mismatch of the zero crossover angles.

The spin-flip probability from ^{32}S measured at 15.9 MeV was even larger, showing a peak value greater than 0.5 (Fig. 12). This is the largest spin-flip probability reported to date. The same optical-model parameters, extended in energy, which fit the data at 17.6 MeV, fall short of reproducing this large value of the spin-flip probability.

The large peak values of $S(\phi)$ in ^{32}S are not understood. A similar experiment on ^{32}S with deuterons[5] does not show such a large value, but is not necessarily inconsistent with our results, since that experiment was done at a very different energy, and we have already noted the rapid change in the peak $S(\phi)$ with energy. Apparently a collective-model approach such as we have used here is incapable of showing the detailed features and behavior of the spin-flip probability.

Even without a spin-orbit interaction term in ΔU, spin-flip inelastic scattering can occur ($\Delta = 0$), and this alone can account for a large part of the effects we observe. Apparently the model is not sufficiently detailed to allow for either the amplitude we have seen in peak value or the variation with energy. There have been recent attempts to apply microscopic models,[3,12] but these have not been especially promising in solving the present problem, because they require accurate and detailed wave functions, and because it is probable that a full consideration of core-polarization effects will be required.

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Concept of the Intrinsic State

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The problem of collective nuclear rotations is discussed in terms of a kinematic transformation to an intrinsic body-fixed coordinate system. Some results are obtained that are equivalent to the classical case. By use of approximate projection operators, an algorithm for calculating successively higher terms in the expansion of the rotational parameter ($\frac{1}{2}$ the inverse inertial moment) is developed. The first-order term is just the Skyrme formula, with the proviso that it be evaluated with respect to the "nonrotational" part of the Hamiltonian.

I. KINETIC TRANSFORMATIONS

The picture one has of the collective motion of a nucleus is that of an ellipsoid slowly rotating within the laboratory reference frame, perhaps executing small vibrations. There are various semi-classical ways of using this picture to approximate nuclear parameters, e.g., the "moment of inertia" or inverse spacing between the few lowest-energy levels. These find their most rigorous expression in terms of approximations to the projection of states of good angular momentum $\vec{J}$ (the

caret is used throughout to distinguish operators) from some intrinsic state Φ.[1] The state Φ describes the oriented ellipsoidal system in terms of a coordinate system fixed in the nucleus, usually taken to coincide with the principal axes of the nuclear inertial moment. This is the same as regarding the intrinsic state as an oriented density distribution corresponding roughly to a deformed potential well; in such a case, the eigenfunctions of the Hamiltonian of the intrinsic frame would no longer be eigenfunctions of $\vec{\hat{J}}$, since $[\vec{\hat{J}}, \hat{U}] \neq 0$ or $[\vec{\hat{J}}, \hat{\rho}] \neq 0$ where $\hat{\rho}$ is the operator corresponding to the density in the intrinsic frame.

Various approximation schemes[2] are based on the purported smallness of the angular velocity parameter ω that expresses the rate of rotation of the deformed system as seen in the laboratory frame. It is true that the rotational level spacings (and hence difference in ω's) are small in comparison to the angular frequency of a transition between vibrational levels, or to the frequencies corresponding to single-particle-hole excitations; however, it is not obvious that a parameter classically identified as being related to the angular momentum by a linear transformation can be varied in a continuous fashion or used as the expansion parameter in presumably rapidly convergent expansions.[3] One of the aims of the present study is to eliminate this dependence on ω.

Such descriptions of rotation in terms of "small ω" usually assume that the rotation takes place about an axis perpendicular to the symmetry axis.[2] At first sight, this is a strange *ad hoc* assumption, since it is evident that the classical rigid ellipsoid would rarely rotate in such fashion; the justification given is that a rotation around the symmetry axis cannot be discerned externally. But a rigid ellipsoid (even a symmetric one) could rotate about any other axis. Classically $\vec{\omega}$ need not be along the direction of $\vec{J}$; it is taken to lie along the instantaneous axis of rotation and usually has nonvanishing components with respect to space-fixed and body axes, as does $\vec{J}$. For a force-free rigid body with an axis of symmetry (two principal inertial moments the same) $\vec{\omega}$ precesses about $\vec{J}$ with constant angular velocity of precession, so that the inertial ellipsoid (which could correspond to a surface with given density value) rolls around in a circle on the invariable space-fixed plane. In the general case (no principal inertial moments the same) the motion is not so regular; it is solvable in terms of Jacobi elliptic functions.[4,5]

