should probably expect[27] substantially bigger differences between the logft values for these Fermi transitions than we find here.

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ACKNOWLEDGMENTS

Two of us (D. E. A. and D. H. W.) are indebted to Professor S. Gorodetzky for the opportunity of participating in this research as visitors at the Institute of Nuclear Research.

PHYSICAL REVIEW VOLUME 132, NUMBER 5 1 DECEMBER 1963

Moments of Inertia and the Shell Model*

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(Received 1 July 1963)

The variational formula of Skyrme for the moment of inertia is analyzed in some detail. The errors in this formula are studied and an upper bound is given. It is found that in the case of the shell model this approach is quite accurate and allows use of general Hamiltonians.

I. INTRODUCTION

THE general problem of using shell-model techniques for investigating collective properties of nuclei is a challenging one whose solution will certainly lead to a more fundamental understanding of collective nuclear models. In a previous paper[1] the emphasis was on the connection between the shell model and the vibrational model.

However, there is a broad class of nuclei with clearly defined rotational properties for low excitation energies whose vibrational levels lie much higher in energy. These are the so-called "strongly deformed" nuclei and the natural parameter describing their low excited states is the moment of inertia. The question considered in this paper is the following: Given a shell-model single-particle well and two-body interaction, how does one go about computing the moment of inertia? One solution that comes to mind is to set up some kind of Hartree-Fock scheme using the given Hamiltonian and then apply the Inglis[2] "cranking formula" for the evaluation of the moment of inertia. Indeed, Nilsson and Prior[3] have carried out such a program where instead of a Hartree-Fock calculation they calculated the wave functions using a given single-particle deformed field plus a pairing force. This approach has been fairly successful. However, in characterizing the underlying shell-model Hamiltonian only in terms of a pairing part and a single-particle deformed well one loses some control of the problem and any systematic disagreements between the theoretical calculations and experiment are hard to study since modifications of the underlying interaction are quite difficult to make. On the other hand, the degree of validity of the cranking formula itself is hard to assess in a real nucleus. In addition, it is not clear that the Nilsson and Prior approach will work at all well for the light-deformed nuclei where pairing theory has not been successfully applied.

Let us review the possibilities open to us if we wish to use a given shell-model Hamiltonian for our calculation. First, consider the Hartree-Fock problem. In general, this is quite difficult since the orbitals can be varied quite arbitrarily. However, if we restrict the possible variations so that the orbitals retain axial symmetry and are made up of components from a single major shell then the resulting calculations are quite feasible. Possibly one can even go farther and include pairing-type degrees of freedom by working with "quasiparticles."

The next problem that arises is how to extract the moment of inertia from these wave functions and the Hamiltonian. Exploratory calculations using the "cranking formula" in the s-d shell indicated insufficient accuracy in cases where one knew beforehand the actual eigenvalues of the Hamiltonian. On the other hand, the variational formula of Skyrme[4] worked out quite well in these cases. This was indeed encouraging and led to a further analysis of this approach. In this paper the problem of finding a variational formula for the moment of inertia under our self-imposed shell-model boundary conditions is investigated. In addition, the accuracy of the final formula is given in terms of an upper bound on the error. The final result presented is, indeed, Skyrme's formula.

For even-even nuclei one thus has a fairly accurate feasible method for computing deformed wave functions and moments of inertia from a given shell-model

* The research reported in this document has been sponsored in part by Office of Scientific Research OAR, through the European Office, Aerospace Research, U. S. Air Force.
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Hamiltonian. In the case of odd-even nuclei somewhat more delicate questions of Corioliss mixing and core polarization effects occur but they present little extra trouble in practice. It is the great advantage of the general procedures advocated here that one is working with a known Hamiltonian and an explicitly computed set of self-consistent wave functions corresponding to that Hamiltonian. The influence of an extra particle on the underlying core can be easily calculated. These last considerations will not be treated in this paper but will appear shortly.

In the following sections the variational calculation of moments of inertia is developed from the point of view of the "focus parameter" discussed in Sec. II. The formal mathematical calculation of this parameter is discussed in the following sections and, finally, the specialization of the method for use with a Hartree-Fock representation is touched upon.

