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**The Villars formalism for nuclear rotation**

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**Abstract.** The paper discusses the method proposed by Villars for describing the rotational states of nuclei. For simplicity only two-dimensional rotation is considered for the ground-state band of an even-even nucleus in which the last occupied sub-shell of the deformed potential is completely filled. It is shown how to avoid inconsistencies arising from the multi-valuedness of the angle variable which appears in the formalism. In the Villars method the moment of inertia appears in terms of a sum over the eigenstates of the 'intrinsic' Hamiltonian. Since these are not calculable exactly, one needs an approximation scheme. A possible scheme based on the Hartree-Fock approximation is used, though for the present this is approximated further by the use of harmonic oscillator wave functions. The case of  $^{28}\text{Si}$  is treated by way of illustration. The detailed model is too unrealistic to expect physically significant results; it does suggest, however, that the method is suitable for practical evaluation. Further steps for improving the accuracy are discussed.

**1. Introduction**

Recently, Villars (1965, 1966) has proposed a new formalism for describing rotational states of nuclei. This problem is still of interest today, in spite of the existence of many important papers both on the practical applications of the concept of rotational states, and on the theoretical basis. Much of the current work is based on the idea of the 'cranking model' first proposed by Inglis, but in spite of its simplicity and intuitive value the theoretical foundations of this model are not very secure, particularly if one wishes to take into account the effects of correlations between the nucleons. Another line of approach (Thouless 1960, Peierls and Thouless 1962) is based on a variational approach; the accuracy of the results therefore depends on how well the trial function used represents the rotational states. In addition, this approach is formulated in terms of an exact solution of the Hartree-Fock equations of the nuclear problem, and when a full Hartree-Fock calculation is too laborious it is not clear how best to use the variational approach (Husain 1967). For these reasons it is still interesting to consider new formulations of the problem. One such possibility has been proposed in a paper by Kerman and Klein (1963), but we shall not follow this in the present study.

The idea of the method of Villars is to extract from the Hamiltonian of the many-body system an 'intrinsic' part which does not contain the rotational energy, so that the remainder relates directly to the rotational properties. This division is carried out, in principle, exactly, though its practical evaluation must, of course, require approximations. No attempt is made to separate the degrees of freedom of the system into intrinsic and collective ones, and the variables used in the formulation of the intrinsic Hamiltonian are still the degrees of freedom of all nucleons. The redundancy arising from this manifests itself in a degeneracy of the intrinsic Hamiltonian, which has the same eigenvalue spectrum for all values of the angular momentum.

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Villars formulated his method only for the case of rotation about a given axis, and we shall retain the same restriction in the present paper. The extension to three-dimensional rotation would make the expressions more complicated, but does not seem to involve any new difficulties of principle.

For rotation about a given axis, say the  $z$  axis, one then needs for the specification of the intrinsic Hamiltonian an angle which is related to the orientation of the deformed nucleus, or rather its projection on the  $xy$  plane. This angle  $\phi$  may be taken as a function of the nucleon coordinates only. Care must, however, be taken because physically such an angle can be defined only mod  $2\pi$ . One may choose to restrict it to an interval of length  $2\pi$ , but this results in a discontinuity which would cause very severe complications. Otherwise the angle is multivalued, and must not be assumed to be a physical observable. Some of the equations of Villars are somewhat ambiguous as they stand because their derivation relies on the existence of  $\phi$  as an observable. The simplest way out is to work, not with the angle  $\phi$  itself, but with a periodic function, such as  $\exp(i\phi)$ . If the intrinsic state of the nucleus has mirror symmetry, as is the case for the ground state of an even-even nucleus, which we shall consider in detail, even a rotation by  $\pi$  causes no physical change, so that  $\phi$  is defined only mod  $\pi$ . We shall therefore have to work with the quantity  $\exp(2i\phi)$ . One object of the present paper is to re-write the Villars formalism with this point in mind.

In this way one obtains an expression for the Hamiltonian of the nucleus in terms of intrinsic operators, in which the angular momentum appears as a parameter. For low angular momentum the dependence of the energy on this parameter can be handled by perturbation theory, yielding an expression for the rotational energy in terms of the eigenstates and eigenvalues of the intrinsic Hamiltonian  $H^{(0)}$ . This expression is, in principle, exact, but its evaluation would require a knowledge of the exact solutions for  $H^{(0)}$ , which are as hard to obtain as those for the original Hamiltonian  $H$ . If we possessed techniques of calculation adequate for this purpose, we could also directly calculate the spectrum of  $H$ , and the rotational energies would be known without any special device.

