

## NUCLEAR STRUCTURE STUDIES OF $^{20}\text{Ne}$ AND $^{24}\text{Mg}$ IN THE VARIATION-AFTER-PROJECTION HARTREE-FOCK METHOD

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**Abstract:** The variation-after-projection Hartree-Fock method is described. Angular momentum projection algorithms which are practical to use in small and large bases, for axially symmetric as well as asymmetric states, for doubly even, doubly odd as well as odd-even nuclei, are discussed in detail. The method is successfully used to calculate the ground band structures of  $^{20}\text{Ne}$  (axial) and  $^{24}\text{Mg}$  (non-axial), in a five-major-shell basis with the Saunier-Pearson semi-realistic N-N interaction. The operators  $J^2$ ,  $Q_2^0$  and  $R_2^2$  are used as cranking constraints. Level schemes, static moments, E2 transition strengths, charge radii, elastic and inelastic electron scattering form factors are computed for the two nuclei studied. Comparisons are made with experimental data, with results obtained in other microscopic calculations, and with predictions in the rotational model.

### 1. Introduction

The Hartree-Fock approximation (HF)<sup>1)</sup> has been seen recently to be a powerful tool for studying both bulk<sup>2)</sup> and detailed<sup>3)</sup> properties of nuclei. In a study of detailed properties, good angular momentum must be projected from the “intrinsic state” obtained in the Hartree-Fock calculation. One of the important questions arising from the use of angular momentum projected states is whether the projected energy is sensitive to variations in the intrinsic Slater determinant. A search for the lowest projected energy will be called a variation after projection. This contrasts with the usual<sup>1)</sup> deformed HF where only the intrinsic energy is minimized. In this paper the method of variation after projection will be studied in some detail. The method is successfully applied to the study of  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  and the results are reported here.

The two-body nucleon-nucleon potential used here is the semi-realistic interaction<sup>††</sup>

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of Saunier and Pearson <sup>4)</sup>. Since these authors have adopted a somewhat novel point of view we comment briefly on their force.

It is well known that most realistic two-body interactions cannot be used to first order in the HF approximation <sup>5)</sup>. This may be remedied <sup>5, 6)</sup> by using Brueckner's *K*-matrix. The *K*-matrix depends on the two-body potential, on the starting energies and also on the density through the exclusion operator. Saunier and Pearson avoided these complications by renormalizing their velocity-dependent interaction to make it produce a good *first order* account of *nuclear matter* properties. Their interaction no. 2 is used here. It should be viewed as an effective *K*-matrix, where the energy and density dependences have been averaged out. One consequence of this is that the single particle energies are affected <sup>7)</sup>. However other nuclear properties remain essentially unchanged.

The basis Hamiltonian *H* is briefly defined in sect. 2. Sect. 3 outlines the projection method and discusses the choices of the intrinsic Hamiltonians used to vary the intrinsic states whose projected energy is to be obtained. The results obtained for <sup>20</sup>Ne and <sup>24</sup>Mg are presented in sects. 4–6. Results for the axially asymmetric, doubly odd nucleus <sup>22</sup>Na have been reported elsewhere <sup>3)</sup>. Sect. 4 gives results for various cranking operators. Sect. 5 analyses the static electromagnetic properties of <sup>20</sup>Ne and <sup>24</sup>Mg. The elastic and inelastic electron scattering form factors are presented in sect. 6. Sect. 7 provides a comparison with the usual rigid rotator model. Finally, sect. 8 summarizes our results.

## 2. The basic Hamiltonian

The Hamiltonian is defined as

$$H = T_{\text{rel}} + \mathcal{V}_{\text{NN}} + \mathcal{V}_{\text{Coul}} + \mathcal{V}_{\text{s.o.}} \quad (1)$$

Here  $T_{\text{rel}}$  is the kinetic energy operator with respect to the centre of mass (c.m.), and may be expressed as either

$$T_{\text{rel}} = \sum_{i=1}^A \sum_{j=1}^A \frac{1}{4mA} (p_i - p_j)^2, \quad (2a)$$

or

$$T_{\text{rel}} = \sum_{i=1}^A \frac{p_i^2}{2m} \left(1 - \frac{1}{A}\right) - \frac{1}{2mA} \sum_{i=1}^A \sum_{j=1}^A p_i p_j. \quad (2b)$$

These two expressions are formally the same and naturally have the same expectation values. However, due to the asymmetric treatment of the one-body and two-body operators in the HF method, slightly different wave functions are obtained depending on which expression is used. In ref. <sup>2)</sup> eq. (2a) was used for the HF iterations but  $T = \sum_i p_i^2/2m$  was used to calculate the single-particle (s.p.) energies. In this work we use eq. (2b) throughout since it converges to the laboratory kinetic energy operator,  $T$ , where  $A \rightarrow \infty$ . The expectation value of the two-body term in eq. (2b) is always small.

The potential  $\mathcal{V}_{NN}$  is the two-body nuclear interaction and as mentioned in the introduction, is represented here by the semi-realistic, velocity-dependent potential no. 2 of Saunier and Pearson <sup>4</sup>).