II. THE FOCUS PARAMETER

An even-even nuclear spectrum with levels of spin $0, 2, 4, 6\cdots$ can be characterized by a parameter $A=1/2I$ where I is the "moment of inertia" of the nucleus when the energies E_J are given by the simple formula:

$$E_J=AJ(J+1). \tag{1}$$

However, in practice, spectra exhibit this behavior only approximately and it is necessary to define a "best" value of A. One approach is to try to fit the spectrum E_J to the form

$$E_J=AJ(J+1)+B(J(J+1))^2. \tag{2}$$

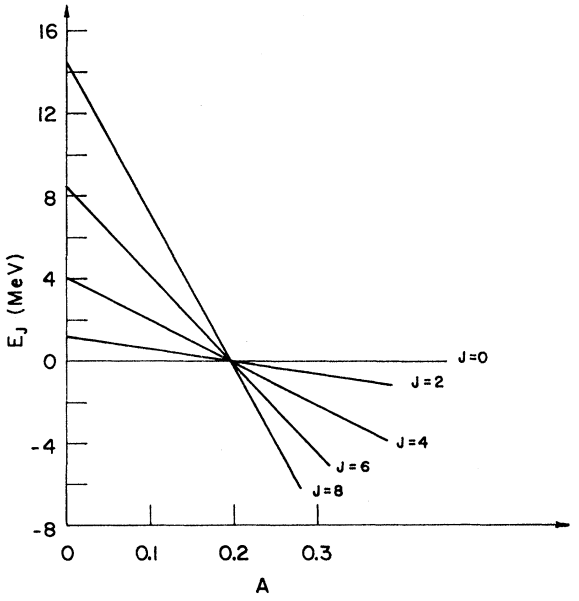

FIG. 1. Idealized focus plot for a spectrum of the form $E_J=0.2J(J+1)$.

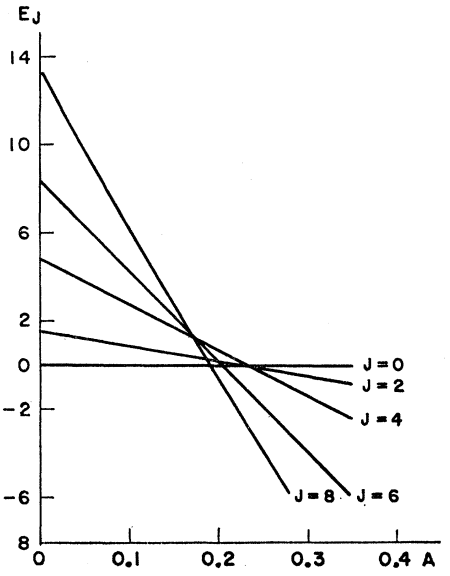

FIG. 2. Focus plot for the nucleus Ne^{20}.

The coefficient B arises in certain models and describes the effect of perturbations on the moment of inertia.

Another method is to draw a "focus" plot.[5] In this plot the energies E_J are placed at points on the vertical axis which is calibrated in energy units. Then a line is drawn through each point E_J with a slope $J(J+1)$. The horizontal axis is also calibrated in energy units.

An example for the case of a spectrum of the exact form (1) is shown in Fig. 1. For a realistic case we show the same plot in Fig. 2 for Ne^{20}. The focus of the lines which was at $A=0.2$ in Fig. 1 is now blurred. However, the eye finds a best focus around $A\sim 0.2$. Mathematically, the focus might be found from the least-square condition derived by minimizing the function

$$F(A)=\sum_J\{E_J-E_0-AJ(J+1)\}^2, \tag{3}$$

or more generally a function

$$G(A)=\sum_J N_J\{E_J-E_0-AJ(J+1)\}^2, \tag{4}$$

where $\sum N_J=1$, and N_J is a set of weighting factors chosen because either the experiment or the theory is more or less dependable for certain values of J. In the following sections a variational method will be derived for evaluating the best A defined by minimizing $G(A)$ in Eq. (4) when one is given a Hamiltonian and a set of variational wave functions. In addition, an upper bound on the width of the focus is given. This method is quite convenient for evaluating moments of inertia in terms of a shell-model Hamiltonian and independent-particle wave functions.

[5] This plot was suggested to the author by H. J. Lipkin.