One must therefore necessarily have recourse to approximate techniques, and the obvious approach is by way of the Hartree-Fock approximation. This is applicable only to non-singular potentials, and we shall discuss a model using non-singular forces. For a treatment using realistic forces, one would have to replace the Hartree-Fock approximation by one of the more modern techniques, such as that of Brueckner, but before proceeding to this degree of elaboration it seems worth studying the method in a model with non-singular forces.

Even then the Hartree-Fock method neglects nucleon-nucleon correlations, which are likely to be important for the moment of inertia. It is therefore essential to have a formalism in which such correlations, in particular pairing correlations, can be incorporated. There seems to be no difficulty of principle in including these in the Villars formalism, and work in this direction is now under way. The present paper will, however, deal only with the Hartree-Fock type of approximation.

It then turns out that the perturbation theory required to determine the rotational energy is somewhat ambiguous, since the Hartree-Fock approximation to  $H^{(0)}$  does not possess the degeneracy appropriate to the exact solution. This difficulty can be avoided by using a variation principle for the second-order perturbation, which makes the result less sensitive to the lack of knowledge of the exact excitation spectrum of  $H^{(0)}$ .

Even with the approximations outlined above, the algebra would be prohibitively complicated, since the angular operator  $\exp(2i\phi)$  is strongly non-linear in the nucleon coordinates. It turns out to be the ratio of a numerator which is a linear combination of one-particle operators and a non-linear denominator which depends on the shape, but not on the orientation, of the two-dimensional mass tensor. While the orientation of this mass tensor is evidently an important dynamical variable for the collective motion, it seems reasonable to expect the fluctuations in the shape of a deformed nucleus to be small. This approximation can be tested and is found to be satisfied for not too small nuclei and not too small deformation.

We shall report numerical results for a simple model by way of illustration.

## 2. The modified Villars method

For a system of  $A$  nucleons with the Hamiltonian

$$H = T + V = \sum_i \frac{p_i^2}{2M} + \sum_{i < j} v_{ij}, \quad i, j = 1, 2, \dots, A \quad (2.1)$$

where  $p_i$  is the momentum of the  $i$ th nucleon and  $v_{ij}$  a two-body interaction potential, the idea of Villars (1965, 1966) is to express the Hamiltonian in the form

$$H = H^{(0)} + JH^{(1)} + \frac{1}{2}J^2H^{(2)} + \dots \quad (2.2)$$

in which  $J$  denotes the  $z$  component of the total angular momentum:

$$J = L_z + S_z \quad (2.3)$$

$L$  and  $S$  being the orbital and spin angular momenta. The operators  $H^{(n)}$  are defined so as to commute both with the angular momentum  $J$  and with a collective angle  $\phi$ , which is conjugate to  $J$ :

$$[J, \phi] = -i. \quad (2.4)$$

(We use units such that  $\hbar = 1$ .) Thus

$$\begin{aligned} [H^{(n)}, J] &= 0 \\ [H^{(n)}, \phi] &= 0. \end{aligned} \quad (2.5)$$

The fact that each of these operators commutes with a pair of mutually non-commuting operators obviously requires it to have a high degree of degeneracy. Indeed, if we regard  $H^{(n)}$  as a matrix in the space of  $J$ , it can easily be seen to be a multiple of the unit matrix, the factor still being a matrix in the space of the remaining 'intrinsic' variables. This property justifies the description of the  $H^{(n)}$  as intrinsic operators, and in particular  $H^{(0)}$  as the intrinsic Hamiltonian.