The quantity  $\mathcal{V}_{\text{Coul}}$  is the two-body Coulomb interaction between protons,

$$\mathcal{V}_{\text{Coul}} = \sum_{i=1}^Z \sum_{j=i}^Z \frac{e^2}{|r_i - r_j|}.$$

The interaction  $\mathcal{V}_{\text{s.o.}}$  is the approximate <sup>8</sup>) one-body electromagnetic spin-orbit interaction due to the Larmor precession of the nucleons as well as the Thomas precession of the protons in the nuclear electric field <sup>9</sup>). Since  $\mathcal{V}_{\text{s.o.}}$  is a small correction to the total Hamiltonian, the electric field is assumed to come from a uniform charge density of radius  $R = 1.2 A^{1/3}$  fm. Furthermore, since the nucleon may be found inside the nucleus most of the time, we replace the static Coulomb field for  $r > R$  by the expression valid in the interior. We thus obtain

$$\mathcal{V}_{\text{s.o.}}^p = - \sum_{i=1}^Z (g_p - 1) \frac{Ze^2}{2m^2 c^2 R^3} l_i \cdot s_i, \quad (3a)$$

$$\mathcal{V}_{\text{s.o.}}^n = - \sum_{i=1}^N g_n \frac{Ze^2}{2m^2 c^2 R^3} l_i \cdot s_i, \quad (3b)$$

where  $g$  is the gyromagnetic ratio, with  $g_p = 5.5856$  and  $g_n = -3.8263$ . Using eq. (3) we get expectation values of  $-42$  keV and  $+35$  keV for the  $0d_{3/2}$  proton and neutron, respectively, in <sup>16</sup>O. This appears to have an observable effect on the  $0d_{3/2}$  and  $1s_{1/2}$  splitting of the  $A = 17$  system <sup>10</sup>).

### 3. The projected Hartree-Fock method

We divide this section into three parts. After the preliminaries contained in the first part the second part contains a brief description of the principle of variation after projection as used here. The third part is a detailed description of the projection technique we employ. It will be seen that variation after projection involves no greater difficulties than those incurred in performing a sequence of angular momentum projection calculations.

#### 3.1. PRELIMINARIES

The following equations and definitions of symbols are given here for ease of later discussion.

The quantity  $H_1$  is the "intrinsic" Hamiltonian,

$$H_1(\lambda) = H - \sum_c \lambda_c \mathcal{M}_c, \quad (4)$$

where the  $\mathcal{M}_c$  are selected constraint or cranking operators such as  $J^2$ ,  $Q_2$ , etc.,

and the  $\lambda_c$  are the cranking parameters;  $H$  is the basic Hamiltonian defined in sect. 2 and  $H_1(0) \equiv H$ .

The state  $|\chi_I(\lambda)\rangle$  is the intrinsic state or Slater determinantal HF solution corresponding to  $H_1(\lambda)$ ;  $|\chi_I(0)\rangle \equiv |\chi\rangle$  is the solution corresponding to  $H$ . In general  $\chi_I$  is a linear combination of many-body states each having good angular momentum  $J$  and projection  $K$  on the body-fixed  $z$ -axis:

$$|\chi_I\rangle = \sum_{JK} |J(K)K\rangle \equiv \sum_{JK} n_{JK} |J(K)K\rangle. \quad (5)$$

In eq. (5) the kets  $| \rangle$  are *unnormalized*. They have the orthonormal property

$$(J(K)M|J'(K')M') = \delta_{JJ'} \delta_{MM'} N_{KK'}^J. \quad (6)$$

In particular  $N_{KK}^J \equiv |n_{JK}|^2$ . The kets  $| \rangle$  are normalized to unity.

The operator  $\hat{R}(\Omega) \equiv \hat{R}(\alpha, \beta, \gamma)$  is the rotation operator specified by the Euler angles <sup>11)</sup>  $(\alpha, \beta, \gamma)$ . The rotation matrix  $\mathcal{D}(\Omega)$  is defined through

$$\hat{R}(\Omega)|JM\rangle = \sum_N \mathcal{D}_{NM}^J(\Omega)|JN\rangle, \quad (7)$$

where  $\mathcal{D}_{NM}^J(\alpha, \beta, \gamma) = e^{-i(\alpha N + \gamma M)} d_{NM}^J(\beta)$ . The  $d$ -function is that of Brink and Satchler <sup>11)</sup>.

The hermiticity property of the electromagnetic operator is the one proposed by Brink and Rose <sup>12)</sup>,

$$(\mathcal{O}_\lambda^\mu)^\dagger = (-1)^{\lambda-\mu+c} \mathcal{O}_\lambda^{-\mu}, \quad (8)$$

where  $c = 1$  for magnetic multipole operators and  $c = 0$  otherwise.

The phase conventions, the definition of s.p. orbits, the density matrix and the calculations of one- and two-body matrix elements are as described in ref. <sup>2)</sup>.