III. ACCURACY OF EIGENVALUE APPROXIMATION

We review a well-known theorem[6] which gives the accuracy of the approximation

$$E\sim\langle\Phi|H|\Phi\rangle, \tag{5}$$

where Φ is a trial wave function and H is the Hamiltonian. Let $\langle\Phi|\Phi\rangle=1$ and define the eigenfunctions ψ_i and eigenvalues E_i of H:

$$H\psi_i=E_i\psi_i; \tag{6}$$

also define

$$P_i\equiv|\langle\psi_i|\Phi\rangle|^2, \tag{7}$$

thus,

$$\sum P_i=1. \tag{8}$$

Then

$$\langle\Phi|H|\Phi\rangle=\sum_i P_iE_i\equiv\bar{E}, \tag{9}$$

next

$$\langle\Phi|(H-\bar{E})^2|\Phi\rangle=\sum_i P_i(E_i-\bar{E})^2. \tag{10}$$

Since $P_i\geqslant 0$, $(E_i-\bar{E})^2\geqslant 0$, if we replace the factors $(E_i-\bar{E})^2$ in Eq. (10) by their smallest value $(E_k-\bar{E})^2$ we conclude, using Eq. (8), that

$$\langle\Phi|(H-\bar{E})^2|\Phi\rangle\geqslant(E_k-\bar{E})^2, \tag{11}$$

where E_k is the eigenvalue of H closest to $\bar{E}$. If we define

$$I^2=\langle\Phi|(H-\bar{E})^2|\Phi\rangle, \tag{12}$$

then Eq. (11) can be rewritten as

$$\bar{E}-I\leqslant E_k\leqslant\bar{E}+I, \tag{13}$$

which shows that there is at least one eigenvalue of H within an energy interval I of $\bar{E}$.

If we define χ by

$$H\Phi=\langle\Phi|H|\Phi\rangle\Phi+\chi, \tag{14}$$

then we see that

$$\langle\Phi|\chi\rangle=0 \qquad \langle\chi|\chi\rangle=I^2; \tag{15}$$

so the length of the "correction" part χ is an upper limit on the error when one approximates E by $\langle\Phi|H|\Phi\rangle$. As one minimizes $(\chi|\chi)$ one is trapping an eigenvalue of H inside a definite interval given by $(\chi|\chi)$. This leads to just the sort of variational principle needed to find the best A of the previous section.

IV. THE FOCUS THEOREM

We are given a Hamiltonian H and a trial wavefunction Φ. H is spherically symmetric. Φ is, in general, not an eigenstate of angular momentum. In later applications it will take the form of a determinant of independent-particle wave functions corresponding to a deformed-field potential. We now consider a new Hamiltonian.

$$\hat{H}(A)=H-A\mathbf{J}^2, \tag{16}$$

where $\mathbf{J}^2$ is the square of the angular momentum operator and A is regarded as a parameter. The eigenvalue spectrum of the Hamiltonian $\hat{H}(A)$ is $E_J(A)$. These are plotted as a function of A on a "focus" plot, (c.f. Figs. 1 and 2) where one starts at $A=0$ with the eigenvalues of H. We seek that value A such that the focus is sharpest. If the focus came to a point as in Fig. 1 then the eigenvalue spectrum of H would be of the form of Eq. (1) with A equal to that value at the focus. (i.e., $A=0.2$). Physically we would regard $\hat{H}(0.2)$ as the "intrinsic" Hamiltonian and $0.2\mathbf{J}^2$ as the rotational part of the Hamiltonian.

We next apply the theorem of the previous section. Defining the correction wave function $\chi(A)$ by

$$\hat{H}(A)\Phi=\langle\Phi|\hat{H}(A)|\Phi\rangle\Phi+\chi(A), \tag{17}$$

and

$$(\chi|\chi)=I^2(A), \tag{18}$$

we can conclude that an eigenvalue of $\hat{H}$ lies within an energy interval $I(A)$ of $\langle\Phi|\hat{H}|\Phi\rangle$. We need information about eigenvalues of specific J, however, and for this purpose we introduce projection operators P^J which project on the subspace with given angular momentum J. Applying P^J to Eq. (7) and noting that the commutator

$$[H,P^J]=0, \tag{19}$$

because $\hat{H}$ is spherically symmetric, we find

$$\hat{H}\Phi_J=\langle\Phi|\hat{H}|\Phi\rangle\Phi_J+\chi_J, \tag{20}$$

where

$$P^J\Phi=\Phi_J, \quad P^J\chi=\chi_J.$$

Applying Φ_J on the left of Eq. (20)

$$\langle\Phi_J|\hat{H}|\Phi_J\rangle=\langle\Phi|\hat{H}|\Phi\rangle\langle\Phi_J|\Phi_J\rangle+\langle\Phi_J|\chi_J\rangle. \tag{21}$$