The intrinsic coordinate system is related to the laboratory system through an explicitly time-dependent rotational transformation.[6] Such a transformation will be termed *kinematic*, in contrast to the transformation of rotation of the system through a finite angle about some axis; the latter transformation amounts to a reorientation of the system and will be termed a *static* rotation in order to distinguish it from the kinematic case. The transformation is given as $e^{-i\vec{\omega}\cdot\vec{J}t}$, where $\hbar = 1$ here and in what follows. This approach has previously been used in the treatment of magnetic-resonance problems.[6] Classically $\vec{J} = \vec{I}\cdot\vec{\omega}$ is the angular momentum, and the energy of rotation is $H_R = \frac{1}{2}\vec{\omega}\cdot\vec{I}\cdot\vec{\omega} = \frac{1}{2}\vec{\omega}\cdot\vec{J}$. The dyadic $\vec{I}$ here represents the inertial tensor.[7] The quantum-mechanical operator for the rotational energy is $H_R = \frac{1}{2}\vec{\omega}\cdot\vec{\hat{J}}$, so the explicitly time-dependent operator for the kinematic rotation becomes $e^{-i\vec{\omega}\cdot\vec{J}t} = e^{-i2H_R t}$, which will enable us to discuss the rotation without reference to the classical parameter $\vec{\omega}$. An additional static (time-dependent) rotation would in general be necessary to orient the coordinate axes along the principal axes of the density distribution in the body-fixed frame.

The state function of the system as viewed from the laboratory frame is then $\psi_J = e^{-i2\hat{H}_R t}\phi_J$ where ϕ_J is the state function in the rotating frame. If $[\hat{H}_R, \vec{\hat{J}}] = 0$, then ϕ_J must be an eigenfunction of $\vec{\hat{J}}$, since ψ_J is.

Let us examine the problem of the excitations of the system as viewed from the intrinsic frame. First we note

$$\hat{H}\psi_J = i\dot{\psi}_J = 2\hat{H}_R e^{-i2\hat{H}_R t}\phi_J + ie^{-i2\hat{H}_R t}\dot{\phi}_J = \hat{H}e^{-i2\hat{H}_R t}\phi_J ,$$

so

$$(e^{i2\hat{H}_R t}\hat{H}e^{-i2\hat{H}_R t} - 2\hat{H}_R)\phi_J = i\dot{\phi}_J = (\hat{H}' - 2\hat{H}_R)\phi_J \qquad (1)$$

is the eigenvalue problem in the rotating frame; this is essentially the same as the classical result.[4] Note that the Hamiltonian for the system $(\hat{H}' - 2\hat{H}_R)$ is no longer to be identified as the total energy of the system, i.e., it is *not* the "energy in the intrinsic frame." The main assumption that has been made thus far is the existence of a nuclear Hamiltonian $\hat{H}_R$ that describes collective rotations. In what follows, we shall have in mind the description of states of even-even nuclei, so that J will be an integer and usually an even integer.

We have now eliminated the dependence of the rotation on $\vec{\omega}$ and obtained the Hamiltonian eigenvalue problem for the rotating frame. In Sec. II, we give a method for finding the coefficients of the series expansion of the rotational energy E_{RJ}, based upon an ansatz for the expansion of the projection operator in terms of powers of $\vec{\hat{J}}$. Some useful properties of these operators and their relation to previously used projection techniques are discussed. An algorithm is developed to generate these operators to any order. In Sec. III,

the identification of E_{RJ} as an expansion in powers of $J(J+1)$ allows us to develop a compact self-consistent method for evaluating the rotational spectrum. In this approximation the eigenvalues of $\hat{H}' - 2\hat{H}_R$ are degenerate (independent of J); the Hamiltonian of the intrinsic frame, rather than that of the lab frame should then be used in the variational procedure if the variational wave function is to represent the wave function of the intrinsic state.