### 3.2. VARIATION AFTER PROJECTION

In the absence of constraints on the Hamiltonian, the intrinsic state  $|\chi\rangle$  is found through the HF equation

$$\delta\langle\chi|H|\chi\rangle = \delta W = 0. \quad (9)$$

We may use eq. (5) to interpret  $|\chi\rangle$  as the intrinsic state which minimizes a weighted mean of the energies of the  $J$ -projected states, the weight factors being the normalization constants  $N_{KK}^J$ , given in eq. (6). Thus it is not guaranteed that each individual  $J$ -state has minimum energy. The simplest way to find a different intrinsic state, such that energies of some  $J$ -states may have lower values than that projected from  $|\chi\rangle$ , is to use the constrained Hamiltonian  $H_1$ , instead of  $H$ . We do this as follows. For a given set of cranking parameters  $(\lambda)$  we find  $|\chi_I(\lambda)\rangle$  by using the HF variational equation

$$\delta\langle\chi_I(\lambda)|H_1(\lambda)|\chi_I(\lambda)\rangle = 0 \quad (\text{for fixed } \lambda). \quad (10)$$

The energies  $E_J(\lambda)$  of states with good  $J$  are calculated from  $|\chi_I(\lambda)\rangle$ . The optimum

values of  $\lambda$ , for a given  $J$ -state, are then determined by the equations

$$\partial E_J(\lambda)/\partial \lambda_c = 0, \quad \text{all } c. \quad (11)$$

It is clear that there is a large number of linearly independent constraint operators which represent all the variational degrees of freedom of a many-body system; thus, it is not practical to consider all of these operators in our calculation. In fact, only those constraint operators which affect the collective properties need be considered. Only three constraint operators have been used in this work. These are  $J^2$ , and the quadrupole operators  $Q_2^0$  and  $Q_2^2$ . Their significance will be discussed later.

The calculation of  $E_J(\lambda)$ , together with some other physically interesting quantities, is discussed in subsect. 3.3.

### 3.3. THE PROJECTION TECHNIQUE

It was seen in ref. <sup>2)</sup> that the basis used for the HF calculation includes the first five harmonic oscillator major shells plus the  $1h_{3/2}$  state of the  $N = 5$  shell. Altogether, then, there are 16 different  $j$ -shells in the basis. Furthermore in order to treat odd, doubly odd, and doubly even nuclei, as well as electromagnetic multipole operators and scalar operators on an equal footing, the use of complex arithmetic is mandatory. These conditions necessitate the use of the most efficient angular momentum projection method. We now describe our choice for this method.

For any spherical tensor operator  $\hat{\mathcal{O}}_\lambda^\mu$ , it is easy to derive from eq. (5) and the properties of the rotation matrix, the following generalized *sum rule*

$$\langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu R(\Omega) | \chi_1 \rangle = \sum_{JK} \sum_{J'K'} C_{K'-\mu, \mu, K'}^{J\lambda J'} \mathcal{D}_{K'-\mu, K}^J(\Omega) (J'(K') || \mathcal{O}_\lambda || J(K)). \quad (12)$$

The double-barred quantity on the right hand side in (12) is the reduced matrix element <sup>11)</sup> and  $C_{\alpha\beta\gamma}^{abc} \equiv \langle ab\alpha\beta | c\gamma \rangle$  is a Clebsch-Gordan coefficient. The inverse of (12) is then the generalized Hill-Wheeler integral of Peierls and Yoccoz <sup>13)</sup>,

$$(J'(K') || \mathcal{O}_\lambda || J(K)) = \frac{2J+1}{8\pi^2} \sum_{\mu=-\lambda}^{\lambda} C_{K'-\mu, \mu, K'}^{J\lambda J'} \int d^3\Omega \mathcal{D}_{K'-\mu, K}^{J*}(\Omega) \langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\Omega) | \chi_1 \rangle. \quad (13)$$

Eqs. (12) and (13) are the two basic equations for projection.

One of the two conditions we impose on the s.p. density is that  $|\chi_1\rangle$  be expressed in the principal axis system of the mass quadrupole tensor; furthermore  $|\chi_1\rangle$ , together with its time-reversed state,  $T|\chi_1\rangle$ , must have the four-group ( $D_2$ ) symmetry. (The other condition is that the proton and neutron numbers be separately conserved.) Following Bar-Touv and Kelson <sup>14)</sup>, this symmetry is insured by dividing the Hilbert space into subspaces which are mutual time-reversal conjugates and expanding any s.p. wave function in either one of these subspaces. An immediate consequence of this is that in the expansion (5) all  $K$  must differ by an *even* integer. Namely

$$|\chi_1\rangle = \sum_{K=1,3,5,\dots}^{K_{\max}} \sum_{J=|K|}^{J_{\max}} |J(K)K\rangle. \quad (5')$$

This property is important and is one of the keys to our projection technique.