Writing Eq. (20) in the form of Eq. (14) and Eq. (15):

$$\hat{H}\Phi_J=\left\{\langle\Phi|\hat{H}|\Phi\rangle+\frac{\langle\Phi_J|\chi_J\rangle}{\langle\Phi_J|\Phi_J\rangle}\right\}\Phi_J+\chi_J-\frac{\langle\Phi_J|\chi_J\rangle}{\langle\Phi_J|\Phi_J\rangle}\Phi_J, \tag{22}$$

where we see from Eq. (21) that the factor in brackets is simply $\langle\Phi_J|\hat{H}|\Phi_J\rangle/\langle\Phi_J|\Phi_J\rangle$, and the "correction" term $\chi_J-(\langle\Phi_J|\chi_J\rangle/\langle\Phi_J|\Phi_J\rangle)\Phi_J$ is orthogonal to Φ_J. In order to apply our theorem we need to use a normalized Φ_J. To this purpose we introduce the normalization constants

$$N_J=\langle\Phi_J|\Phi_J\rangle, \tag{23}$$

and write

$$\Phi_J{}^N=\frac{\Phi_J}{N_J{}^{1/2}}. \tag{24}$$

[6] The author wishes to thank Professor L. Wilets for pointing out to him the existence of this theorem.

Finally Eq. (22) can be divided by $N_J^{1/2}$ to give

$$\hat{H}\Phi_J{}^N=\left\{\langle\Phi|\hat{H}|\Phi\rangle+\frac{\langle\Phi_J|\chi_J\rangle}{N_J}\right\}\Phi_J{}^N+\frac{\chi_J}{N_J{}^{1/2}}-\frac{\langle\Phi_J|\chi_J\rangle}{N_J}\Phi_J{}^N, \quad (25)$$

where the factor in brackets is simply $\langle\Phi_J{}^N|\hat{H}|\Phi_J{}^N\rangle$.

$$\epsilon_J\equiv\langle\Phi_J{}^N|\hat{H}|\Phi_J{}^N\rangle=\langle\Phi|\hat{H}|\Phi\rangle+\frac{\langle\Phi_J|\chi_J\rangle}{N_J}. \quad (26)$$

The error interval corresponding to this approximation for the energy E_J is I_J where $I_J{}^2$ is given by

$$I_J{}^2=\left\langle\frac{\chi_J}{N_J{}^{1/2}}-\frac{\langle\Phi_J|\chi_J\rangle}{N_J}\Phi_J{}^N\middle|\frac{\chi_J}{N_J{}^{1/2}}-\frac{\langle\Phi_J|\chi_J\rangle}{N_J}\Phi_J{}^N\right\rangle=\frac{\langle\chi_J|\chi_J\rangle}{N_J}-\frac{|\langle\Phi_J|\chi_J\rangle|^2}{N_J{}^2}, \quad (27)$$

and by the theorem of Sec. III

$$|E_J(A)-\epsilon_J|\leqslant I_J, \quad (28)$$

where $E_J(A)$ are eigenvalues of $\hat{H}(A)$ with angular momentum **J**.

From Eqs. (26) and (27) we derive a remarkable equality, namely,

$$\sum_J\{(\epsilon_J-\langle\Phi|\hat{H}|\Phi\rangle)^2+I_J{}^2\}N_J=I^2(A), \quad (29)$$

where

$$I^2(A)=\sum_J\langle\chi_J|\chi_J\rangle=\langle\chi|\chi\rangle, \quad (30)$$

because

$$\textstyle\sum_J P^J=1.$$

From Eq. (28) we conclude that

$$\sum_J\{(\epsilon_J-\langle\Phi|\hat{H}|\Phi\rangle)^2+(E_J(A)-\epsilon_J)^2\}N_J\leqslant I^2(A). \quad (31)$$

Using the relation

$$\tfrac{1}{2}(y-z)^2\leqslant(y-x)^2+(z-x)^2, \quad (32)$$

we finally conclude

$$\sum_J(E_J(A)-\langle\Phi|\hat{H}|\Phi\rangle)^2N_J\leqslant 2I^2(A), \quad (33)$$

writing

$$E_J(A)=E_J-AJ(J+1), \quad (34)$$

where $E_J=E_J(0)$ are eigenvalues of H. We have

$$\sum_J(E_J-A\mathbf{J}(\mathbf{J}+1)-\langle\Phi|\hat{H}(A)|\Phi\rangle)^2N_J\leqslant 2I^2(A). \quad (35)$$

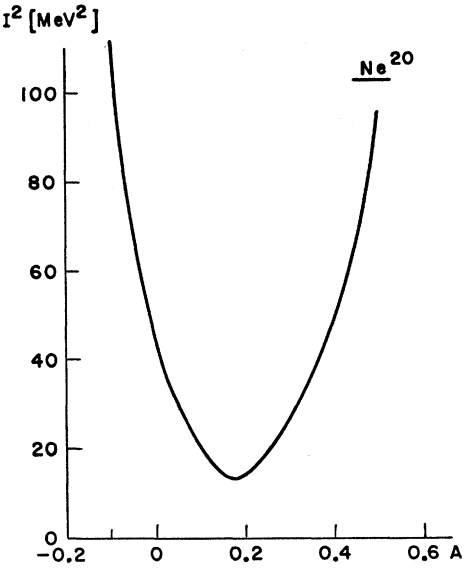

FIG. 3. Plot of $I^2(A)=(\chi(A)|\chi(A))$ for the case of Ne^{20}.