II. APPROXIMATE PROJECTION OPERATORS

We assume that the intrinsic state is $\Phi = \sum_{J=0}^{\infty} \alpha_J \phi_J$. The true projection operator given by $\hat{O}_J \Phi = \alpha_J \phi_J$ has the following properties:

$$\begin{aligned}
&\langle \Phi | \hat{O}_J | \Phi \rangle = \alpha_J \langle \Phi | \phi_J \rangle = \alpha_J^* \alpha_J , \\
&\langle \Phi | \hat{O}_J^2 | \Phi \rangle = \alpha_J \langle \Phi | \hat{O}_J | \phi_J \rangle = \alpha_J \langle \Phi | \phi_J \rangle = \alpha_J^* \alpha_J , \\
&\langle \Phi | \hat{O}_{J'}^{\dagger} \hat{O}_J | \Phi \rangle = \alpha_{J'}^* \langle \phi_{J'} | \phi_J \rangle \alpha_J = \delta_{JJ'} \alpha_J^* \alpha_J , \\
&\langle \Phi | \sum_J \hat{O}_J | \Phi \rangle = \sum_J |\alpha_J|^2 = 1 .
\end{aligned} \tag{2}$$

The operator $\hat{O}_J$ has the following explicit representation[8]:

$$\hat{O}_J = \prod_{K \neq J} \{ [\hat{J}^2 - K(K+1)] / [J(J+1) - K(K+1)] \} ,$$

which clearly annihilates all eigenfunctions with $K \neq J$.

Perhaps the most popular representation of $\hat{O}_J$ (actually $\hat{O}_{JM}$) is that used by Peierls and Yoccoz,[1] who write it in the form of a Hill-Wheeler-Griffin integral.[9] Discussions of this method as applied to the projection of angular momenta after Hartree-Fock (HF) variation are well covered in the lectures of Ripka[10] and Villars[11]; Faessler and Plastino[12] use it to derive a scheme for HF variation after angular momentum projection. These methods essentially average the HF single-particle functions over the total solid angle, using the rotation matrix $\mathfrak{D}^{J\dagger}_{MM'}(\Omega)$ as a weighting function. They also require a prohibitive number (Ref. 12, p. 77) of matrix or determinant calculations. Since our approach here is to be formal and approximate, and the formal aspects of the projection integral have been well described elsewhere,[13] we shall not use this method.

For calculations restricted to a finite basis, the ladder calculation scheme of Kelson and Levinson,[14] Ripka,[10] and Löwdin[8] based on the properties of continued products of $\hat{J}_- \hat{J}_+$ should provide sufficient accuracy.[10] Actually the solution of the set of linear equations

$$\langle \Phi | \hat{J}^{2n} | \Phi \rangle = \sum_{J \neq 0}^{N} J^n (J+1)^n \alpha_J^* \alpha_J , \tag{3}$$

might prove to be a convenient approach in certain cases. The normalization requirement could be used to find $|\alpha_0|^2$.

The approach used here is patterned after that of Hu[15]; a similar approach is developed independently by Das Gupta and Van Ginneken.[16] Define the operator $\hat{P}_J = \hat{O}_J^2 / |\alpha_J|^2$. Then $\langle \Phi | \hat{P}_J | \Phi \rangle = 1$ for all J. We would like to have $\langle \Phi | \hat{P}_K \hat{P}_J | \Phi \rangle = 0$ for $K \neq J$. We intend to approximate

$$\langle \phi_J | (\hat{H}' - 2\hat{H}_R) | \phi_J \rangle = \frac{\langle \Phi | \hat{O}_J (\hat{H}' - 2\hat{H}_R) \hat{O}_J | \Phi \rangle}{\langle \Phi | \hat{O}_J^2 | \Phi \rangle} , \tag{4}$$

by $\langle \Phi | (\hat{H}' - 2\hat{H}_R) \hat{P}_J | \Phi \rangle$. In general $[(\hat{H}' - 2\hat{H}_R), \hat{O}_J] = 0$ only if the angular momentum projection is to eigenstates of the Hamiltonian involved, so $\hat{P}_J$ is being used to simulate the effect of a commuting $\hat{O}_J^2$. From this point forward, we understand that all expectation values (represented by the angular brackets) are to be taken with respect to Φ unless otherwise stated.