Returning now to eq. (13) it is seen that, in order to extract the reduced matrix elements a three-dimensional integration over the Euler angles  $(\alpha, \beta, \gamma)$  must be performed. Only when considering axially symmetric  $\chi_1$  can the integration be greatly simplified<sup>13</sup>, since in this case there is only one  $K$  in the sum in (5') and the integrations over  $\alpha$  and  $\gamma$  can be carried out analytically. In general this reduction is not possible. A brute force three-dimensional numerical integration should, however, be avoided at all costs because in a large basis such as ours, the calculation of the integrand in (13), or more precisely  $\langle \chi_1 | \hat{\mathcal{O}} \hat{R}(\Omega) | \chi_1 \rangle$ , is very time consuming. The computation time is roughly proportional to  $N^4$  if  $\hat{\mathcal{O}}$  is a two-body operator, and to  $N^2 A^2$  if  $\hat{\mathcal{O}}$  is a one- or zero-body operator. Here  $N$  is the number (82 in this work) of s.p. oscillator states in the basis, and  $A$  is the particle number. In addition, there is *no* guarantee of accuracy if this approach is taken.

We replace the three integrals in (13) by

$$\frac{1}{2\pi} \int_0^{2\pi} f(\alpha) d\alpha \rightarrow \frac{1}{m'} \sum_{r=0}^{m'-1} f\left(\frac{r\pi}{m'}\right), \quad (14a)$$

$$\frac{1}{2\pi} \int_0^{2\pi} f(\gamma) d\gamma \rightarrow \frac{1}{m} \sum_{r=0}^{m-1} f\left(\frac{r\pi}{m}\right), \quad (14b)$$

$$\int_{-1}^{+1} f(x) dx \rightarrow \sum_{i=1}^{N_\beta} f(x_i) w_i, \quad x = \cos \beta, \quad (14c)$$

where  $m$  and  $m'$  are the number of  $K$ -bands in  $|\chi_1\rangle$  and  $|\chi_1'\rangle$  respectively,  $m = \frac{1}{2}(K_{\max} - K_{\min}) + 1$ ,  $m' = \frac{1}{2}(K'_{\max} - K'_{\min}) + 1$ ,  $N_\beta$  is the smallest integer not less than  $\frac{1}{2}(J_{\max} + J'_{\max}) + 1$ , and  $x_i$  and  $w_i$  are nodes and weight of the  $N_\beta$ -point Gaussian quadratures. It can be shown that the replacement (14) is *exact* to the extent that the finite expansion in (5') is exact. The replacement (14a, b) is sufficient because of the identity

$$\frac{1}{m} \sum_{r=0}^{m-1} \exp\left(i \frac{2kr\pi}{m}\right) = \delta_{k,0}, \quad k = 0, 1, \dots, m-1. \quad (15)$$

By substituting (12) into (13) it is easily verified that the integrand relevant to the integration over  $\alpha$  has the form  $\sum_i e^{i2k'_i\alpha}$ , where  $k'_i = \frac{1}{2}(K' - K'_i)$ ,  $K'_{\min} \leq K'_i \leq K'_{\max}$ . From (14a) and (15) the term  $K'_i = K'$  is then projected out. A similar argument can be made for the  $\gamma$ -integral. It is seen that if the  $\Delta K = \text{even}$  integer restriction mentioned earlier were not realized, the number of  $\alpha$ -angles at which the integrand is to be evaluated would be almost doubled since we must then let  $m' = K'_{\max} - K'_{\min} + 1$ , etc. Also, the equation (14c) is adequate because the integrand in (13) is a polynomial in  $\cos \beta$  of order  $J_{\max} + J'_{\max}$  if (and only if)  $\Delta K = \text{even}$  integer.

It is now clear that, in order to make use of eq. (14), one must first determine what  $K$ -bands are present in a given  $|\chi_1\rangle$ . This is done via a preliminary  $K$ -projection to

determine  $n_K$  in

$$|\chi_1\rangle = \sum_K n_K |\chi_1(K)K\rangle, \quad \sum_K n_K^2 = 1, \quad (16)$$

where, from (5),

$$n_K |\chi_1(K)K\rangle \equiv \sum_J n_{JK} |J(K)K\rangle, \quad \sum_J n_{JK}^2 = n_K^2. \quad (17)$$

It is easily verified that

$$n_K^2 = \frac{1}{2\pi} \int_0^{2\pi} d\alpha e^{iK\alpha} \langle \chi_1 | \hat{R}(\alpha, 0, 0) | \chi_1 \rangle. \quad (18)$$

The integrand of eq. (18) is relatively easy to compute, thus any reasonable method can be used to do the integration. In practice we truncate the sum over  $K$ , in (16), so that  $\sum_K n_K^2 \geq 0.995$ . These  $K$  are then included in the formal expansion (5'), and taken into account in eqs. (14a, b). For the  $\beta$ -integration we use  $N_\beta = 16$  Gaussian points. This is sufficient for all  $|\chi_1\rangle$  containing  $J_{\max} \leq \frac{3}{2}$ . We see, from the above discussion, that the reduced matrix elements of any tensor operator can be accurately calculated by evaluating the integrand in (13) at  $N_\Omega = mm'N_\beta$  sets of Euler angles. We now show that this expression for  $N_\Omega$  is an upper limit, which in most cases can be reduced through judicious use of the symmetry properties of the  $|\chi_1\rangle$  involved. To illustrate this we consider the simpler case where  $|\chi_1'\rangle = |\chi_1\rangle$ . We have from eq. (8)

