Moment of Inertia in Hartree-Fock Theory*

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The conditions under which a Hartree-Fock wave function may be a good description of the intrinsic state of a rotational nucleus are discussed from two points of view; first by studying the fluctuations of the modified Hamiltonian $H-\alpha \mathbf{J}^2$ as a function of α, and second by studying the response of the wave function to a small external perturbation $-\omega J_x$. Following Thouless and Valatin, this response is given in terms of an anti-Hermitian cranking operator S. We demonstrate that, when the Hartree-Fock wave function is adequate, S is of the form $[J_x, \rho]/\epsilon$, where ρ is the single-particle density operator and ϵ is twice the rotational energy content of the intrinsic state. These considerations lead to simple tests of the adequacy of the Hartree-Fock wave function as a rotational intrinsic wave function. A comparative study of various formulas for the moment of inertia, utilizing the aforementioned result for S, is presented.

1. INTRODUCTION

DURING recent years attempts have been made to provide a microscopic description of the intrinsic wave functions of deformed nuclei with Hartree-Fock (HF)[1] or Hartree-Fock-Bogoliubov[2] (HFB) wave functions. These efforts have been rewarded with both quantitative success and better qualitative understanding. Once a reliable intrinsic wave function is obtained, the calculation of physical quantities, e.g., energies of the rotational levels, electromagnetic moments, etc., is straightforward in principle; it requires projection of good angular-momentum states from the intrinsic wave function. In practice this can be very laborious. Alternatives to projection calculations, even at the expense of some accuracy, are therefore desirable. A well-known example is the use of a moment of inertia when the spectrum is rotational. But it is necessary to know whether the spectrum is rotational before calculating the moment of inertia. One of the objects of this paper is to establish the conditions under which one can obtain states exhibiting a rotational spectrum from an intrinsic wave function. The conditions are stated in terms of an operator S which describes the response of the intrinsic wave function to cranking. We also examine and compare the various available formulas for the moment of inertia.

We confine our discussions to the HF theory. The extension of the basic ideas developed in this paper to the HFB theory should be apparent. We frequently use simple HF calculations in the $2s$-$1d$ shell to illustrate some of the points under discussion. Since there is no particularly striking example of a rotational spectrum in this shell, the choice is not very fortunate. HF calculations in the rare-earth region would have been preferable, but these are beyond the resources available to the present authors.

Our HF calculations assume that O^{16} serves as an inert core and that the extra core particles are confined to the $2s$-$1d$ oscillator shell. The Hamiltonian, to be referred to as H throughout the paper, contains a single-particle term and a two-particle interaction term. The parameters of the single-particle term are fixed from the appropriate level spacings in O^{17}. The interaction between the extra core particles, denoted as v, is taken to be a purely central force with a Yukawa radial dependence with a range of 1.4 fm. The strengths in the singlet-even, triplet-even, singlet-odd, and triplet-odd states are -34.4, -46.9, 40.8, and 19.4 MeV, respectively. Oscillator functions, with the length parameter adjusted to give the root-mean-square radius correctly, have been used for the radial wave functions of the single-particle states. For simplicity, most of the general discussions and remarks in the paper pertain to axially symmetric HF wavefunctions. We discuss the triaxial cases explicitly only when necessary.

In Sec. 2, we discuss the conditions for the validity of the HF approximation for the intrinsic wave function. In Sec. 3, we develop the conditions which the response operator S must satisfy in order that the spectrum be rotational. The significance of these conditions is discussed in Sec. 4, and the various formulas for the moment of inertia have been examined in Sec. 5. $\hbar$ is set equal to one in the formulas throughout the paper.

2. VALIDITY OF HF APPROXIMATION

A. Fluctuation

The concept of an intrinsic wave function is a very useful tool in the theory of rotational nuclei. For clarity we will specialize the following discussion to axially symmetric nuclei. The underlying conjecture is that the states of a rotational band are well described by the wave functions $\Phi_M{}^{IK}$ obtained by projecting good

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[1] For a good review of the situation see G. Ripka, in *Advances in Physics*, edited by M. Baranger and E. Vogt (Pergammon Press, Inc., New York, 1968), Vol. 1.

[2] M. Baranger, *1962 Cargèse Lectures* (W. A. Benjamin, Inc., New York, 1963).

angular-momentum states from the intrinsic wave function Φ.

$$\Phi_M{}^{IK}=\frac{2I+1}{C_I 8\pi^2}\int d\Omega\, D_{MK}{}^{I*}(\Omega)R(\Omega)\Phi, \quad (2.1)$$

where $R(\Omega)$ is the operator of rotation through the Eulerian angles Ω, $D_{MK}{}^{I}(\Omega)$ is the usual representation of the rotation operator, K is the band quantum number of the axially symmetric wave function Φ, and C_I is the normalization constant such that

$$\Phi=\sum_I C_I\Phi_K{}^{IK}, \quad (2.2)$$

where Φ and $\Phi_M{}^{IK}$ are normalized wave functions. Since the $\Phi_M{}^{IK}$ are supposed to be eigenfunctions of the Hamiltonian

$$H\mid\Phi_M{}^{IK}\rangle=E_I\mid\Phi_M{}^{IK}\rangle, \quad (2.3)$$

the idea of an intrinsic wave function becomes useful if there is a simple prescription for constructing it. HF and HFB theories have been used extensively as approximations to the intrinsic wave function; here we confine our attention to the HF theory. In general the intrinsic wave function Φ, obtained by a HF variational calculation, will not be an eigenfunction of the Hamiltonian H for two reasons. The intrinsic wave function, when it exists at all, may contain correlations not present in a HF determinantal wave function. Such a defect is partly remedied in the HFB approach. The second reason, which is more pertinent to the present discussion, is that even when (2.3) is true the eigenvalues E_I are, in general, nondegenerate. Therefore, a linear combination of the $\Phi_K{}^{IK}$ will not be an eigenfunction of H. The eigenvalues can be brought into degeneracy by substracting from the Hamiltonian a polynomial $F(\mathbf{J}^2)$ of $\mathbf{J}^2$, where the polynomial $F(I(I+1))$ gives the dependence of E_I on I. Here we are interested in a rotational spectrum, i.e., $F(\mathbf{J}^2)\sim A\mathbf{J}^2$. We may write

$$(H-A\mathbf{J}^2)\mid\Phi_M{}^{IK}\rangle=E_0\mid\Phi_M{}^{IK}\rangle, \quad (2.4)$$

and now a linear combination of the $\Phi_K{}^{IK}$ will be an eigenfunction of $H-A\mathbf{J}^2$. It is not essential that the intrinsic wave function be an eighefunction of a modified Hamiltonian in order that its projections be eigenfunctions of H. However, if Φ is an eigenfunction of $H-A\mathbf{J}^2$ then the $\Phi_M{}^{IK}$ are guaranteed to satisfy (2.3). The real advantage of considering a modified Hamiltonian, of which the intrinsic wave function may be an eigenfunction, is that it justifies the use of a variational procedure to find Φ. Skyrme[3] and Levinson[4] used these ideas to develop methods of determining the inertial parameter A, introduced in (2.4), which is half the reciprocal of the moment of inertia. We review these methods briefly.

Let Φ_α be the HF wave function of the Hamiltonian $H-\alpha\mathbf{J}^2$. Then,

$$(H-\alpha\mathbf{J}^2)\mid\Phi_\alpha\rangle=E_\alpha\mid\Phi_\alpha\rangle+\mid\chi_\alpha\rangle, \quad (2.5)$$

where $\mid\chi_\alpha\rangle$ is a sum of two-particle–two-hole states only and may be written as

$$\mid\chi_\alpha\rangle=\sum_{ij\lambda\mu}\langle i_\alpha j_\alpha\mid v-2\alpha\mathbf{J}_1\cdot\mathbf{J}_2\mid\lambda_\alpha\mu_\alpha\rangle\mid i_\alpha j_\alpha;\lambda_\alpha\mu_\alpha\rangle, \quad (2.6)$$

where the Greek letters denote occupied and the Latin letters denote unoccupied single-particle states, and the state $\mid i_\alpha j_\alpha;\lambda_\alpha\mu_\alpha\rangle$ is a two-particle–two-hole state built on $\mid\Phi_\alpha\rangle$. The subscript α serves to remind us that all these quantities are for the HF solution of $H-\alpha\mathbf{J}^2$. If the intrinsic wave function can be a determinant at all, then there will exist a value of α, viz., $\alpha=A$, such that $\mid\Phi_\alpha\rangle$ is an eigenfunction of $H-\alpha\mathbf{J}^2$ and, therefore, $\mid\chi_\alpha\rangle$ will vanish for that value of α. Levinson pointed out that the value of α which minimizes $\langle\chi_\alpha\mid\chi_\alpha\rangle$ may be taken as the best estimate of the inertial parameter and the corresponding Hartree-Fock wavefunction Φ_α is the best determinantal approximation to the intrinsic wave function. The resulting inertial parameter is denoted by A_L. Neglecting the dependence of Φ_α on α, Skyrme obtained the following approximate formula for the inertial parameter from the condition of minimization of $\langle\chi_\alpha\mid\chi_\alpha\rangle$:

$$A_S=\sum_{ij\lambda\mu}\langle ij\mid v\mid\lambda\mu\rangle\langle\lambda\mu\mid\mathbf{J}^2\mid ij\rangle/\sum_{ij\lambda\mu}\mid\langle ij\mid\mathbf{J}^2\mid\lambda\mu\rangle\mid^2, \quad (2.7)$$

where all the quantities are evaluated at $\alpha=0$.