Hu[15] claims that the operator

$$\hat{P}_J^H = 1 + \frac{\hat{J}^2 - \langle \hat{J}^2 \rangle}{\langle \hat{J}^4 \rangle - \langle \hat{J}^2 \rangle^2} [J(J+1) - \langle \hat{J}^2 \rangle] \tag{5}$$

with the properties $\langle \Phi | \hat{P}_J^H | \Phi \rangle = 1$ and $\langle \Phi | \hat{J}^2 \hat{P}_J^H | \Phi \rangle = J(J+1)$ projects out eigenstates of the Hamiltonian H with eigenvalue $E_K + J(J+1)/(2\mathfrak{I}_K)$ for the case where the z' component of the angular momentum is K in the intrinsic frame. Leaving aside the question of normalization, such an operator cannot be a true projection operator, because it is not idempotent:

$$\langle (\hat{P}_J^H)(\hat{P}_{J'}^H) \rangle = 1 + [J(J+1) - \langle \hat{J}^2 \rangle][J'(J'+1) - \langle \hat{J}^2 \rangle] . \tag{6}$$

Suppose that one writes

$$\hat{P}_J = 1 + \sum_{n=1}^{\infty} \hat{A}_n B_n . \tag{7}$$

Since $\langle \hat{P}_J \rangle = 1$, $\langle \hat{A}_n \hat{J}^2 \rangle = 0$. If we choose the normalization on the operator $\hat{A}_n$ such that $\langle \hat{J}^{2n} \hat{A}_n \rangle = 1$, then

$$\hat{A}_n = \frac{\hat{J}^{2n} - \langle \hat{J}^{2n} \rangle}{\langle \hat{J}^{4n} \rangle - \langle \hat{J}^{2n} \rangle^2} \tag{8}$$

appears to be the simplest such operator. The coefficients B_n are then chosen to yield approximately the correct eigenvalues of functions of $\hat{J}^2$ and still keep the error at any stage of the calculation relatively [to $J(J+1) - \langle \hat{J}^2 \rangle$] small. Set

$$\begin{aligned}
B_1 &= J(J+1) - \langle \hat{J}^2 \rangle , \\
B_2 &= J^2(J+1)^2 - \langle \hat{J}^4 \rangle - \langle \hat{J}^4 \hat{A}_1 \rangle B_1 , \\
B_3 &= J^3(J+1)^3 - \langle \hat{J}^6 \rangle - \langle \hat{J}^6 \hat{A}_1 \rangle B_1 - \langle \hat{J}^6 \hat{A}_2 \rangle B_2 , \\
B_n &= J^n(J+1)^n - \langle \hat{J}^{2n} \rangle - \langle \hat{J}^{2n} \sum_{j=1}^{n-1} \hat{A}_j B_j \rangle .
\end{aligned} \tag{9}$$

It is important for subsequent steps that B_n be of

this form, with a small remainder. Then

$$\langle \hat{J}^{2k}\hat{P}_J\rangle = \langle \hat{J}^{2k}\rangle + \sum_{n=1}^{\infty}\langle \hat{J}^{2k}\hat{A}_n\rangle B_n$$
$$= \langle \hat{J}^{2k}\rangle + J^k(J+1)^k - \langle \hat{J}^{2k}\rangle - \langle \hat{J}^{2k}\sum_{j=1}^{k-1}\hat{A}_jB_j\rangle$$
$$+ \sum_{j=1}^{k-1}\langle \hat{J}^{2k}\hat{A}_jB_j\rangle + \sum_{n=k+1}^{\infty}\langle \hat{J}^{2k}\hat{A}_n\rangle B_n \ . \quad (10)$$