$$\langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\alpha\beta\gamma) | \chi_1 \rangle = (-1)^{i+c} \sum_{\mu'} \mathcal{D}_{\mu', -\mu}^\lambda(\gamma\beta\alpha) \langle \chi_1 | \hat{\mathcal{O}}_\lambda^{-\mu'} \hat{R}(\gamma\beta\alpha) | \chi_1 \rangle, \quad (19)$$

thus reducing  $N_\Omega$  to  $\frac{1}{2}m(m+1)N_\beta$ . If in addition,  $|\chi_1\rangle$  is *invariant* under the four-group, then the identities

$$\langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\alpha\beta\gamma) | \chi_1 \rangle = (-1)^\mu \langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\alpha, \pi - \beta, \pi - \gamma) | \chi_1 \rangle \quad (20a)$$

$$= (-1)^\mu \langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\alpha, \pi - \beta, -\gamma) | \chi_1 \rangle \quad (20b)$$

$$= \langle \chi_1 | \hat{\mathcal{O}}_\lambda^\mu \hat{R}(\pi - \alpha, \pi - \beta, \gamma) | \chi_1 \rangle^* \quad (20c)$$

will further reduce the number of essential angles to  $\frac{1}{4}(m+1)^2[N_\beta/2]$ , where  $[x]$  is the smallest integer not less than  $x$ . It should be pointed out that a four-group invariant, non-axially symmetric  $|\chi_1\rangle$  contains  $K = -K_0, -K_0+2, \dots, 0, \dots, K_0$ ,  $K_0 = K_{\max} = -K_{\min}$ , in such a way that the  $K$  and  $-K$  bands are not distinct. In this case the number of bands in  $|\chi_1\rangle$  is  $m = K_0 + 1$ , but the number of *independent* bands is  $\frac{1}{2}(m+1)$ .

For any given  $|\chi_1\rangle$  the lower limit of  $N_\Omega$  is always given by the number of non-zero and independent matrix elements  $\langle J'(K') || \mathcal{O} || J(K) \rangle$  of a scalar operator  $\hat{\mathcal{O}}$ . If we call this number  $N_<$ , the ratio  $N_</N_\Omega \leq 1$  is then a measure of the efficiency of the projection method. The efficiencies of the present method for some typical doubly even, doubly odd and even-odd nuclei are shown in table 1. We see that for an axial nucleus with  $K = K_{\min} = 0$  or  $\pm\frac{1}{2}$ , the efficiency is 1. In fact the efficiency can be

made to be 1 for any axial  $|\chi_1\rangle$  with any  $K$  since, in this case, the integrand in (13) (taken for  $|\chi'_1\rangle = |\chi_1\rangle$ ) has the form  $x^{2|K|}P(x)$ , where  $x = \cos \beta$  and  $P(x)$  is a polynomial of order  $2(J-|K|)$ . This last property is however not reflected in table 1 because it was not used in the actual computer code.

TABLE 1  
Examples of efficiency ratio  $N_</N_\Omega$  for the projection method ( $N_\beta = 16$ )

| Case | Type <sup>a)</sup> | Symmetry <sup>a)</sup> | $K_{\min}$     | $K_{\max}$    | $m$ | $J_{\max}$ <sup>b)</sup> | $N_<$ <sup>c)</sup> | $N_\Omega$ <sup>d)</sup> | $N_</N_\Omega$ |
|------|--------------------|------------------------|----------------|---------------|-----|--------------------------|---------------------|--------------------------|----------------|
| 1    | e-e                | A, IV                  | 0              |               | 1   | 14                       | 8                   | 8                        | 1              |
| 2    | e-e                | NA, IV                 | -6             | 6             | 7   | 15                       | 104                 | 128                      | 0.81           |
| 3    | o-o                | A                      | 0              |               | 1   | 15                       | 16                  | 16                       | 1              |
| 4    | o-o                | A                      | 3              |               | 1   | 15                       | 13                  | 16                       | 0.81           |
| 5    | o-o                | NA                     | -1             | 3             | 3   | 15                       | 84                  | 96                       | 0.88           |
| 6    | o-e                | A                      | $\frac{1}{2}$  |               | 1   | $\frac{31}{2}$           | 16                  | 16                       | 1              |
| 7    | o-e                | NA                     | $-\frac{5}{2}$ | $\frac{7}{2}$ | 4   | $\frac{31}{2}$           | 140                 | 160                      | 0.88           |

<sup>a)</sup> The symbols have the following meaning: e - even, o - odd (proton-neutron number), A - axial, NA - non-axial, IV - four-group invariant.

<sup>b)</sup> Assume  $J_{\max}$  to be as large as possible, but no greater than  $\frac{31}{2}$ .

<sup>c)</sup> For the enumeration of non-zero reduced matrix elements see ref. <sup>15)</sup>.