The representation (2.2) of the Hamiltonian is an identity if  $J$  is regarded as an operator. We may, however, also consider the expression (2.2) with  $J$  a parameter. Calling this parameter  $J'$ , we can write

$$H(J') = H^{(0)} + J'H^{(1)} + \frac{1}{2}J'^2H^{(2)} + \dots \quad (2.2a)$$

For given  $J'$ ,  $H(J')$  has eigenstates which may also be chosen to be eigenstates of the angular momentum operator  $J$ , with any value of  $J$ . The value of (2.2a) for such a state will, because of the degeneracy, be independent of  $J$ , but will depend on the value of the parameter  $J'$ . Only states with  $J' = J$  have physical meaning, and are eigenstates of the original Hamiltonian  $H$ . Because of the degeneracy, we may, however, compute the energy also from states with  $J' \neq J$  (e.g. with  $J = 0$ ). Alternatively, we may use linear combinations of states with different  $J$ , even going as far as making  $\phi$  diagonal, although this extreme and rather singular choice would not usually be convenient. In this sense it may be claimed that the method has separated the description of the rotation from the intrinsic dynamics.

Simple algebra shows that, in order to make (2.2) an identity and to satisfy the commutativity conditions (2.5), the operators  $H^{(n)}$  must have the following form:

$$\begin{aligned} H^{(0)} &= H - JH^{(1)} - \frac{1}{2}J^2H^{(2)} - \dots \\ H^{(1)} &= i[H, \phi] - JH^{(2)} + \dots \\ H^{(2)} &= -[[H, \phi], \phi] + \dots \end{aligned} \quad (2.6)$$

The dots stand for higher terms which contain powers of  $J$  higher than the second, and multiple commutators of higher order. If  $\phi$  is a function of the nucleon coordinates only, and if the two-nucleon potential  $v_{ij}$  is static,  $\phi$  commutes with the potential energy, so that the first commutator  $[H, \phi]$  comes only from the kinetic energy part of  $H$  and is linear in the particle momenta. The second commutator  $[[H, \phi], \phi]$  then is a function of the

coordinates only, and the higher terms vanish. This is true even if the potential contains exchange forces, so that in  $v_{ij}$  there is a term containing  $P_{ij}$ , the operator exchanging particles  $i$  and  $j$ , multiplied by a function of the coordinates. In that case  $P_{ij}$  still commutes with  $\phi$  provided the definition of  $\phi$  contains all the nucleons symmetrically, which is a reasonable restriction. Genuine velocity-dependent terms, such as the spin-orbit part of the force, would give rise to higher-order terms in (2.6). We have not investigated the effect of such terms, and we shall neglect them in what follows.

For the reasons discussed in the introduction it is not satisfactory to assume the existence of an operator  $\phi$ , and we have to work with a periodic function of  $\phi$ . For the intrinsic ground state of an even-even nucleus, to which we shall restrict ourselves, we must choose a function of period  $\pi$ , the simplest choice being

$$B = e^{2i\phi}. \quad (2.7)$$

(Any other function with the same period can, of course, be written as a function of  $B$ .) The commutation law (2.4) must then be replaced by

$$[J, B] = 2B. \quad (2.8)$$

We also require the Hermitian conjugate to  $B$ ,

$$B^* = e^{-2i\phi}$$

and evidently  $B^*B = 1$ .

The expansion (2.2) then remains valid, with

$$[H^{(n)}, J] = [H^{(n)}, B] = 0 \quad (2.9)$$

provided we choose

$$\begin{aligned} H^{(0)} &= H - JH^{(1)} - \frac{1}{2}J^2H^{(2)} - \dots \\ H^{(1)} &= \frac{1}{2}B^*[H, B] - (J+1)H^{(2)} + \dots \\ H^{(2)} &= \frac{1}{4}B^*[B^*[H, B], B] + \dots \end{aligned} \quad (2.10)$$

If  $B$  is a symmetric function of the nucleon coordinates it follows, as before, that the higher commutators indicated by the dots in (2.2) and (2.10) are zero for a static internucleon potential including exchange terms. All previous statements which do not contain  $\phi$  explicitly thus remain valid.

The rotational energy can now be expressed as the dependence of the eigenvalues of (2.2a) on the parameter  $J'$ . The moment of inertia is related to the quadratic term in  $J'$  (the linear term vanishes for reasons of symmetry). If we wish to evaluate (2.2a) to order  $J'^2$  we may treat the second and third terms as small perturbations. The quadratic term need be taken only to first order of perturbation theory, but the linear term has to be carried to second order.

