2 (E_{J_n} - E_{J_2}) . \end{aligned} \tag{A1}$$

First consider the case of $J=0$. Using the value of $a_{J_1}{}^2 = 0.017$ and $E_{J_1} - E_{J_2} = -6$ MeV from Sec. V in Eq. (A1) we get

$$E^J_{\rm TD} - E_{J_2} = -0.102 + \sum_{n=3} a_{J_n}{}^2 (E_{J_n} - E_{J_2}) . \tag{A2}$$

From this equation it follows that

$$E^J_{\rm TD} \geq E_{J_2} , \tag{A3}$$

unless the second term on the right side in Eq. (A2) is smaller than 0.102, which is highly unlikely. For example, assuming $E_{J_3} - E_{J_2}$ to be 3.5 MeV and $\sum_{n=3} a_{J_n}{}^2$ to be 0.03, we get from Eq. (A2)

$$E^J_{\rm TD} - E_{J_2} > 0.003 .$$

The case of $J=2$ needs no discussion, because in this case $a_{J_1}{}^2 = 0.0007$, which can be taken as zero for all practical considerations. For $J=4$ we get

$$E^J_{\rm TD} - E_{J_2} = -0.08 (E_{J_2} - E_{J_1}) + \sum_{n=3} a_{J_n}{}^2 (E_{J_n} - E_{J_2}) . \tag{A4}$$

It is quite likely that the second term is greater than the first term in Eq. (A4), which implies that Eq. (A3) for the upper bound can be used in the case of the $J=4$ state also.

The derivation of the formula for the lower bound on the energy of the excited states is based on Eq. (14) of Sec. II. It can be easily verified that this equation remains valid even if we assume a_0, $a_1, a_2, \ldots, a_{k-1}$ to be nonzero in Eq. (7), i.e.,

$$\Phi_K = \sum_{n=0} a_n \Psi_n .$$

Hence, our estimate for the lower bound on the energy of the states of the excited $K=0$ band is fully justified despite the lack of complete orthogonality between $\Psi^J_{\rm TD}$ and ψ_{J_1}.

The effect of a small overlap between $\Psi^J_{\rm TD}$ and ψ_{J_1} on formula (31) can be examined in a similar way, and it can be demonstrated that we are justified in using this formula for calculating the upper bound on the error in the wave functions of the $J=0$ and 2 states of the excited $K=0$ band.

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Structure of the Odd-Mass Gallium Isotopes with a Particle-Phonon Coupling Model

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The structure of the low-lying levels in odd-mass gallium isotopes is investigated within the framework of the semimicroscopic model, assuming three protons coupled to a quadrupole vibrator. A detailed comparison with experiments is performed for ^{69}Ga.

I. INTRODUCTION

The present investigation was stimulated by the following facts:

(1) In recent years, the structure of odd-mass Ga isotopes has been studied experimentally using different methods: the nuclear reactions (^{3}He, d),[1,2] (d, n),[3,4] and ($n, n'\gamma$)[5]; $\beta^\pm$ decays[6-8]; nuclear resonance fluorescence[9] and other spectroscopic techniques.[10] The electric quadrupole moment and magnetic dipole moment for the ground states are also known from previous measurements.[10]

(2) Intermediate coupling between particle field and collective modes has been successfully applied to account for the structure of nuclei near closed shells.[11-32] In particular, it is a generally accepted point of view that the low-lying states in the odd-mass Cu isotopes can be described in terms of multipole structure and the mixing of multiplets.[11-18] This fact has also been confirmed in a recent comparison with a shell-model calculation using a realistic effective interaction.[33] It is the purpose of the present analysis to take a further step in the application of the semimicroscopic model and propose it for the description of the gallium odd-mass isotopes.

From the above-mentioned experiments it can be seen that the distribution of the single-particle strengths and electromagnetic properties are similar for the low-lying states in odd-mass gallium isotopes (from $A = 65$ to $A = 71$) even if their energy spectra change gradually as the $N = 40$ subshell is filled up. This effect is due to the excitation modes not contained in the particle-vibrator picture (for example, pairing-vibrational mode).

We shall discuss mainly the ^{69}Ga isotope, whose energy spectrum is better known. Obviously, many results and conclusions will also be valid for the other gallium nuclei.

II. MODEL

Since a detailed description of the model can be found in several review articles,[31] only a brief survey of the main formulas and notation will be presented in this section. In particular, a calculation with three extracore particles has been previously performed by Alaga and Ialongo for the gold isotopes.[30]

The total Hamiltonian of the system is written as

$$H = H_0 + H_p + H_{\mathrm{int}}, \tag{1}$$

where H_0 represents the energy of the quadrupole harmonic vibrator and that of the extracore protons. The residual interaction between protons, H_p, is approximated by a pairing force. It will affect only the seniority-one states.[34] The interaction Hamiltonian H_{int} is linear in collective and particle variables and has the form

$$H_{\mathrm{int}} = -\left(\frac{\hbar\omega}{2C}\right)^{1/2} \sum_{\mu=-2}^{2} [b^{\mu\dagger} + (-)^{\mu} b^{-\mu}] \times \sum_{p} k(r_p) Y_2{}^{\mu *}(\theta_p, \phi_p), \tag{2}$$

where the summation p extends over the outside protons and $k(r) = r\,dV(r)/dr$. The potential $V(r)$ is the average shell-model potential usually taken as a Woods-Saxon potential. The symbols $b^{\mu\dagger}$ (b^{μ}) are the operators for the creation (destruction) of the quadrupole phonon field.

The quantity $(\hbar\omega/2C)^{1/2}$, where $\hbar\omega$ is the energy of the phonon and C is the restoring force of the vibrator, measures the amplitude of the vibration-