<sup>d)</sup> For e-e,  $N_\Omega = \frac{1}{8}(m+1)^2 N_\beta$ ,  $N_\Omega = \frac{1}{2}m(m+1)N_\beta$  otherwise.

A projection method, very similar to the one described here, was proposed by Raynal <sup>14)</sup>. The main difference between his method and ours is that Raynal did not take advantage of the fact that the integrand in (13) is a polynomial in  $\cos \beta$  of finite order. Consequently instead of using the nodes of Gaussian quadratures random values for  $\beta$  were used. This necessitates the solving of sets of simultaneous equations successively which not only is less transparent than the direct summation proposed here but may also lead to numerical difficulties [such as would arise when  $\beta = \frac{1}{2}\pi$  is used <sup>14)</sup>].

So far we have only discussed the use of the symmetries in the case  $|\chi'_1\rangle = |\chi_1\rangle$ . The generalization of eq. (11) for the cases  $|\chi'_1\rangle \neq |\chi_1\rangle$  is straightforward when one of  $|\chi_1\rangle$  and  $|\chi'_1\rangle$  is or both are four-group invariant.

We now consider the computation of the matrix element  $\langle \chi'_1 | \hat{\mathcal{O}}^\mu \hat{R}(\Omega) | \chi_1 \rangle$ . Löwdin <sup>16)</sup> has shown that the matrix element of any many-body operator between two Slater determinants  $|\chi\rangle$  and  $|\chi'\rangle$  can be obtained from the overlap  $D$  and the "cross-density" matrix  $\rho^*$ , defined as follows:

$$D \equiv \langle \chi' | \chi \rangle, \quad \rho_{\alpha\beta}^* \equiv \langle \chi' | c_\beta^\dagger c_\alpha | \chi \rangle / D. \quad (21)$$

Here, as in ref. <sup>2)</sup>,  $\alpha, \beta$  are the labels of our basis s.p. states. In terms of these states the  $\mu$ th occupied state in  $|\chi\rangle$  and the  $v$ th occupied state in  $|\chi'\rangle$  are expanded as

$$|\mu\rangle = \sum_\alpha u_{\alpha\mu} |\alpha\rangle, \quad |v\rangle = \sum_\alpha v_{\alpha v} |\alpha\rangle.$$

We then find

$$D = \det(d_{\mu\nu}), \quad (22)$$

and

$$\rho_{\alpha\beta}^{\times} = \sum_{\nu\mu} u_{\alpha\nu}(d^{-1})_{\nu\mu}(v^{\dagger})_{\mu\beta}, \quad (23)$$

where the matrix  $d$  has elements

$$d_{\mu\nu} = \sum_{\alpha} v_{\alpha\mu}^* u_{\alpha\nu} = \sum_{\alpha} (v^{\dagger})_{\mu\alpha} u_{\alpha\nu}. \quad (24)$$

It can be easily verified that  $\rho^{\times}$  has the usual properties of a density matrix, namely that  $\rho^{\times} \cdot \rho^{\times} = \rho^{\times}$  and  $\text{Tr } \rho^{\times} = A$ , the number of particles. If  $\mathcal{O}^{(1)}$  is any one-body operator and  $\mathcal{O}^{(2)}$  is any two-body operator, we find

$$\langle \chi' | \hat{\mathcal{O}}^{(1)} | \chi \rangle = D \sum_{\alpha\beta} \mathcal{O}_{\alpha\beta}^{(1)} \rho_{\beta\alpha}^{\times}, \quad (25a)$$

$$\langle \chi' | \hat{\mathcal{O}}^{(2)} | \chi \rangle = \frac{1}{2} D \sum_{\alpha\beta\gamma\delta} \mathcal{O}_{\alpha\beta\gamma\delta}^{(2)} \rho_{\gamma\alpha}^{\times} \rho_{\delta\beta}^{\times}, \quad (25b)$$

where  $\mathcal{O}_{\alpha\beta\gamma\delta}^{(2)}$  is antisymmetrized. Eqs. (21)–(25) can be used for our purpose if we let  $|\chi\rangle = \hat{R}(\Omega)|\chi_1\rangle \equiv |\chi_1(\Omega)\rangle$  and  $|\chi'\rangle = |\chi_1'\rangle$ . Instead of the  $u$  above we now use

$$u_{\alpha\mu}(\Omega) = \sum_{\beta} \mathcal{D}_{\alpha\beta}(\Omega) u_{\beta\mu}, \quad (26)$$

where  $\mathcal{D}_{\alpha\beta}(\Omega) = \delta_{j_{\alpha}j_{\beta}} \mathcal{D}_{m_{\alpha}m_{\beta}}^{j_{\alpha}}(\Omega)$  is the appropriate rotation matrix element. The expressions in eq. (25) are easily evaluated except when  $D = 0$ . However if  $|\chi\rangle$  and  $|\chi'\rangle$  are orthogonal by less than two orbitals a numerical scheme can be devised so that l'Hospital's rule is accurately simulated, and eq. (25) remains valid.