Because of the degeneracy we need not perform this calculation with angular momentum eigenstates for each  $J'$ , but may choose states of any angular momentum  $J$ , or linear combinations. Assume for the moment, for definiteness, that we know the eigenstates of  $H^{(0)}$  which also have  $J = 0$ , and that these are labelled by a symbol  $n$ :

$$H^{(0)}|n\rangle = E_n|n\rangle, \quad J|n\rangle = 0. \quad (2.11)$$

Then the  $J'^2$  term in the energy, which is by definition related to the moment of inertia, is

$$\frac{1}{2I} J'^2 = J'^2 \sum_{n \neq 0} \frac{\langle 0|H^{(1)}|n\rangle \langle n|H^{(1)}|0\rangle}{E_0 - E_n} + \frac{1}{2} J'^2 \langle 0|H^{(2)}|0\rangle \quad (2.12)$$

or symbolically

$$\frac{1}{2I} = \langle 0|H^{(1)} \frac{P}{E_0 - H^{(0)}} H^{(1)}|0\rangle + \frac{1}{2} \langle 0|H^{(2)}|0\rangle \quad (2.13)$$

where  $P$  is a projection operator excluding the state  $n = 0$ .

The summation in (2.12) should extend only over those eigenstates of  $H^{(0)}$  which have value zero for the angular momentum operator, but this takes care of itself because  $H^{(1)}$  commutes with  $J$ , so that it has no matrix elements connecting states of different angular momentum. We may therefore leave the sum in (2.12) unrestricted, except for the exclusion of the ground state, for which the denominator would vanish. For the same reason it is in order to take the projection operator  $P$  in (2.13) as excluding only the state  $|0\rangle$ . If the system has time-reversal invariance the projection operator  $P$  is unnecessary since  $H^{(1)}$  is odd under time reversal, so that  $H^{(1)}|0\rangle$  and  $|0\rangle$  must be orthogonal.

Evidently we could have chosen as our initial state some eigenstate of  $H^{(0)}$  with eigenvalue  $E_0$  and any arbitrary value of the angular momentum, since all the operators which occur in the calculation are degenerate. It then follows further that we may also choose a state which is not an eigenstate of angular momentum at all, but any linear combination of such states. The projection operator in (2.13) then again excludes only the initial state.

It is a separate question for what values of  $J'$  the quadratic approximation is adequate and how large are the terms containing higher powers of  $J'$ . Apart from the additional terms in (2.2) which arise from velocity-dependent terms in the internucleon potential, this is a question of the rapidity of convergence of the perturbation series. This is governed by the magnitude of the collective terms  $H^{(1)}$  and  $H^{(2)}$  relative to the energy difference between intrinsic states. This is just what one would expect intuitively from the idea that these higher effects represent a distortion of the nucleus due to the Coriolis and centrifugal forces, the stiffness of the nucleus for deformations being related to its spectrum of intrinsic energy levels. It is quite straightforward to write down higher terms in the perturbation series.

The expression (2.12) makes it particularly evident that it is important not to assume the existence of an angle operator  $\phi$ . If we interpret (2.12) as expressed in the  $J = 0$  representation, the second term in  $H^{(1)}$  in (2.6) vanishes because the operator  $J$  multiplying it has eigenvalue zero. Thus

$$\langle 0|H^{(1)}|n\rangle = \langle 0|H\phi - \phi H|n\rangle.$$

But both  $|0\rangle$  and  $|n\rangle$  have  $J = 0$ , and the first line of (2.6) shows that, acting on such states,  $H$  and  $H^{(0)}$  are identical. Hence the matrix element is also

$$\langle 0|H^{(0)}\phi - \phi H^{(0)}|n\rangle = (E_0 - E_n)\langle 0|\phi|n\rangle.$$

But  $\phi$  commutes with  $H^{(0)}$  and therefore cannot have matrix elements between states belonging to different eigenvalues of this operator. Hence the first term in (2.12) would vanish if  $\phi$  existed as an operator. The remaining term containing  $H^{(2)}$  will later be seen to yield by itself a value for  $I$  close to the 'hydrodynamic' one. It would indeed be very surprising if such a simple result were generally valid.