The quantity $\langle\chi_\alpha\mid\chi_\alpha\rangle$ is actually the fluctuation of $H-\alpha\mathbf{J}^2$ in Φ_α, i.e.,

$$\langle\chi_\alpha\mid\chi_\alpha\rangle=\langle\Phi_\alpha\mid(H-\alpha\mathbf{J}^2)^2\mid\Phi_\alpha\rangle-\langle\Phi_\alpha\mid H-\alpha\mathbf{J}^2\mid\Phi_\alpha\rangle^2. \quad (2.8)$$

Naturally each of the two considerations which, in general, prevent $\mid\Phi_\alpha\rangle$ from being an eigenfunction of $H-\alpha\mathbf{J}^2$ contributes to $\langle\chi_\alpha\mid\chi_\alpha\rangle$. Minimization of $\langle\chi_\alpha\mid\chi_\alpha\rangle$ with respect to α eliminates to a large extent the role of the nondengeneracy of the projected spectrum. The minimized value of $\langle\chi_\alpha\mid\chi_\alpha\rangle$ is essentially a measure of the extent to which the projected states are eigenfunctions. A more direct way of studying this point would be to calculate the quantities $\langle\Phi_\alpha{}^I\mid H^2\mid\Phi_\alpha{}^I\rangle-\langle\Phi_\alpha{}^I\mid H\mid\Phi_\alpha{}^I\rangle^2$. It is much easier to calculate the following weighted sum of these fluctuations:

$$\sum_I\mid C_I{}^\alpha\mid^2\{\langle\Phi_\alpha{}^I\mid H^2\mid\Phi_\alpha{}^I\rangle-\langle\Phi_\alpha{}^I\mid H\mid\Phi_\alpha{}^I\rangle^2\}$$
$$=\langle\Phi_\alpha\mid H^2\mid\Phi_\alpha\rangle-\sum_I\mid C_I{}^\alpha\mid^2\langle\Phi_\alpha{}^I\mid H\mid\Phi_\alpha{}^I\rangle^2. \quad (2.9)$$

B. Numerical Examples

We have calculated the minimized fluctuation for Ne^{20}, Mg^{24}, Si^{28}, S^{32}, and Ar^{36} using the Hamiltonian and the restricted single-particle space described in Sec. 1.

[3] T. H. R. Skyrme, Proc. Phys. Soc. (London) **A70**, 433 (1957).
[4] C. A. Levinson, Phys. Rev. **132**, 2184 (1963).

TABLE I. Fluctuations and the Levinson inertial parameter. Column 2 contains the value of the fluctuation of the original Hamiltonian, and columns 3, 4, and 5 contain the values of α_i such that the fluctuation of the modified Hamiltonian $\hat{H}=H-\Sigma_i\alpha_i J_i^2$ is minimized. Column 6 contains this minimum value of the fluctuation of $\hat{H}$, Δ in column 7 is the energy gap between the last-occupied and first-unoccupied Hartree-Fock orbitals. The ratio presented in column 8, discussed in the text, is in some sense a measure of the goodness of the Hartree-Fock wave function.

Nucleus	$\langle H^2\rangle-\langle H\rangle^2$ (MeV^2)	Levinson parameters (in MeV) α_x	α_y	α_z	$\langle\hat{H}^2\rangle-\langle\hat{H}\rangle^2$ (MeV^2)	Δ (MeV)	$\frac{\langle\hat{H}^2\rangle-\langle\hat{H}\rangle^2}{4\Delta^2}$
Ne^{20}	10.8	0.177	0.177	0	2.6	8.61	0.009
Mg^{24}	17.0	0.134	0.103	0.300	6.7	6.85	0.036
Si^{28}	19.5	0.115	0.115	0	12.3	6.68	0.069
S^{32}	15.8	0.097	0.097	0.097	11.6	7.54	0.051
Ar^{36}	9.0	0.138	0.138	0	2.8	6.04	0.019

These nuclei exhibit several simplifying features so far as the HF calculation is concerned. First of all, in these cases HFB calculations converge to normal solutions.[5] Second, the HF density in each of the these cases has time-reversal symmetry and three orthogonal planes of reflection symmetry.[6] The nuclei Ne^{20}, Si^{28}, and Ar^{36} are axially symmetric, while the other two are triaxial. Finally, the neutrons and the protons have similar orbits. The minimized fluctuations and the Levinson parameters are presented in Table I. It is a little difficult to pick a parameter with which the minimized fluctuation should be compared to decide if it is large or small. If the spectrum of the states contained in the intrinsic wave function is truly rotational, then the wave function can be an eigenfunction of $H-A\mathbf{J}^2$, where A is the true inertial parameter. If the value of α in $H-\alpha\mathbf{J}^2$ at which the fluctuation is minimized coincides with A, then the lowest-order corrections to the HF wave function $|\Phi_\alpha\rangle$ are the two-particle–two-hole states $|i_\alpha j_\alpha;\lambda_\alpha\mu_\alpha\rangle$ with coefficients $\langle i_\alpha j_\alpha|v-\alpha\mathbf{J}^2|\lambda_\alpha\mu_\alpha\rangle/(\epsilon_i+\epsilon_j-\epsilon_\lambda-\epsilon_\mu)$. The minimum value of the denominator in the coefficient is 2Δ, where Δ is the gap in the HF spectrum between the last-coccupied and the first-unoccupied states. Hence we may say that the HF wave function $|\Phi_\alpha\rangle$ is a good approximation to the intrinsic wave function when

$$\langle\chi_\alpha|\chi_\alpha\rangle/4\Delta^2\ll 1. \tag{2.10}$$

This ratio is presented in column 8 of Table I. It is clear that the HF theory works better for Ne^{20}, Mg^{24}, and Ar^{36} than for the other two nuclei. We also present, in Figs. 1 and 2, plots of $\langle\chi_\alpha|\chi_\alpha\rangle$ and the quantity (2.9) as functions of α for Ne^{20} and Si^{28}. We see that the nature of $|\Phi_\alpha\rangle$ is not affected very strongly by varying α. In the case of Ne^{20} the minimum value of the quantity (2.9) is 60% of its value at $\alpha=0$. The corresponding number for Si^{28} is 90%.

The foregoing remarks are relevant only to a comparison of the results of the HF approximation with those of a shell-model calculation with the same Hamiltonian and the same set of single-particle states. A comparison of the HF results with experimental data can be made only if we use the correct effective-interaction matrix elements and allow for core polarization,[7] major shell mixing, etc. The parameters of the simple Hamiltonian used in these illustrative calculations were adjusted to fit the low-lying level spectra of O^{18} and F^{18}. Noting that only the $2s$-$1d$ shell states were considered, it may be argued that the matrix elements of the Hamiltonian used in these calculations compare well with the actual effective matrix elements incorporating the core-polarization corrections suggested by Kuo and Brown.[7] Even if the claim is valid, these matrix elements are useful only for a few particles outside of O^{16}. As the number of extra core particles becomes comparable to the number of strongly polarizable core particles, the effect of the major shell mixing in the single-particle states of the extra core particles becomes important. The Hamiltonian which we used suffers from the further limation that it contains no noncentral forces. It is known that the two-body spin-orbit force affects the strength of the effective single-particle spin-orbit force as more and more nucleons are added. These considerations prevent us from comparing the results of the HF theory with experimental data. While quantitative comparison is not permissible, the Hamiltonian employed is not unrealistic. In fact, for the case of Ne^{20}, the excitation energies of the low-lying even-even states calculated with states projected from the best HF wave function compare well with the experimental data, as shown in Table II. The difference of the binding energies of Ne^{20} and O^{16}, after correcting for the Coulomb energies, is 39.7 MeV. The value for the same quantity obtained from the HF calculation is 40.4 MeV. Hence the qualitative conclusions based on these HF calculations are acceptable.