The left side of (35) has the same form as Eq. (4). We see that the weighting factor N_J is a measure of how much of the state $P^J\Phi$ is contained in Φ. This is fortunate since Φ will be determined variationally and the dominate $P^J\Phi$ of Φ will be best represented. Returning to Eq. (33) we see that the focus condition can be replaced by the condition that $I^2(A)$ be minimized. Our new problem then is to find a Φ and an A such that $(\chi|\chi)$ is a minimum where these quantities are related by the equation

$$(H-A\mathbf{J}^2)\Phi=\langle\Phi|H-A\mathbf{J}^2|\Phi\rangle\Phi+\chi. \quad (36)$$

Physically, we are subtracting rotational energy $AJ(J+1)$ from the original E_J so that the differences $E_J-AJ(J+1)$ are as independent of J as possible and cluster about the value $\langle\Phi|H(A)|\Phi\rangle$, which may be interpreted as the intrinsic energy of the system. In practice, this procedure is carried out in two steps. First we minimize $\langle\Phi|H-AJ^2|\Phi\rangle$ for fixed A and varying Φ. If Φ is cast in the form of a determinant of independent-particle orbitals we have a Hartree-Fock type problem. Designate the best Φ obtained this way by Φ_A and the corresponding χ by χ_A. Next we minimize $(\chi_A|\chi_A)$ as a function of A. We finally arrive at a best value of A and an upper limit, $2(\chi_A|\chi_A)$ for the focus defined as the left side of Eq. (33). The particular advantage of this procedure is that the evaluation of

$$(\chi_A|\chi_A)=\langle\Phi_A|(\hat{H}-\langle\Phi_A|\hat{H}|\Phi_A\rangle)^2|\Phi_A\rangle=\sum_{|n\rangle}\langle\Phi_A|\hat{H}-\langle\Phi_A|\hat{H}|\Phi_A\rangle|n\rangle\times\langle n|\hat{H}-\langle\Phi_A|\hat{H}|\Phi_n\rangle|\Phi_A\rangle \quad (37)$$

only involves intermediate states n corresponding to 2-particle excitations. The contribution for $|n\rangle=\Phi_A$ is

obviously zero and for a single-particle excitation we know that $\langle\Phi_A|H|n\rangle=0$ because Φ_A is the Hartree-Fock solution for H. Finally, we only need evaluate

$$(\chi_A|\chi_A)=\sum_{|II\rangle}|\langle\Phi_A|H-A\mathbf{J}^2|II\rangle|^2, \tag{38}$$

where $|II\rangle$ are the set of 2-particle excitations.

Detailed calculations using this approach will be reported on shortly. As an example, however, we show in Fig. 3 the plot of $I^2(A)=(\chi(A)|\chi(A))$ for the case again of Ne^{20}. An Elliott-Flower's[7] type shell-model Hamiltonian was used and only the orbitals outside the O^{16} core were varied. The value A at which the minimum occurs does indeed coincide with the focus of Fig. 2. The value of $I^2(A)$ at the minimum is $\sim$12 MeV. So $2I\sim7$ MeV. The focus width in the physical situation is $\sim$2 MeV. Hence, our theoretical upper limit is quite a bit larger than the observed width in this case.

[7] J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) **A229**, 536 (1955).

V. CONCLUSIONS

If one sets out on the program of computing collective properties with a given shell-model Hamiltonian then the moment of inertia formula of Skyrme is a convenient and accurate tool. The error committed in using this formula has an upper bound which is easily ascertained without performing any extra calculations. The natural parameter that arises in this method is a "focus" point which can be simply extracted from the physical data.

ACKNOWLEDGMENTS

The author would like to thank Professor H. J. Lipkin for many instructive and stimulating conversations. Professor L. Wilets gave several crucial suggestions and really started the work going when he suggested the use of the theorem in Sec. III. Many thanks to Dr. I. Kelson for kindly computing the results shown in Fig. 3.