### 3. The angular operator

The most plausible choice for the directional operator  $B$  introduced in the last section is based on the direction of the major axis of the two-dimensional tensor of inertia:

$$B \equiv e^{2i\phi} = \frac{\Sigma(x_j^2 - y_j^2) + 2i\Sigma x_j y_j}{\{(\Sigma x_j^2 - y_j^2)^2 + 4(\Sigma x_j y_j)^2\}^{1/2}} \equiv \frac{\xi + i\eta}{D^{1/2}} \quad (3.1)$$

where the suffix  $j$  runs over all nucleons. This evidently satisfies the commutation law (2.8).

This function possesses, in principle, a singularity. For configurations in which the tensor of inertia is isotropic both the numerator and the denominator vanish and  $B$  becomes indeterminate. This kind of singularity is hard to avoid for any definition of an angle. It is not likely to be serious for cases in which the concept of rotational states is interesting, because these are cases of fairly heavy and strongly deformed nuclei, for which the probability of finding isotropic configurations should be very small. This complication is certainly negligible if it is permissible to use the approximate method by which we propose to evaluate  $B$ , since the approximation ignores the possibility of such configurations.

Accepting this choice of  $B$ , the operators defined in (2.10) take the form:

$$H^{(0)} = H - J\{\Sigma(x^2 - y^2)\Sigma(xp_y + yp_x) - 2\Sigma xy\Sigma(xp_x - yp_y)\} \frac{1}{MD} + \frac{1}{2}J^2\Sigma(x^2 + y^2) \frac{1}{MD} \quad (3.2)$$

$$H^{(1)} = 2\{\Sigma x^2\Sigma yp_x - \Sigma y^2\Sigma xp_y - \Sigma xy(\Sigma xp_x - \Sigma yp_y)\} \frac{1}{MD} \quad (3.3)$$

$$H^{(2)} = \Sigma(x^2 + y^2) \frac{1}{MD}. \quad (3.4)$$

These expressions are identical with those which would follow from (2.6), not surprisingly, since, while  $\phi$  is ill-defined, its derivatives may be regarded as single-valued. Expressions (3.2) and (3.3) differ in detail from the expressions given by Villars; this is due to a slight algebraic error in Villars' algebra concerning the order of non-commuting factors, but this difference involves no point of principle.

A direct evaluation of the matrix elements of (3.2) to (3.4) would be prohibitively complicated, because of the occurrence of  $D$  in the denominator. We note, however, that this denominator does not depend on the orientation of the tensor of inertia; it is a scalar function of its shape, i.e. of its eigenvalues. It may therefore be expected that the rotation will not substantially affect the value of  $D$ . Variations in  $D$  can come only from vibrational motion and other changes in the intrinsic state. Since these have high excitation energies one may expect that the fluctuations in  $D$  will be small, and this suggests that it may be a reasonable approximation to treat  $D$  as constant and replace it by its average value. This approximation would not, of course, be expected to apply to nuclei near the edge of the region in which the ground states of nuclei are deformed, since there the energy required to change the deformation is small, and fluctuations in the shape may be considerable.

The approximation of treating  $D$  as a constant should certainly not be used in evaluating commutators such as those occurring in (2.10), since the stiffness of the system in resisting shape deformation, on which the approximation relies, implies also that the restoring force, and hence the frequency of such vibrations, is high. The commutators must be computed from the exact expression (3.1), which fortunately is possible, and the approximation for  $D$  used only in the result.

To test the fluctuations of  $D$ , we computed the mean square fluctuation

$$\langle D^2 \rangle - (\langle D \rangle)^2 \quad (3.5)$$

for the ground state of a system of independent nucleons in a deformed harmonic oscillator potential. The calculation was done for a prolate shape, with the axis of symmetry in the  $x$  direction, so that

$$\omega_x = a, \quad \omega_y = \omega_z = b \quad (3.6)$$

with

$$d = a/b < 1. \quad (3.7)$$

We considered only nucleon numbers which were just sufficient to fill one of the sub-shells of the deformed oscillator, in order to avoid the complications of a degenerate ground state. For example, the largest number considered related to a case in which the shells with total quantum number up to 4 were filled, and in addition the sub-shells with  $(n_x, n_y + n_z) = (5, 0)$ ,  $(4, 1)$ ,  $(3, 2)$  and  $(2, 3)$ , respectively, of the main shell with  $n = 5$ .