[5] L. Satpathy, D. Goss, and M. K. Banerjee, Phys. Rev. (to be published).

[6] M. K. Banerjee, C. A. Levinson, and G. J. Stephenson, Jr., Phys. Rev. **178**, 1709 (1969).

[7] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).

3. CRANKING AND TEST FOR ROTATIONAL SPECTRUM

In Sec. 2 we have seen that, by studying the fluctuation of the Hamiltonian in the intrinsic wave function, we not only can test the validity of the model for the intrinsic wave function, but we can also obtain a value for the inertial parameter when the model wave function is acceptable. However, for heavier nuclei, calculations of the fluctuation of the Hamiltonian is an extremely time consuming task on account of the very large number of possible two-particle–two-hole states. Therefore, it is useful to attempt to develop a simpler and more practical test to see if the intrinsic wave function describes a rotational band adequately.

The discussions in this section will be limited to HF wave functions which have the symmetries

$$T\,|\,\Phi\rangle = P\exp(-i\pi J_y)\,|\,\Phi\rangle = P\exp(-i\pi J_x)\,|\,\Phi\rangle = |\,\Phi\rangle, \tag{3.1}$$

where T is the time reversal operator and P is the parity operator. These symmetries guarantee[6] that the single-particle density has a principal axis coordinate system

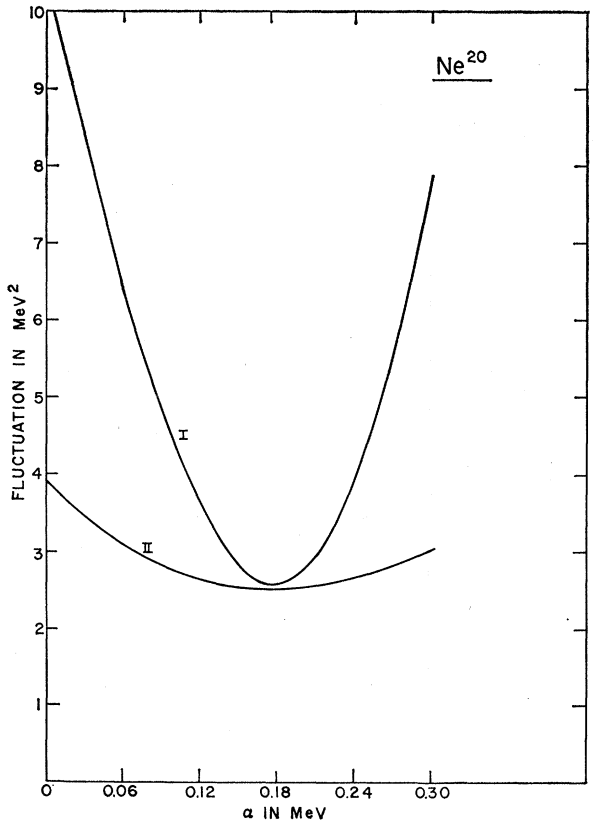

FIG. 1. Plots of the fluctuation of $H-\alpha \mathbf{J}^2$ as a function of α for Ne^{20}. Curve I is the fluctuation in the intrinsic Hartree-Fock state $|\,\Phi_\alpha\rangle$, and curve II is the weighted sum of the fluctuations in the states of sharp angular momentum projected from $|\,\Phi_\alpha\rangle$ given by Eq. (2.9).

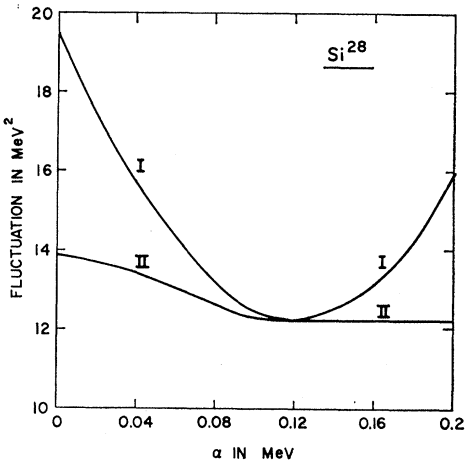

FIG. 2. Plots of the fluctuation of $H-\alpha \mathbf{J}^2$ as a function of α for Si^{28}. Curve I is the fluctuation in the intrinsic Hartree-Fock state $|\,\Phi_\alpha\rangle$, and curve II is the weighted sum of the fluctuations in the states of sharp angular momentum projected from $|\,\Phi_\alpha\rangle$ given by Eq. (2.9).

and that, in the expansion of the HF single-particle states in terms of a complete set of real radial functions with spin-angular functions in the Condon and Shortley phase convention, the expansion coefficients are all real. Again, for simplicity, we consider the axially symmetric nuclei; the changes necessary for triaxial cases will be pointed out wherever appropriate.

A. Conditions for Rotational Spectrum

From the discussions in Sec. 2, we see that, if the HF wave function $|\,\Phi\rangle$ of a Hamiltonian H is a satisfactory model for the intrinsic wave function of a rotational band, then the relation

$$H\,|\,\Phi\rangle = (E_0 + A\mathbf{J}^2)\,|\,\Phi\rangle \tag{3.2}$$

should be approximately true. Equation (3.2) has two implications:

(i) The one-particle–one-hole matrix elements $\langle i;\lambda\,|\,\mathbf{J}^2\,|\,\Phi\rangle$ are negligibly small because the corresponding matrix elements of H are zero. The symbol $|\,i;\lambda\rangle$ stands for a one-particle–one-hole state. (3.3a)

(ii) The two-particle–two-hole matrix elements of H should be proportional to those of $\mathbf{J}^2$, i.e.,

$$\langle ij;\lambda\mu\,|\,H\,|\,\Phi\rangle = \langle ij\,|\,v\,|\,\lambda\mu\rangle = A\langle ij\,|\,\mathbf{J}^2\,|\lambda\mu\rangle. \tag{3.3b}$$

It is rather unlikely that the first of the two conditions will ever be exactly satisfied except for the uninteresting case where Φ is an eigenfunction of $\mathbf{J}^2$. But it is possible that the norm of the one-particle–one-hole states may be small compared to that of the other terms in $\mathbf{J}^2\,|\,\Phi\rangle$.

TABLE II. Comparison of the excitation energies of the states projected from the Hartree-Fock intrinsic wave function with the experimental excitation energies in Ne^{20}.

	Excitation energy (in MeV)	
J	Projected	Expt
2	1.34	1.63
4	3.95	4.25
6	8.13	7.65
8	11.68	11.86

The wave function $\mathbf{J}^2 \mid \Phi\rangle$ may be written as a sum of three terms

$$\mathbf{J}^2 \mid \Phi\rangle = \langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle \mid \Phi\rangle + \sum_{i\lambda} \langle i;\lambda \mid \mathbf{J}^2 \mid \Phi\rangle \mid i;\lambda\rangle + \sum_{ij\lambda\mu} \langle ij;\lambda\mu \mid \mathbf{J}^2 \mid \Phi\rangle \mid ij;\lambda\mu\rangle. \quad (3.4a)$$

Let

$$F = \sum_{ij\lambda\mu} |\langle ij;\lambda\mu \mid \mathbf{J}^2 \mid \Phi\rangle|^2 \quad (3.4b)$$

and

$$G = \sum_{i\lambda} |\langle i;\lambda \mid \mathbf{J}^2 \mid \Phi\rangle|^2 \quad (3.4c)$$

be the norms of the two-particle–two-hole states and the one-particle–one-hole states, respectively. A crude estimate of the quantity G relative to $|\langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle|^2$ and F may be obtained in the following manner. The matrix element

$$\langle i;\lambda \mid J_x^2 \mid \Phi\rangle = \langle i \mid J_x^2 \mid \lambda\rangle - 2 \sum_{\mu} \langle i \mid J_x \mid \mu\rangle\langle\mu \mid J_x \mid \lambda\rangle.$$

For our purpose we may regard $\langle i;\lambda \mid J_x^2 \mid \Phi\rangle$ to be of the same order as $\langle i \mid J_x^2 \mid \lambda\rangle$. It then follows that $G \approx \sum_\lambda \langle\lambda \mid \mathbf{J}^4 \mid \lambda\rangle = N\langle j^4\rangle$, where $\langle j^4\rangle$ stands for the average value of $\langle\lambda \mid \mathbf{J}^4 \mid \lambda\rangle$ in the occupied orbitals and N is the number of particles. Similar arguments would show that $\langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle \approx N\langle j^2\rangle$, where $\langle j^2\rangle$ is the average value of $\langle\lambda \mid \mathbf{J}^2 \mid \lambda\rangle$. Since $\langle j^4\rangle/\langle j^2\rangle^2$ is likely to be of the order of unity it follows that $G/|\langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle|^2 \sim 1/N$.