For systems such that $\langle \hat{J}^{2n}\rangle/\langle \hat{J}^2\rangle^n \to 0$ as $n\to\infty$ (although $\langle \hat{J}^{2n}\rangle > \langle \hat{J}^{2n-2}\rangle$) one has

$$\langle \hat{J}^{2k}\hat{A}^n\rangle = \frac{\langle \hat{J}^{2(k+n)}\rangle - \langle \hat{J}^{2n}\rangle\langle \hat{J}^{2k}\rangle}{\langle \hat{J}^{4n}\rangle - \langle \hat{J}^{2n}\rangle^2} < 1 \quad (11)$$

for $k<n$ because this goes essentially as $\langle \hat{J}^{2k}\rangle/\langle J^{2n}\rangle$ for large enough n. Because the accuracy of estimates made with the series depends sensitively on $\langle \hat{J}^{2n}\rangle$, no general guarantee can be given as to the rate of convergence. While it would be convenient for the purposes of a calculation if the series converged in a few terms for well-chosen Φ, for the purpose of formal manipulation it is sufficient to identify the first-order coefficient with "reasonable" accuracy. That is, one is given an operator $\hat{F}(\hat{J}^2)$ such that if

$$\langle \phi_J|\hat{F}(\hat{J}^2)|\phi_J\rangle = a + bJ(J+1) + cJ^2(J+1)^2 + \cdots ,$$

then (12)

$$\langle \Phi|\hat{F}(\hat{J}^2)\hat{P}_J|\Phi\rangle = a' + b'J(J+1) + c'J^2(J+1)^2 + \cdots , \quad (13)$$

where $a = a' + \delta a$ and $\delta a \ll a_1$, etc.

III. APPLICATIONS TO HF THEORY

Let

$$E_{RJ} = \langle \phi_J|\hat{H}_R|\phi_J\rangle = AJ(J+1) + BJ^2(J+1)^2 + \cdots \quad (14)$$

and

$$\hat{H} = \hat{H}_0 + \hat{H}_R \ ,$$

so that

$$\hat{H}' - 2\hat{H}_R = \hat{H}_0 - \hat{H}_R \ .$$

If we replace the Hamiltonian matrix for the intrinsic frame by its projected approximation,

$$\langle \phi_J|(\hat{H}_0 - \hat{H}_R)|\phi_J\rangle \simeq \langle \Phi|\hat{H}_0\hat{P}_J|\Phi\rangle - E_{RJ} \ , \quad (15)$$

and if $\hat{P}_J$ is such that the expansion is of the form

$$\langle \Phi|\hat{H}_0\hat{P}_J|\Phi\rangle = \langle \Phi|\hat{H}_0|\Phi\rangle + A[J(J+1) - \langle \hat{J}^2\rangle]$$
$$+ B[J^2(J+1)^2 - \langle \hat{J}^4\rangle] + \cdots , \quad (16)$$

we can make the identification

$$\langle \Phi|\hat{H}_0\hat{P}_J|\Phi\rangle = \langle \Phi|(\hat{H}_0 - A\langle \hat{J}^2\rangle - \cdots)|\Phi\rangle$$
$$+ AJ(J+1) + \cdots$$
$$= \langle \Phi|(\hat{H}_0 - \hat{H}_R)|\Phi\rangle + E_{RJ} \ . \quad (17)$$

Our present choice of approximate projection operator yields

$$\sum_{n=1}^{\infty}\langle \Phi|\hat{H}_0\hat{A}_nB_n|\Phi\rangle$$
$$= \langle \Phi|\hat{H}_0|\Phi\rangle + \left\{\frac{\langle \hat{H}_0\hat{J}^2\rangle - \langle \hat{H}_0\rangle\langle \hat{J}^2\rangle}{\langle \hat{J}^4\rangle - \langle \hat{J}^2\rangle}\right\}[J(J+1) - \langle J^2\rangle]$$
$$+ \text{higher-order terms} \ , \quad (18)$$

where the coefficient A is given by the term in curly brackets. It corresponds to the Skyrme formula[17] for the rotation operator, except that the "non-rotational" Hamiltonian is used in place of the full Hamiltonian $\hat{H}$.

From our identification of corresponding terms in E_{RJ} and $\langle \hat{H}_0\hat{P}_J\rangle$ we have

$$\langle \Phi|(\hat{H}' - 2\hat{H}_R)\hat{P}_J|\Phi\rangle = \langle \Phi|(\hat{H}' - 2\hat{H}_R)|\Phi\rangle$$
$$= \sum_J |\alpha_J|^2\langle \phi_J|(\hat{H}' - 2\hat{H}_R)|\phi_J\rangle$$
$$\simeq \langle \phi_J|(\hat{H}' - 2\hat{H}_R)|\phi_J\rangle \quad (19)$$

for all J, or one might say that the eigenvalues of $(\hat{H}' - 2\hat{H}_R)$ are degenerate in this approximation.