For an axial  $|\chi_1\rangle$ , the calculation of the *unnormalized* reduced matrix elements  $(J'(K')||\mathcal{O}_{\lambda}||J(K))$  essentially concludes the computation, since the *normalized* reduced matrix elements are simply obtained as

$$\langle J'(K')||\mathcal{O}_{\lambda}||J(K) \rangle = (J'(K')||\mathcal{O}_{\lambda}||J(K))/n_{J'K'}n_{JK} \quad (27)$$

and  $n_{JK}^2 = N_{KK}^J$ , where

$$N_{K'K}^J \equiv (J(K')|J(K)) = (J(K')||1||J(K)), \quad (28)$$

1 being the identity. Thus, for example, the projected energy for a  $J(K)$  state of an axial  $|\chi_1\rangle$  is

$$E_{J(K)} = H_{KK}^J/N_{KK}^J, \quad H_{K'K}^J \equiv (J(K')||H||J(K)). \quad (29)$$

For a non-axial  $|\chi_1\rangle$ , neither  $H^J$  nor  $N^J$  are in general diagonal in  $K$ , thus  $K$  is generally not a good quantum number. This leads to the following secular equation<sup>17)</sup> for each  $J$ :

$$\sum_{K'} (H_{KK'}^J X_{K'}^{J\sigma} - N_{KK'}^J X_{K'}^{J\sigma} E_{J\sigma}) = 0, \quad (30)$$

which can be solved by first diagonalizing  $N_{KK'}^J$ , then normalizing and finally diag-

normalizing the transformed Hamiltonian matrix in the new orthonormal basis. This results in the  $K$ -mixed states,

$$|J(\sigma)M\rangle = \sum_K X_K^{J\sigma} |J(K)M\rangle = \sum_K x_K^{J\sigma} |J(K)M\rangle, \quad (31)$$

where  $x_K^{J\sigma} \equiv X_K^{J\sigma} n_{JK}$ . The normalization condition is

$$\sum_{KK'} X_{K'}^{J\sigma'*} N_{K'K}^J X_K^{J\sigma} = \delta_{\sigma'\sigma}. \quad (32)$$

The eigenvalues,  $E_{J\sigma}$ , and the normalized reduced matrix elements

$$\langle J'(\sigma') || \mathcal{O}_\lambda || J(\sigma) \rangle = \sum_{KK'} X_{K'}^{J'\sigma'*} (J'(K') || \mathcal{O}_\lambda || J(K)) X_K^{J\sigma} \quad (33)$$

are the quantities we shall use to compare with experimental data.

The accuracy of the projection procedure can be checked by computing the reduced matrix elements of the two-body scalar  $J^2$ , or more easily, the one-body vector  $J$ , both of which have known reduced matrix elements. A *sum rule*, which is eq. (12) specialised to  $\Omega = 0$ ,

$$\langle \chi_I | \hat{\mathcal{O}}_\lambda^\mu | \chi_I \rangle = \sum_{JJ', K'-K=\mu} C_{K\mu K'}^{J\lambda J'} (J'(K') || \mathcal{O}_\lambda || J(K)), \quad (12')$$

can also be used as an internal consistency check. With  $N_\beta = 16$ , we find the accuracy to be better than one part in  $10^7$ , for all axial  $|\chi_I\rangle$ .

For non-axial doubly even nuclei with  $A \leq 24$ , it was found that four or fewer (independent)  $K$ -bands would usually give an accuracy which was better than  $10^{-6}$ , for states with  $J \leq 4$ ; an accuracy of  $10^{-5}$  was found for states with higher  $J$ . For doubly odd and odd-even, non-axial nuclei the accuracy was a factor of ten to one hundred worse than for doubly even nuclei.

In the following sections, we shall discuss results obtained for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$ , using the methods described above. A systematic study of light nuclei using the PHF method will be reported elsewhere.

#### 4. Results of the variation after projection

Our first example of the method of variation after projection (VPHF) is concerned with the subtraction of the rotational energy in the intrinsic state. Namely, we consider the constrained Hamiltonian

$$H_I(\lambda) = H - \lambda J^2. \quad (34)$$

We may view  $\lambda$  as a variational parameter; for each projected state of energy and spin  $E_J(\lambda)$ , the value of  $\lambda$  may be determined by demanding  $\partial E_J(\lambda)/\partial \lambda = 0$ , as mentioned earlier. The results for the axially symmetric nucleus,  $^{20}\text{Ne}$ , are shown in fig. 1. We see that the optimum value of  $\lambda$  for the  $0^+$  state is  $\approx 0.4$  MeV. This value gradually decreases with increasing spin, and is  $\approx 0.15$  MeV for the  $8^+$  state. How-