Writing out the matrix element of $\langle ij;\lambda\mu \mid \mathbf{J}^2 \mid \Phi\rangle$ explicitly and carrying out the sum in (3.4b), it may be seen that $F = |\langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle|^2 +$ terms of the order of N. Hence G/F and $G/|\langle\Phi \mid \mathbf{J}^2 \mid \Phi\rangle|^2$ are both of the order of $1/N$ and hence small for large nuclei. Even for light nuclei G/F is fairly small. For Ne^{20} it is ~ 0.17 and for Si^{28} it is ~ 0.07.

B. Response to Cranking

The most obvious way of testing (3.3) would appear to be to determine the inertial parameter A by least-squares fitting which gives precisely the Skyrme formula (2.7) for A, and then to use it to evaluate the quantity

$$\sum_{ij\lambda\mu} |\langle ij \mid v - A\mathbf{J}^2 \mid \lambda\mu\rangle|^2$$

and see if it is small. However, the work involved is the same as that in the calculations discussed in Sec. 2. Fortunately, the validity of (3.3) can be tested by another method which is considerably simpler and entails far less work. The method involves examination of the structure of the operator S, which describes the response of the HF wave function to cranking. The operator S is defined as follows. For small values of ω the HF wave function of $H - \omega J_x$ may be written as

$$\mid \Phi_\omega\rangle = e^{\omega S} \mid \Phi\rangle, \quad (3.5)$$

where $S = \sum_i S_i$ is an anti-Hermitian single-particle operator. It is convenient to represent S in terms of the HF single-particle states associated with $\mid \Phi\rangle$. The only relevant matrix elements of S are those between the occupied states $\mid \lambda\rangle$ and the unoccupied states $\mid i\rangle$. In terms of the creation and annihilation operators for these states

$$S = \sum_{i\lambda} \{s_{i\lambda} a_i^\dagger a_\lambda - s_{i\lambda}^* a_\lambda^\dagger a_i\}. \quad (3.6)$$

These matrix elements are determined with the following equations given by Thouless[8]

$$\sum_{j\mu} \{\delta_{ij}\delta_{\lambda\mu}(\epsilon_i - \epsilon_\lambda) + \langle i\mu \mid v \mid j\lambda\rangle\} s_{j\mu} + \sum_{j\mu} \langle ij \mid v \mid \lambda\mu\rangle s_{j\mu}^* = \langle i \mid J_x \mid \lambda\rangle,$$

$$\sum_{j\mu} \{\delta_{ij}\delta_{\lambda\mu}(\epsilon_i - \epsilon_\lambda) + \langle i\mu \mid v \mid \lambda j\rangle^*\} s_{j\mu}^* + \sum_{j\mu} \langle ij \mid v \mid \lambda\mu\rangle^* s_{j\mu} = \langle\lambda \mid J_x \mid i\rangle. \quad (3.7)$$

This set of equations may be represented in matrix form in the space of one-particle–one-hole states. We associate with S the column vector

$$\begin{pmatrix} s \\ -s^* \end{pmatrix},$$

where the top half contains the elements $s_{i\lambda}$ and the bottom half contains the elements $s_{\lambda i} = -s_{i\lambda}^*$. Similarly, the matrix elements of J_x may be represented as the column vector

$$\begin{pmatrix} \mathcal{J}_x \\ \mathcal{J}_x^* \end{pmatrix}.$$

We also introduce the matrices Γ and Λ, defined by

$$\langle i;\lambda \mid \Gamma \mid j;\mu\rangle = \delta_{ij}\delta_{\mu\lambda}(\epsilon_i - \epsilon_\lambda) + \langle i\mu \mid v \mid \lambda j\rangle \quad (3.8)$$

and

$$\langle i;\lambda \mid \Lambda \mid j\mu\rangle = -\langle ij \mid v \mid \lambda\mu\rangle. \quad (3.9)$$

As a consequence of the symmetries (3.1), both Γ and Λ are real Hermitian matrices and the column vectors s

[8] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).

and $\mathcal{J}_x$ are real. Equations (3.7) may now be written as

$$\mathcal{H}\begin{pmatrix} s \\ -s \end{pmatrix}=\begin{pmatrix} \Gamma & \Lambda \\ \Lambda & \Gamma \end{pmatrix}\begin{pmatrix} s \\ -s \end{pmatrix}=\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix}, \quad (3.10)$$

where $\mathcal{H}$ stands for the Hermitian matrix shown with submatrices Γ and Λ.

We now examine the consequence of (3.3) on the structure of s. For this purpose it is convenient to exhibit the isospin of the states explicitly. Since the one-hole–one-particle state $|i;\lambda\rangle$ is created by the operator J_x the states $|i\rangle$ and $|\lambda\rangle$ must have the same isospin. Conservation of isospin requires that $|j\rangle$ and $|\mu\rangle$ must also have the same isospin. The states $|i\rangle$ and $|j\rangle$ (or $|\lambda\rangle$ and $|\mu\rangle$ need not have the same isospin. If (3.3) is true, it follows from (3.9) that

$$\begin{aligned}\langle i;\lambda\tau\,|\,\Lambda\,|\,j;\mu\tau'\rangle&=-\langle i\tau,j\tau'\,|\,v\,|\,\lambda\tau,\mu\tau'\rangle\\&=-A\langle i\tau,j\tau'\,|\,\mathbf{J}^2\,|\,\lambda\tau,\mu\tau'\rangle\\&=-2A\{\langle i\tau\,|\,J_x\,|\,\lambda\tau\rangle\langle j\tau'\,|\,J_x\,|\,\mu\tau'\rangle\\&\quad-\delta_{\tau\tau'}\langle i\tau\,|\,J_x\,|\,\mu\tau\rangle\langle j\tau\,|\,J_x\,|\,\lambda\tau\rangle\\&\quad+\text{similar terms for the } y \text{ component}\}. \quad (3.11)\end{aligned}$$

Since we have assumed axial symmetry, the z-component terms do not appear.

The matrix Λ may be written as a sum of two matrices: Λ_D, made up of the direct matrix elements, and Λ_E, made up of the exchange matrix elements,

$$\Lambda=\Lambda_D+\Lambda_E, \quad (3.12a)$$

where

$$\begin{aligned}\langle i;\lambda\tau\,|\,\Lambda_D\,|\,j;\mu\tau'\rangle&=-2A\langle i\tau\,|\,J_x\,|\,\lambda\tau\rangle\langle j\tau'\,|\,J_x\,|\,\mu\tau'\rangle\\&\quad-2A\langle i\tau\,|\,J_y\,|\,\lambda\tau\rangle\langle j\tau'\,|\,J_y\,|\,\mu\tau'\rangle \quad (3.12b)\end{aligned}$$

and

$$\begin{aligned}\langle i;\lambda\tau\,|\,\Lambda_E\,|\,j;\mu\tau'\rangle&=2A\delta_{\tau\tau'}\langle i\tau\,|\,J_x\,|\,\mu\tau\rangle\langle j\tau\,|\,J_x\,|\,\lambda\tau\rangle\\&\quad+2A\delta_{\tau\tau'}\langle i\tau\,|\,J_y\,|\,\mu\tau\rangle\langle j\tau\,|\,J_x\,|\,\lambda\tau\rangle. \quad (3.12c)\end{aligned}$$

The x and the y component parts of Λ_D commute since

$$\sum_{i\lambda\tau}\langle i\tau\,|\,J_x\,|\,\lambda\tau\rangle\langle i\tau\,|\,J_y\,|\,\lambda\tau\rangle=\langle\Phi\,|\,J_xJ_y\,|\,\Phi\rangle=0. \quad (3.13)$$