It is then clear that the best variational approximation to this equation then solves the problem: Minimization of $\langle \Phi|(\hat{H}' - 2\hat{H}_R)|\Phi\rangle$ determines a Φ such that E_{RJ} can be calculated from A, B, etc. This implies that what should be minimized in the usual HF approach to the rotational problem is $\hat{H}' - 2\hat{H}_R$ instead of $\hat{H}$.

In using the Skyrme method, one assumes roughly the following: Let $\hat{H}_R = A_S\hat{J}^2$, $E_{RJ} = A_SJ(J+1)$. If this is true, calculation of A_S from the formula using the full Hamiltonian results in

$$A_S = \frac{\langle(\hat{H}_0 + A_S\hat{J}^2)\hat{J}^2\rangle - \langle(\hat{H}_0 + A_S\hat{J}^2)\rangle\langle \hat{J}^2\rangle}{\langle \hat{J}^4\rangle - \langle \hat{J}^2\rangle^2} \ ,$$
$$A_S = \frac{\langle \hat{H}_0\hat{J}^2\rangle - \langle \hat{H}_0\rangle\langle \hat{J}^2\rangle}{\langle \hat{J}^4\rangle - \langle \hat{J}^2\rangle^2} + A_S\frac{\langle \hat{J}^4\rangle - \langle \hat{J}^2\rangle^2}{\langle \hat{J}^4\rangle - \langle \hat{J}^2\rangle^2} \ . \quad (20)$$

As there is no reason why the numerator of the first term should vanish, this would indicate that such a procedure is inconsistent if one assumes Φ is the variational approximation to the eigenfunction of the Hamiltonian of the intrinsic frame. But this is not what the authors of Ref. 17 set out to do; their variation minimizes $(\hat{H} - \hat{H}_R)$ with respect to projected wave functions, such that the deviation from the pure $J(J+1)$ spectrum is minimized in a particular way. Their method is similar in function to projection of angular moments followed by variation.

On the other hand, if Eq. (19) is an exact eigen-

value equation, $(\hat{H}_0 - \hat{H}_R)|\Phi\rangle = E_0|\Phi\rangle$, and $\hat{H}_R = A\hat{J}^2$, then

$$\langle \hat{H}_0 \hat{J}^2 \rangle - \langle \hat{H}_0 \rangle \langle \hat{J}^2 \rangle = \langle (E_0 + \hat{H}_R)\hat{J}^2 \rangle - \langle (E_0 + \hat{H}_R) \rangle \langle \hat{J}^2 \rangle , \tag{21}$$

so that

$$A = \frac{A\langle \hat{J}^4 \rangle - A\langle \hat{J}^2 \rangle^2}{\langle \hat{J}^4 \rangle - \langle \hat{J}^2 \rangle^2}$$

which is obviously self-consistent.

The state which is obtained by minimizing the Hamiltonian in the lab frame without requiring a sharp angular momentum cannot be considered a truly intrinsic state; it should not, for example, be considered to have a particular shape, because it consists of a superposition of densities rotating with differing angular momenta and rotational energies. The method of variation after angular momentum projection serves to obtain an antisymmetric variational wave function which is also an angular momentum eigenfunction referred to the lab frame. The reason this method seems to work better than the usual HF variation followed by projection may be because the Hamiltonian $\hat{H}$ is not the correct one to use in the intrinsic frame.

The projection of angular momenta from a properly antisymmetrized wave function that has minimized an operator related additively to the Hamiltonian of the system in question may in fact be a reasonable approximation for calculating various parameters of interest for such a system. The author feels that the minimization of the correct Hamiltonian for the system might yield a better approximation (numerical studies are underway to check this) and should surely provide more physical understanding of the nature of nuclear collective excitations. Discussion concerning the proper Hamiltonian $\hat{H}_0$ to be used and a detailed variational calculation are left to a future publication.

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