The results, which were obtained by means of the KDF9 computer of the University of Oxford, are shown in figure 1 against the ratio  $d$  of the frequencies. It should be noted that for the more extreme deformations (small  $d$ ) the filling assumed is not correct, since the highest filled sub-shell has higher energy than some of the sub-shells of the major shell with  $n = 6$ . The deformations for which this occurs are not very realistic, but in any case the correct filling would further reduce the magnitude of the fluctuations. Similarly, it is to be expected that the nucleon-nucleon correlations which are neglected in this

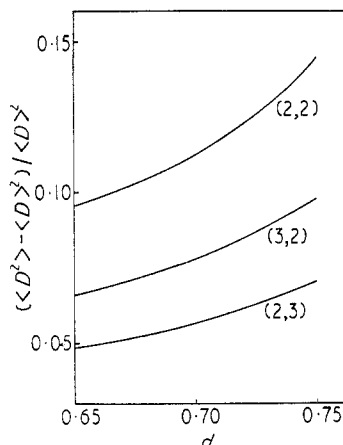


Figure 1. Fluctuation of the shape parameter  $D$  (see equation (3.1)) as a function of the deformation. The labels on the curves indicate the last filled sub-shell.

estimate (apart from those caused by the Pauli principle) would further reduce the result.

We conclude from figure 1 that for not too small nuclei and not too small deformation the fluctuations in  $D$  are reasonably small.

#### 4. Approximate evaluation of the moment of inertia

The moment of inertia is given by (2.12) or (2.13) in which now all the operators are well-defined and, with the aid of the approximation introduced in § 3, manageable. However, the evaluation requires some knowledge of the eigenstates and eigenvalues of the intrinsic Hamiltonian  $H^{(0)}$ .

The most obvious idea would be to use the Hartree–Fock approximation, and to replace the matrix elements of  $H^{(1)}$  in (2.12) by those calculated between the Hartree–Fock ground state and determinants formed from all possible one-particle wave functions in the Hartree–Fock potential. However, this procedure meets with a difficulty, which is particularly obvious for small deformation, i.e. for an almost spherical nucleus.

The excited states,  $|n\rangle$ , occurring in (2.12) will then include states of very low excitation, which differ from the ground state by the transfer of one or more nucleons from the last filled to the lowest empty sub-shell within the same main shell. Such transitions affect predominantly the rotational aspect of the problem, which is supposed to have been eliminated in our construction of the intrinsic Hamiltonian  $H^{(0)}$ . One would not expect to find states of such low intrinsic excitation, but this kind of excitation should be in part contained in the degenerate ground states of  $H^{(0)}$  which, as was discussed in § 2, do not contribute to (2.12), and perhaps in part in the intrinsic excitations, which should have excitation energies comparable with the splitting of the main shells.

The complete orthonormal set of states based on the Hartree–Fock potential does not possess the exact degeneracy required of the eigenstates of  $H^{(0)}$ , and this presumably accounts for the appearance of states of low excitation. Such states are, of course, important for the sum in (2.12) since they occur with small denominators. One possible way to overcome this difficulty would be to omit from (2.12) all terms arising from transitions within the partly filled main shell, on the grounds that such states would in a more exact treatment be degenerate with the ground state. However, this procedure seems rather arbitrary; moreover, it becomes ill-defined for larger deformation, when the spacing of the sub-shells becomes comparable with the spacing of the main shells, or may even exceed it.

To illustrate this point, we carried out calculations in which the Hartree–Fock potential was again replaced by a deformed oscillator potential, which has a very similar structure. If all terms were retained in (2.12) the sum became so large as to exceed the last term, so that the rotational energy became negative. If the transitions within the last main shell



were omitted, one obtained a positive value for the moment of inertia, of a reasonable order of magnitude, but it seems clear that no great reliance can be placed on these results.

Instead, it is preferable to base our evaluation on (2.13) and to deal with our lack of knowledge of the precise eigenstates of the intrinsic Hamiltonian by using a variation principle. We require three pieces of information for the evaluation of (2.13): (i) some approximation to the ground state  $|0\rangle$  of the intrinsic Hamiltonian; (ii) a knowledge of the ground-state energy  $E_0$ ; (iii) some approximation to the Green function  $(E_0 - H^{(0)})^{-1}$ .