Because of (3.13) and the factorable form of the matrix elements it follows that

$$\begin{aligned}\Lambda_D\mathcal{J}_x&=-2A\langle\Phi\,|\,J_x^2\,|\,\Phi\rangle\mathcal{J}_x\\ \text{and}\quad\Lambda_D\mathcal{J}_y&=-2A\langle\Phi\,|\,J_y^2\,|\,\Phi\rangle\mathcal{J}_y,\end{aligned} \quad (3.14)$$

and that all the other eigenvalues of Λ_D are zero. The column vectors $\mathcal{J}_x$ and $\mathcal{J}_y$ in general will not be exact eigenfunctions of Λ because Λ_E may mix $\mathcal{J}_x$ and $\mathcal{J}_y$ with other eigenfunctions of Λ_D with zero eigenvalues. The upper limit on the weight of such admixture is given by

$$[(\mathcal{J}_x\,|\,\Lambda_E^2\,|\,\mathcal{J}_x)(\mathcal{J}_x\,|\,\mathcal{J}_x)-(\mathcal{J}_x\,|\,\Lambda_E\,|\,\mathcal{J}_x)^2]/4A^2(\mathcal{J}_x\,|\,\mathcal{J}_x)^4.$$

A rough estimate of this quantity may be obtained by ignoring the cross terms involving matrix elements of both J_x and J_y. Let us introduce the Hermitian matrix P defined as follows:

$$\langle\lambda\tau\,|\,P\,|\,\mu\tau'\rangle=\sum_j\langle\lambda\tau\,|\,J_x\,|\,j\tau\rangle\langle j\tau\,|\,J_x\,|\,\mu\tau\rangle\delta_{\tau\tau'},$$

$$\langle\lambda\tau\,|\,P\,|\,j\tau'\rangle=0.$$

In terms of this matrix P, the estimate of the weight of the above mixture is

$$[\mathrm{Trace}P^3\times\mathrm{Trace}P-(\mathrm{Trace}P^2)^2]/(\mathrm{Trace}P)^4.$$

This quantity vanishes when either P is a multiple of the unit matrix or P^2 is a multiple of P. In general, it is of order $1/N^2$, where N is the number of nucleons present. Therefore, $\mathcal{J}_x$ and $\mathcal{J}_y$ will be approximate eigenfunctions of Λ, the error being of order $1/N^2$. We may write

$$\Lambda\mathcal{J}_x\simeq-\tfrac{1}{2}\epsilon\mathcal{J}_x; \qquad \Lambda\mathcal{J}_y=-\tfrac{1}{2}\epsilon\mathcal{J}_y, \quad (3.15)$$

where

$$\epsilon=4A\langle\Phi\,|\,J_x^2\,|\,\Phi\rangle=2A\langle\Phi\,|\,\mathbf{J}^2\,|\,\Phi\rangle. \quad (3.16)$$

On the other hand, since the Hamiltonian H is scalar,

$$\langle i,\lambda\,|\,[H,J_x]\,|\,\Phi\rangle=0. \quad (3.17)$$

In terms of the quantities Γ and Λ, (3.17) reads

$$\mathcal{H}\begin{pmatrix} \mathcal{J}_x \\ \mathcal{J}_x \end{pmatrix}=\begin{pmatrix} \Gamma & \Lambda \\ \Lambda & \Gamma \end{pmatrix}\begin{pmatrix} \mathcal{J}_x \\ \mathcal{J}_x \end{pmatrix}=0 \quad (3.18)$$

or

$$(\Gamma+\Lambda)\mathcal{J}_x=0. \quad (3.19)$$

Combining (3.19) with the approximate relation (3.15) we get

$$\Gamma\mathcal{J}_x\simeq\tfrac{1}{2}\epsilon\mathcal{J}_x \quad (3.20)$$

and, therefore,

$$\mathcal{H}\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix}=\epsilon\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix}. \quad (3.21)$$

In its turn (3.21) implies that

$$\begin{pmatrix} s \\ -s \end{pmatrix}=\mathcal{H}^{-1}\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix}=\epsilon^{-1}\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix}. \quad (3.22)$$

In terms of the operators S and J_x, (3.22) may be written as

$$S\simeq\epsilon^{-1}[J_x,\rho], \quad (3.23)$$

where

$$\rho=\sum_\lambda a_\lambda^\dagger a_\lambda \quad (3.24)$$

is the single-particle density operator. Another equivalent statement is

$$\begin{aligned}S\,|\,\Phi\rangle&=\epsilon^{-1}J_x\,|\,\Phi\rangle\\ \text{and}\quad\langle\Phi\,|\,S&=-\epsilon^{-1}\langle\Phi\,|\,J_x.\end{aligned} \quad (3.25)$$

TABLE III. Overlaps of the relevant eigenvectors of the matrices $\Gamma+\Lambda$, $\Gamma-\Lambda$, Γ, and Λ with the vector $|\mathcal{J}_x\rangle$. ϵ is the eigenvalue of $\Gamma-\Lambda$, ϵ_Γ and ϵ_Λ the eigenvalues of Γ and Λ, respectively.

Nucleus	Shape	σ	$\sigma_{\Gamma-\Lambda}$	σ_Γ	σ_Λ	ϵ	ϵ_Γ/ϵ	$-\epsilon_\Lambda/\epsilon$
Ne^{20}	axial	0.9977	0.9943	0.9990	0.9772	4.83	0.505	0.528
Mg^{24}	triaxial	0.9932	0.9674	0.9966	0.9636	4.51	0.510	0.566
		0.9994	0.9931	0.9991	0.9823	4.89	0.506	0.524
		0.9937	0.9707	0.9962	0.9476	3.75	0.518	0.571
Si^{28}	axial	0.9885	0.9070	0.9924	0.9703	4.22	0.540	0.585
S^{32}	triaxial	0.9882	0.8968	0.9913	0.9699	3.92	0.541	0.592
		0.9974	0.8100	0.9899	0.9969	3.98	0.523	0.588
		0.9885	0.9667	0.9945	0.9355	3.63	0.529	0.620
Ar^{36}	axial	0.9892	0.9419	0.9419	0.9633	3.84	0.530	0.581

The physical significance of the quantity ϵ follows directly from (3.16) which shows that $\frac{1}{2}\epsilon=A\langle\Phi\,|\,\mathbf{J}^2\,|\,\Phi\rangle$ is the rotational energy content of $|\,\Phi\rangle$.

For triaxial nuclei, Eq. (3.1) should read

$$H\,|\,\Phi\rangle=(E_0+A_xJ_x^2+A_yJ_y^2+A_zJ_z^2)\,|\,\Phi\rangle. \quad (3.26)$$

One now has to crank about the three principal axes and, for each direction, obtain equations analogous to (3.15) and (3.20). Instead of (3.23) one gets

$$S_x\simeq(1/\epsilon_x)[J_x,\rho],$$
$$S_y\simeq(1/\epsilon_y)[J_y,\rho], \quad (3.27)$$

and

$$S_z\simeq(1/\epsilon_z)[J_z,\rho].$$

C. Simple Test for Rotational Spectrum

The preceding discussion shows that, if (3.3) is valid, (3.15) and (3.20) are correct up to terms of the order of $1/N^2$. Therefore, (3.15) or (3.20) may be used to test the adequacy of the model for the intrinsic wave function for a rotational band. That is to say, either the matrix Γ or the matrix Λ may be diagonalized and the overlap of the appropriate eigenvector with $\mathcal{J}_x$ may be calculated. While the present discussion is specialized to the HF theory, it can be extended to the HFB theory without difficulty.

The test proposed here involves far less work than the calculation of the fluctuation of the Hamiltonian. The number of one-hole–one-particle states excited by J_x is very much smaller than the possible number of two-particle–two-hole states which must be considered in the calculation of the fluctuation. Of course, one pays a price for this reduction of labor. Equation (3.2) demands that $\langle ij\,|\,v\,|\,\lambda\mu\rangle$ be zero if $\langle ij\,|\,\mathbf{J}^2\,|\,\lambda\mu\rangle$ is zero. But the matrix Λ involves only those matrix elements $\langle ij\,|\,v\,|\,\lambda\mu\rangle$ for which $\langle ij\,|\,\mathbf{J}^2\,|\,\lambda\mu\rangle$ are nonzero. It is possible that in a certain case (3.2) is satisfied reasonably well for the matrix elements for which $\langle ij\,|\,\mathbf{J}^2\,|\,\lambda\mu\rangle$ are nonzero, but not otherwise. Then the quantity

$$\sum_{ij\lambda\mu}|\langle ij\,|\,v-A\mathbf{J}^2\,|\,|\,\lambda\mu\rangle|^2,$$

with A given by (2.7), may turn out to be large. This quantity is equal to the fluctuation of $H-\alpha\mathbf{J}^2$, minimized with respect to α, if the dependence of $|\,\Phi_\alpha\rangle$ on α can be ignored. A large fluctuation implies that the choice of the intrinsic wave function is inadequate, even though the proposed test is satisfied. One may hope that this is not a serious practical problem.

We also see that it is not necessary to set up both the Γ and Λ matrices in order to evaluate the elements $s_{i\lambda}$. It is sufficient to construct either of the two matrices and use (3.15) or (3.20), as the case may be, to determine ϵ. Finally one uses (3.22) to obtain the elements $s_{i\lambda}$.

D. Numerical Results

We have tested the two conditions for the validity of (3.2) for some of the $N=Z$ even-even nuclei in the $2s$-$1d$ shell. The stablest HF wave functions for these nuclei have the symmetries displayed in (3.1). The first condition, viz., that the norm of the one-hole–one-particle states in $\mathbf{J}^2\,|\,\Phi\rangle$ be small, has been tested for Ne^{20} and Si^{28}. The quantity $G/\langle\Phi\,|\,\mathbf{J}^2\,|\,\Phi\rangle^2$ was calculated and found to be $\sim1/16$ for Ne^{20} and $\sim1/36$ for Si^{28}.

The second condition may be expressed with anyone of the Eqs. (3.15), (3.20), (3.21), and (3.22). To test the condition in detail, all of these equations were tested. The elements $s_{i\lambda}$ were calculated with the Thouless equations (3.10) and the overlap

$$\sigma=(s\,|\,\mathcal{J}_x)/[(s\,|\,s)(\mathcal{J}_x\,|\,\mathcal{J}_x)]^{1/2} \quad (3.28)$$

was calculated. The matrices Γ, Λ, and $\Gamma-\Lambda$ were separately diagonalized and in each case the eigenfunction with the best overlap with $\mathcal{J}_x$ was isolated. The overlap and the eigenvalue are denoted with σ_Γ and ϵ_Γ for the matrix Γ, σ_Λ, and ϵ_Λ for the matrix Λ, and $\sigma_{\Gamma-\Lambda}$ and ϵ for the matrix $\Gamma-\Lambda$. As a check on the calculations, (3.19) was verified. If the second condition for

TABLE IV. Deviations of the projected energies from a pure $\alpha I(I+1)$ spectrum using intrinsic wave functions for Ne^{20} and Si^{28} which minimize the fluctuations of $H-\alpha J^2$.

J	Ne^{20} (MeV)	Si^{28} (MeV)
0	−0.33	−0.00
2	−0.05	+0.02
4	+0.09	+0.06
6	+0.4	+0.02
8		−0.21
10		−0.87
12		−2.23

(3.2) is satisfied, all the overlaps should be unity and the ratios ϵ_Γ/ϵ and $-\epsilon_A/\epsilon$ should equal $\frac{1}{2}$. The values of these quantities are presented in Table III. For the triaxial nuclei (Mg^{24} and S^{32}) three numbers are listed under each column. These correspond to cranking along the three principal axes.

As mentioned before, these calculations are presented solely for the purpose of illustration. While the $2s$-$1d$ shell nuclei are deformed, their spectra are not markedly rotational. Furthermore, the discussions in Sec. 2 show that the HF wave function is useful for Ne^{20} only. An examination of Table III shows that the tests are satisfied better for Ne^{20} than for the other nuclei. On the other hand, the first condition for the validity of (3.2), viz., the smallness of the norm of one-hole–one-particle terms in $\mathbf{J}^2 \mid \Phi\rangle$, is not satisfied so well for Ne^{20}.

Unfortunately, we are unable to present a quantitative criterion for the degree to which the proposed tests should be satisfied in a rotational situation. One should investigate the possible relationship of the ratio of the coefficient of $\mathbf{J}^4$ to that of $\mathbf{J}^2$ in the spectrum with the quantities $1-\sigma_\Delta$, $1-\sigma_\Gamma$, etc.

The case of Si^{28} is interesting. In Sec. 2 we have seen that the HF wave function is rather inadequate for Si^{28}. At the same time Table IV shows that the projected spectrum is rotational to a high degree. (Of course, the experimental spectrum is very far from being rotational.) This is reflected in the fact that, for Si^{28}, not only is the norm of the one-hole–one-particle states in $\mathbf{J}^2 \mid \Phi\rangle$ small, but the tests presented in Table III are satisfied fairly well. This is an illustration of the limitations, discussed earlier, of this proposed test.

4. Rotating Densities

In order to appreciate the physical significance of the properties of the operator S, deduced in Sec. 3, it is useful to review briefly the phenomenology of a rotating density distribution.[9] Let $\rho_A(t)$ be a time-dependent HF single-particle density operator associated with a system of particles being observed in a stationary frame A. The equation of motion of $\rho_A(t)$ is

$$[h_A(t), \rho_A(t)]=i[\partial\rho_A(t)/\partial t], \tag{4.1}$$

where $h_A(t)$ is the HF single-particle Hamiltonian due to the density $\rho_A(t)$. Let us assume that $\rho_A(t)$ actually describes a rotating density, i.e., there exists a rotating frame where the density would appear stationary. For simplicity, we assume that in its body-fixed coordinate system the density is axially symmetric. The symmetry axis will be labeled as the z axis. The object is rotating about the x axis with an angular velocity ω. The x axis of the body fixed coordinate system coincides with that of A. If we transform our description from the frame A to another frame B which is rotating with respect to A about the x axis with angular velocity ω, the transformed density

$$\rho_B(t) = \exp(i\omega J_x t)\rho_A(t)\exp(-i\omega J_x t) \tag{4.2}$$

satisfies the equation

$$[h_B(t)-\omega J_x, \rho_B(t)]=i(\partial/\partial t)\rho_B(t). \tag{4.3}$$

If our supposition that $\rho_A(t)$ is a spinning density is correct, $\rho_B(t)$ should be stationary, i.e.,

$$[h_B-\omega J_x, \rho_B]=0. \tag{4.4}$$

ρ_B describes the density distribution of the spinning system in its body-fixed coordinate system. The density distribution ρ_0 of the same system, when it is not spinning, is given by the stationary HF equation

$$[h_0, \rho_0]=0. \tag{4.5}$$

For small angular velocities ω the relationship between ρ_B and ρ_0 is

$$\rho_B=e^{\omega S}\rho_0 e^{-\omega S}, \tag{4.6}$$

where S is given by (3.6) and (3.7). The definition (3.5) is equivalent to (4.6).

In the time-dependent HF theory (TDHF), any time dependence in the density is customarily ascribed to the presence of vibrational states. Since ρ_B is claimed to be stationary, the implication is that the $\mid\Phi_\omega\rangle$ [see Eq. (3.5)] associated with ρ_B does not contain any vibrational mode. This requires that $S \mid \Phi\rangle$ be orthogonal to all vibrational intrinsic states built on the ground intrinsic state $\mid\Phi\rangle$.

Since a pure determinant is being used for the ground intrinsic state, it is not quite consistent to describe the vibrational states with TDHF theory [which is equivalent to the random-phase-approximation (RPA) theory].[10] However, if one ignores the resulting error, the requirement on S appears to be satisfied. Let $\mid\psi_0\rangle$ be the correlated ground state and let us assume that the differential response to cranking is still $S \mid \psi_0\rangle$. The intrinsic vibrational states $\mid\psi_\alpha\rangle$ are written as

$$\mid\psi_\alpha\rangle=C_\alpha^\dagger \mid\psi_0\rangle, \tag{4.7}$$

[9] D. J. Thouless and J. G. Valatin, Nucl. Phys. **31**, 211 (1962).