As regards (i) it seems likely that the operator whose ground-state expectation value is required in (2.13) is not too sensitive to the precise form of the ground-state wave function, and we shall therefore replace  $|0\rangle$  by a wave function of the Hartree-Fock type, which, for the present purpose, we shall further simplify by using a determinant of harmonic oscillator states, say  $|\chi\rangle$ .

We therefore replace the first term of (2.13) by  $-F_0$ , where

$$F_0 = \langle \chi | H^{(1)} \frac{1}{H^{(0)} - E_0} H^{(1)} | \chi \rangle. \quad (4.1)$$

The projection operator  $P$  in (2.13) may be omitted, provided the symmetry of  $\langle \chi |$  is such that

$$\langle 0 | H^{(1)} | \chi \rangle = 0 \quad (4.2)$$

as is the case for the exact intrinsic ground state  $|0\rangle$ . Since  $H^{(1)}$  changes sign under the transformation  $(x, y, z) \rightarrow (-x, y, z)$  or  $(x, -y, z)$ , this condition is satisfied provided  $|\chi\rangle$  is either even or odd in  $x$  and  $y$  separately. This ensures at the same time that there is no linear term in  $J$  in the perturbation expansion of (2.2a).

We now remark that (4.1) can also be expressed as the value of the functional

$$F(v) = -\langle v | H^{(0)} - E_0 | v \rangle + \langle v | H^{(1)} | \chi \rangle + \langle \chi | H^{(1)} | v \rangle \quad (4.3)$$

for the function  $v$  defined by the equation

$$(H^{(0)} - E_0) | v \rangle = H^{(1)} | \chi \rangle. \quad (4.4)$$

It is easy to verify that (4.4) is also the condition that  $v$  be the function which maximizes the functional (4.3), provided all eigenvalues of  $H^{(0)}$  belonging to the appropriate symmetry lie above  $E_0$ .† The quantity  $F_0$  defined by (4.1) is therefore the maximum of the functional (4.3).

We therefore obtain an approximation to  $F_0$  by maximizing the functional within a suitable class of functions, for which we shall choose a limited number of the Slater determinants of harmonic oscillator functions in the same potential which yields our approximation to the ground-state eigenfunction. If the class of functions within which  $F$  is maximized forms a linear set, the last two terms of (4.3) are equal to each other and equal and opposite to the first at the restricted maximum.

## 5. A numerical example

We have carried out a calculation for a simple example to test the procedure outlined in § 4. The nucleon number chosen for this corresponds to the nucleus  $^{28}\text{Si}$ . Since our method requires a non-singular nucleon-nucleon potential, we have followed Husain (1967) in choosing a Rosenfeld mixture of Gaussian shape:

$$v_{ij} = \tau_i \cdot \tau_j (g^2 + f^2 \sigma_i \cdot \sigma_j) \exp\{-(r_i - r_j)^2\} \quad (5.1)$$

with  $g^2 = 0.424$  and  $f^2 = 0.965$ . The unit of length is 1.791 fermis, and the unit of energy 12.93 mev. These force parameters agree with low-energy nucleon-nucleon scattering data. The force leads to saturation, and would be suitable for a Hartree-Fock-type calculation.

† The same maximum property, which allows one to put a lower bound on the magnitude of the second-order perturbation term for the ground-state energy when the unperturbed ground-state wave function is known, is also derived in a recent paper by Sharma (1967).

The ground-state wave function was taken to be that for a harmonic oscillator well with a prolate deformation, for which 28 particles fill the sub-shells (0, 0), (1, 0), (0, 1), (2, 0) and (1, 1). The number of nucleons is really too small to make the fluctuations of the denominator  $D$  negligible (see § 3), so that our results for this case can be of only preliminary value. The oscillator parameters should then, strictly speaking, be chosen in such a way as to minimize  $\langle \chi | H^{(0)} | \chi \rangle$ . For simplicity we have instead chosen the values given by Husain (1967), which minimize the expectation value of  $H$ .

To obtain the rotational energy of this model, we must first compute the second term in (2.12). This is given by the expectation of (3.4) in which  $D$  will be replaced by its expectation value, as discussed in § 3.

$D$  is in fact very closely related to the velocity distribution for irrotational flow, at least for uniform density and an ellipsoidal shape, and the rotational energy from the second term of (2.12) alone gives a value very close to the 'hydrodynamic' value quoted by Bohr and Mottelson (1953). In our model this second term corresponds to a moment of inertia of

$$I_{\text{hydro}} = 14.2 \quad (5.2)$$

in our units ( $76.2 \times 10^{-50}$  g cm<sup>2</sup>), and we shall express the other term relative to this.

According to (3.3),  $H^{(1)}$  contains only two-nucleon operators and will lead from the initial state  $\chi$  only to states where either one or two nucleons are transferred to higher states. It is therefore reasonable to restrict the trial function  $v$  in (4.3) to be a sum of one-particle, one-hole and two-particle, two-hole states. The largest matrix elements of  $H^{(1)}$  lead from the initial state to states in which one particle has changed its oscillator quantum number in the  $x$  and  $y$  direction by  $\pm 1$  unit each, while its  $z$  vibration is unchanged. We have therefore restricted  $v$  to be a linear combination of these states only. There are 32 such states, but since the operators are independent of spin and charge, there are only eight independent coefficients.

The matrix elements were computed algebraically, and the set of linear equations determining the maximum of (4.3) were solved on the University of Washington computer.

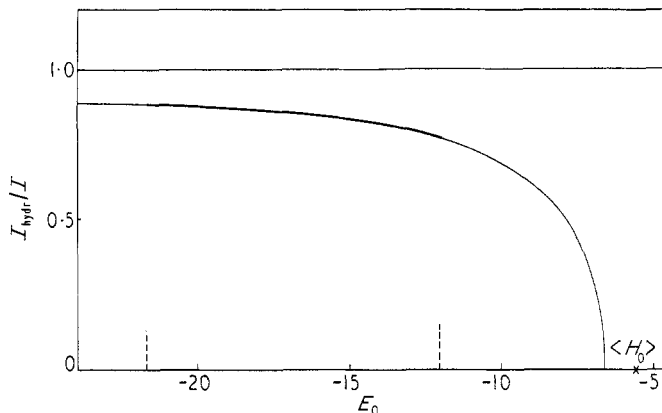


Figure 2. Inverse moment of inertia, compared with the 'hydrodynamic' value, against the ground-state energy  $E_0$ . The heavy part of the curve extends over the likely range of values of  $E_0$  for the model used.

The resulting values of the rotational energy are shown in figure 2 against the value of  $E_0$ , in units of the hydrodynamic value. It is obvious that the curve must approach unity for very low  $E_0$ , since the first term in (2.12) then becomes negligible. For increasing  $E_0$  the curve must go down, approaching  $-\infty$  when  $E_0$  reaches the value of the first intrinsic state with the same symmetry as  $H^{(1)}|\chi\rangle$ .

Finally, we require an estimate of  $E_0$ , the true ground-state eigenvalue of  $H^{(0)}$ . The variational estimate based on the expectation value of  $H^{(0)}$  for our approximate function  $|\chi\rangle$  is too high, and a better estimate could be obtained by correcting this to second order

of perturbation theory. A rough estimate of this second-order correction can be taken from the work of da Providencia (1961), who finds, with a very similar interaction, that the second-order correction for  $^{16}\text{O}$  lies between  $-0.23$  and  $-0.54$  units per particle. This would place the result on the heavy part of the curve in figure 2, leading to a moment of inertia of about 1.2 times the 'hydrodynamic' value. This is rather too low compared with the data for real nuclei, but in view of the preliminary nature of our calculation this is not surprising.

## 6. Discussion

We have shown that the formalism of Villars not only gives in principle an exact expression for the moment of inertia, but that it can be used for an approximate evaluation with a reasonable effort.

Our calculation needs improvements in several respects:

- (i) One must test the effect of widening the subspace of functions included in  $v$ . Because of the variational nature of (4.3), this must increase  $I$ .
- (ii) The calculation should be extended to heavier nuclei, since the approximation of constant  $D$  is only then convincing. One should also test this approximation further by estimating the corrections arising from the fluctuations in  $D$ .
- (iii) One should use a better approximation for the ground-state function  $\chi$  by allowing particularly for pairing correlations.
- (iv) The approximation should ultimately be adapted to the use of realistic, i.e. singular, internucleon potentials.

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