[10] G. E. Brown, *Unified Theory of Nuclear Models and Forces* (North-Holland Publishing Co., Amsterdam, 1967).

where

$$C_\alpha^\dagger = \sum_{i\lambda} (A_{i\lambda}^\alpha a_i^\dagger a_\lambda + B_{i\lambda}^\alpha a_\lambda^\dagger a_i). \quad (4.8)$$

It is assumed that

$$C_\alpha \mid \psi_0\rangle = 0. \quad (4.9)$$

The coefficients $A_{i\lambda}^\alpha$ and $B_{i\lambda}^\alpha$ are determined by the eigenvalue problem

$$\mathcal{H}\begin{pmatrix} A_\alpha \\ B_\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} A_\alpha \\ -B_\alpha \end{pmatrix}, \quad (4.10)$$

where the column vectors are made up of the coefficients $A_{i\lambda}^\alpha$ and $B_{i\lambda}^\alpha$. The solutions with $E_\alpha > 0$ correspond to $C_\alpha^\dagger$. To demonstrate the orthogonality of $S \mid \psi_0\rangle$ to every $\mid \psi_\alpha\rangle$ we have to show that

$$\langle \psi_\alpha \mid S \mid \psi_0\rangle = \langle \psi_0 \mid [C_\alpha, S] \mid \psi_0\rangle = (A^\alpha - B^\alpha)\begin{pmatrix} S \\ -S \end{pmatrix} = 0. \quad (4.11)$$

But

$$(A^\alpha - B^\alpha)\begin{pmatrix} S \\ -S \end{pmatrix} = E_\alpha^{-1}(A^\alpha \quad B^\alpha)\mathcal{H}\begin{pmatrix} S \\ -S \end{pmatrix}$$

$$= E_\alpha^{-1}(A^\alpha \quad B^\alpha)\begin{pmatrix} \mathcal{J}_x \\ -\mathcal{J}_x \end{pmatrix} = 0. \quad (4.12)$$

In the last step we have used the Thouless equation (3.10) and the fact that all $\mid \psi_\alpha\rangle$'s with $E_\alpha > 0$ are orthogonal to $J_x \mid \psi_0\rangle$ which is a spurious solution of (4.10) with zero eigenvalue. Since $E_\alpha \neq 0$, (4.12) proves (4.11). When $\mid \psi_0\rangle$ and $\mid \psi_\alpha\rangle$ are exact intrinsic wave functions for the ground and a vibrational band, i.e., there is no eigenstate of the Hamiltonian common to both, (3.25) follows from (4.11) for a general Hamiltonian. If the descriptions are not exact, (3.25) does not necessarily follow from (4.11).

The Tamm-Dancoff approximation for the vibrational states is actually more consistent with the use of an uncorrelated wave function for the ground intrinsic state, even though both descriptions are less accurate than the ones discussed above. In the Tamm-Dancoff theory, the vibrational phonon-creation operators $C_\alpha^\dagger$ do not contain the backward-going terms $B_{i\lambda}^\alpha a_\lambda^\dagger a_i$. The coefficients $A_{i\lambda}^\alpha$ and the eigenvalues are obtained by diagonalizing the matrix Γ. Normally the spurious state $J_x \mid \Phi\rangle$ does not drop out as a separate solution of the eigenvalue problem, as it does in the RPA theory. However, if (3.3) is satisfied then we find from (3.20) that the spurious state $J_x \mid \Phi\rangle$ does drop out as a separate and recognizable solution. The other eigenfunctions, to be interpreted as vibrational states, are orthogonal to $S \mid \Phi\rangle$.

5. MOMENT OF INERTIA

A. Formulas for Inertial Parameter

The moment of inertia is a very useful parameter inasmuch as its use avoids laborious projection calculations, however, it can only be used when the rotational criteria discussed in Sec. 3 are satisfied. There are several formulas to calculate this parameter or, equivalently, the inertial parameter $A = (2\mathcal{I})^{-1}$. One of these, due to Levinson[4] and based on the minimization of the fluctuation of $H - \alpha \mathbf{J}^2$, has been discussed in Sec. 2. This formula does not lead to any significant reduction in labor. Another due to Skyrme,[3] was presented in Eq. (2.7). In this section, we present additional formulas for this parameter and discuss their relative merits.

A variety of formulas have been developed based on the following idea. If the Hartree-Fock wave function is a linear combination of the eigenfunctions of the members of a rotational band then

$$\langle \Phi \mid H \mid \Phi\rangle = E_0 + A\langle \Phi \mid \mathbf{J}^2 \mid \Phi\rangle. \quad (5.1)$$

If one can find another wave function Φ', which is also a linear combination of the same eigenfunctions, then one has the second equation

$$\langle \Phi' \mid H \mid \Phi'\rangle = E_0 + A\langle \Phi' \mid \mathbf{J}^2 \mid \Phi'\rangle. \quad (5.2)$$

From these two equations we obtain the following formula for the inertial parameter

$$A = (\langle \Phi' \mid H \mid \Phi'\rangle - \langle \Phi \mid H \mid \Phi\rangle)/(\langle \Phi' \mid \mathbf{J}^2 \mid \Phi'\rangle - \langle \Phi \mid \mathbf{J}^2 \mid \Phi\rangle). \quad (5.3)$$

The well known Inglis[11] formula falls in this category. He suggested the use of cranking to generate the second wave function Φ'. Using (3.5) and (3.7) for Φ', we find that (5.3) reduces to

$$A_{\mathrm{BDS}} = \frac{\langle \Phi \mid [S, [S, H]] \mid \Phi\rangle}{\langle \Phi \mid [S, [S, \mathbf{J}^2]] \mid \Phi\rangle} = \frac{\langle \Phi \mid [J_x, S] \mid \Phi\rangle}{\langle \Phi \mid [S, [S, \mathbf{J}^2]] \mid \Phi\rangle} \quad (5.4)$$

in the limit of vanishingly small ω. This is, however, not the Inglis formula which is obtained through two approximations. First, one equates the change of the expectation value of $\mathbf{J}^2$ to twice the square of the change of the expectation value of J_x, i.e.,

$$\langle \Phi \mid [S, [S, \mathbf{J}^2]] \mid \Phi\rangle \simeq 2 \mid \langle \Phi \mid [J_x, S] \mid \Phi\rangle \mid^2. \quad (5.5)$$

This approximation is equivalent to using the classical definition of the moment of inertia as the ratio of the angular momentum along the x axis to the angular velocity ω about the same axis. The resulting formula is

$$\mathcal{I} = 1/2A = \langle \Phi \mid [J_x, S] \mid \Phi\rangle. \quad (5.6)$$

[11] D. R. Inglis, Phys. Rev. **96**, 1059 (1954); **97**, 701 (1955).

TABLE V. Values of the inertial parameters for Ne^{20} and Si^{28} calculated with the formulas discussed in the text.

Nucleus	Skyrme	Das Gupta–VanGinneken	BDS	Thouless–Valatin	Inglis
Ne^{20}	0.214	0.182	0.194	0.161	0.320
Si^{28}	0.122	0.114	0.113	0.103	0.191

The second approximation of Inglis involves treating $-\omega J_x$ as a perturbation on the Hartree-Fock field of the nonspinning system. The result is

$$s_{i\lambda}=\langle i \mid J_x \mid \lambda\rangle/(\epsilon_i-\epsilon_\lambda), \tag{5.7}$$

which leads to the well known Inglis formula

$$\mathcal{I}_{\text{Inglis}}=(2A_{\text{Inglis}})^{-1}=2\sum_{i\lambda}|\langle i \mid J_x \mid \lambda\rangle|^2/(\epsilon_i-\epsilon_\lambda). \tag{5.8}$$

Thouless[8] pointed out the lack of self-consistency in this second approximation and showed that Eqs. (3.7) are the correct equations for the determination of the elements $s_{i\lambda}$. In fact, the second Inglis approximation involves ignoring the two-particle interaction terms in (3.7). Thouless and Valatin[9] retained the first approximation leading to (5.6), and obtained

$$A_{\text{TV}}=1/2\langle\Phi\,|[J_x, S]|\,\Phi\rangle. \tag{5.9}$$

Das Gupta and Van Ginneken[12] have recently suggested a formula for the inertial parameter based on the use of $J_+\mid\Phi\rangle$ for $\mid\Phi'\rangle$. This formula is

$$A_{\text{DV}}=\frac{\langle\Phi \mid HJ^2 \mid \Phi\rangle-\langle\Phi \mid H \mid \Phi\rangle\langle\Phi \mid J^2 \mid \Phi\rangle}{\langle\Phi \mid J^4 \mid \Phi\rangle-\langle\Phi \mid J^2 \mid \Phi\rangle^2}. \tag{5.10}$$

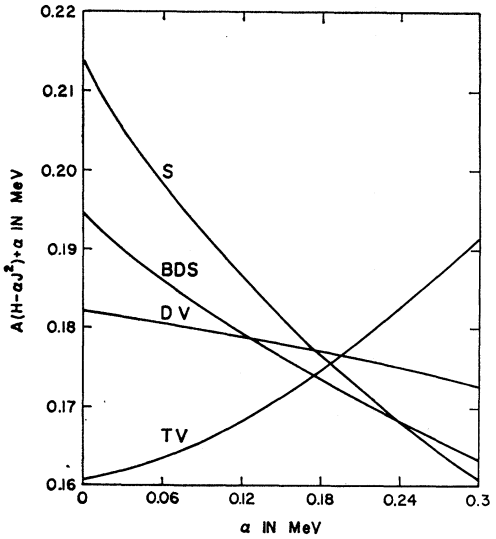

FIG. 3. Inertial parameter calculated in the intrinsic state $\mid\Phi_\alpha\rangle$ using the four formulas indicated plotted against α for Ne^{20}.

[12] S. Das Gupta and A. Van Ginneken, Phys. Rev. **164**, 1320 (1967).

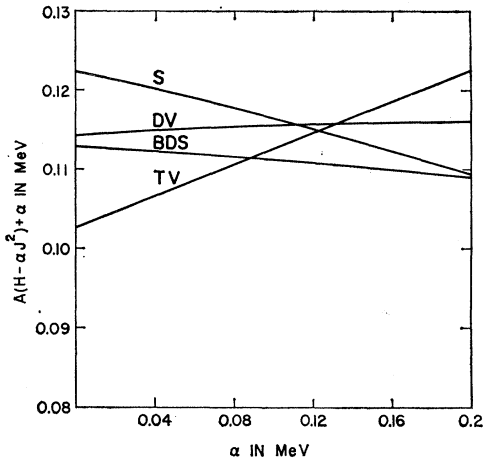

FIG. 4. Inertial parameter calculated in the intrinsic state $\mid\Phi_\alpha\rangle$ using the four formulas indicated plotted against α for Si^{28}.

Using (3.4) and (3.25) we find that

$$\langle\Phi\,|[S,[S,J^2]]|\,\Phi\rangle=(1/\epsilon^2)(2F+G) \tag{5.11}$$

and

$$\langle\Phi \mid J^4 \mid \Phi\rangle-\langle\Phi \mid J^2 \mid \Phi\rangle^2=F+G. \tag{5.12}$$

Using (3.25) we find that the numerator of (5.4) is

$$\langle\Phi\,|[J_x, S]|\,\Phi\rangle=\epsilon^{-1}\langle\Phi \mid J^2 \mid \Phi\rangle. \tag{5.13}$$

The numerators of (2.7) and (5.11) are the same and one can also see that

$$\begin{aligned}&\langle\Phi \mid HJ^2 \mid \Phi\rangle-\langle\Phi \mid H \mid \Phi\rangle\langle\Phi \mid J^2 \mid \Phi\rangle\\&=\sum_{ij\lambda\mu}\langle\lambda\mu \mid v \mid ij\rangle\langle ij \mid J^2 \mid \lambda\mu\rangle \qquad (5.14)\\&=-(\mathcal{J}_x \mid \Lambda \mid \mathcal{J}_x)-(\mathcal{J}_y \mid \Lambda \mid \mathcal{J}_y)=\tfrac{1}{2}\epsilon\langle\Phi \mid J^2 \mid \Phi\rangle.\end{aligned}$$

In the last step (3.15) has been used. Combining these results we find that

$$\begin{aligned}A_{\text{DV}}&=\tfrac{1}{2}\epsilon\langle\Phi \mid J^2 \mid \Phi\rangle/(F+G),\\A_{\text{BDS}}&=\tfrac{1}{2}\epsilon\langle\Phi \mid J^2 \mid \Phi\rangle/(F+\tfrac{1}{2}G),\end{aligned} \tag{5.15}$$

and

$$A_S=\tfrac{1}{2}\epsilon\langle\Phi \mid J^2 \mid \Phi\rangle/F.$$

In other words the three moments of inertia are in arithmetic progression. In actual practice there will be some deviation from the simple rule because Eq. (3.15) is never satisfied exactly.

If condition (3.3a) is satisfied exactly, then $G=0$. In this ideal limit not only are the three formulas in (5.15) equal to each other, but they are also numerically equal to the Levinson moment, as pointed out in Sec. 2.

From (5.13) it follows that

$$A_{\text{TV}}=\epsilon/2\langle\Phi \mid J^2 \mid \Phi\rangle. \tag{5.16}$$

For heavy nuclei this formula becomes equal to those in (5.15) since

$$F\approx\langle\Phi \mid J^2 \mid \Phi\rangle^2\{1+O(1/N)\}. \tag{5.17}$$

The values of the inertial parameter using the five formulas are presented in Table V for Ne^{20} and Si^{28}. All the formulas, except the Levinson moment, were evaluated with H without any modifying $\alpha \mathbf{J}^2$ term. We find less spread in the values of the inertial parameter for Si^{28} than for Ne^{20} since (3.3a) is better satsified for the former.

Kelson[13] proposed a criterion to determine the validity of various formulas for the inertial parameter. The criterion is that, if $A(H)$ is a correct formula for the inertial parameter, then the following relation should hold

$$A(H)=A(H-\alpha \mathbf{J}^2)+\alpha.$$

Thus to test a particular formula, say the one proposed by Das Gupta and Van Ginneken, one would calculate $A(H)$ with Eq. (5.10) and calculate $A(H-\alpha \mathbf{J}^2)$ with the same equation replacing H and $H-\alpha \mathbf{J}^2$ and $|\Phi\rangle$ with $|\Phi_\alpha\rangle$. The Inglis formula, which is positive definite, clearly cannot satisfy this criterion. For the remaining formulas, this criterion really tests the dependence of $|\Phi_\alpha\rangle$ on α. If the rotational criterion that this dependence should be weak is satisfied, all the formulas give nearly the same values and satisfy Kelson's criterion reasonably well. To illustrate this point, the values of $A(H-\alpha \mathbf{J}^2)+\alpha$ as a function of α for the various formulas are presented for Ne^{20} in Fig. 3 and for Si^{28} in Fig. 4. If the Kelson criterion is satisfied, these quantities should be constant. We see that this condition is better satisfied for Si^{28}, where the relevant rotational criterion is better satisfied.

Since all of these formulas are determined self-consistently and with the use of the HF wave functions, the inertial parameter will reflect a weighted average of the excitation energies of the members of the ground band and will give the best results when applied to the spacing of levels with $I\sim[\langle\Phi|\mathbf{J}^2|\Phi\rangle]^{1/2}$. Inasmuch as purely rotational spectra are rarely observed in nature and a more adequate description of the spectrum is of the form

$$E_I=E_0+AI(I+1)+BI^2(I+1)^2,$$

where A is positive and B is negative, these formulas will generally underestimate the spacing E_2-E_0 of the ground- and first-excited states.

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Fluctuations in Nuclear Elastic Scattering Cross Sections*

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A method of fluctuation analysis is developed for elastic scattering of spin-zero particles from spin-zero nuclei. The principal difference between this model and the one proposed by Ericson is that some unitarity is included. It is shown that all features of conventional fluctuation analysis are modified to a small extent. Analysis of the phase shift may show entirely different behavior from that predicted by an Ericson model. Because of the simplicity of the elastic-scattering reaction, it is possible to obtain not only the total width but also the level spacing and partial width (as defined within the context of the model). These quantities are obtained as a function of angular momentum. This method is only applicable if a phase-shift analysis can be done on the data.

I. INTRODUCTION

THE representation of compound-nucleus reaction cross sections by stochastic processes as first proposed by Ericson[1] and Brink and Stephen[2] has had a great deal of success in the interpretation of excitation functions.

The method commonly employed to obtain such a representation is as follows. A general form is given expressing the amplitude in terms of a large number of resonance parameters. The resonance parameters are then assumed to be random variables with appropriate properties. In order to make the resulting process as simple as possible it is desirable to have all of the random variables independent. The choice of form has a strong bearing on the allowability of the independence assumption, as we shall see.

The success achieved by fluctuation theory has been in spite of the fact that the form used, together with the independence assumption, allows unitarity to be

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