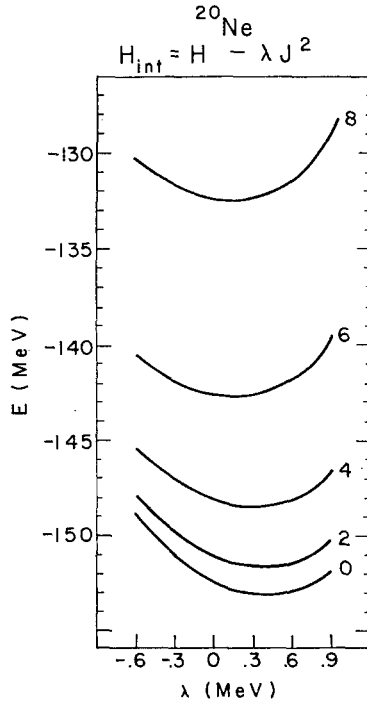


Fig. 1. Projected binding energies of the ground state rotational band of  $^{20}\text{Ne}$ , versus the moment of inertia parameter  $\lambda$  used in the constrained Hamiltonian  $H_I = H - \lambda J^2$ .

ever, in the range  $0.15 \leq \lambda \leq 0.4$ , the energies  $E_J(\lambda)$  vary very smoothly, and do not change by more than 500 keV. Therefore a median value of  $\lambda = 0.27$  MeV for all spins was adopted for the exploration of the other degrees of freedom.

The Hamiltonian used in eq. (34) has another important feature. If we know the spectrum of  $H$  to be rotational, i.e.  $E_J = E_0 + J(J+1)/2\mathcal{I}$ , where  $\mathcal{I}\hbar^2$  is the moment of inertia of the system, then the spectrum calculated with  $H_I(\lambda)$  will be degenerate if we use  $\lambda = 1/2\mathcal{I}$ . Villars<sup>18)</sup> has shown that the exploitation of this property leads to the Thouless-Valatin estimate<sup>19)</sup> of  $\mathcal{I}$ . This estimate does not require a projection calculation, but restricts us to a pure rotational spectrum. Since we already have the projected spectrum here, we may ask whether it is indeed purely rotational. Fig. 2 shows the excitation energies plotted versus  $J(J+1)$ . The plot would be a straight line if the spectrum were rotational. We see that this is not the case either experimentally or theoretically. However, whereas the slope of the experimental curve decreases with spin, all theoretical curves have curvatures of the *opposite* sign. The theoretical spectrum comes closest to being rotational when  $\lambda = 0.27$  MeV, in which case all energies, except that of the  $8^+$  state, fall on a straight line. Presumably this happens because at  $\lambda = 0.27$   $H_I(\lambda)$  is close to being intrinsic<sup>18)</sup>, namely  $\lambda \cong 1/2\mathcal{I}$ . This value of  $\lambda$  corresponds to a moment of inertia of  $90.1 \text{ fm}^2$

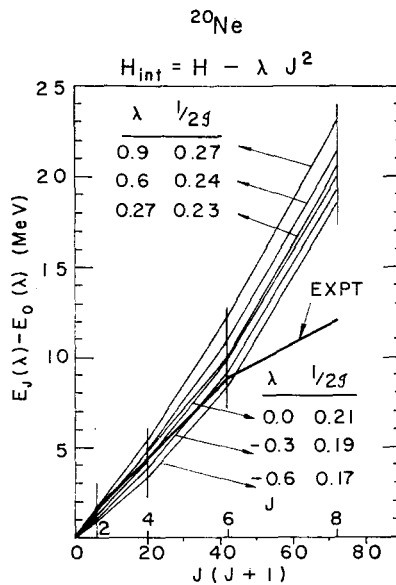


Fig. 2. Calculated excitation energies (thin lines) of  $^{20}\text{Ne}$ , plotted against  $J(J+1)$ , for various values of the moment of inertia parameter  $\lambda$ . The values listed for  $1/2J$  are the slopes of the corresponding theoretical lines at the origin. If the line were straight, then  $J\hbar^2$  would be the moment of inertia of the nucleus. We note that the theoretical line is straight only when  $\lambda = 0.27$ ,  $1/2J = 0.23$ , up to  $J = 6$ . The thick line represents the observed spectrum.

$m_N$ , as compared to the rigid-body value of  $111 \text{ fm}^2 m_N$ , calculated from  $\mathcal{J}_{\text{rig}} = \langle \sum_i^A (x_i^2 + z_i^2) \rangle m_N$ , with  $m_N$  being the mean nucleon mass. The ratio  $\mathcal{J}/\mathcal{J}_{\text{rig}} = 0.81$  lies between one and the value  $(45/16\pi)\beta^2 = 0.18$  ( $\beta = 0.45$ ) obtained by assuming irrotational fluid motions inside the nucleus. The experimental value for  $1/2J$  is 0.27 MeV or 0.21 MeV, depending on whether it is calculated from the excitation energy of the  $2^+$  (1.63 MeV) state or that of the  $4^+$  (4.25 MeV) state.

The fact that the error in the projected energy increases with  $J$  suggests that perhaps the high spin states cannot be represented by a single Slater determinant, or that the N-N interaction used here is inadequate, or that there are terms of importance in the intrinsic Hamiltonian which have not yet been included. The success of recent large scale shell model calculations using effective  $^{20})$  or renormalized realistic  $^{21})$  interactions certainly lends support to the first two possibilities. An obvious change to the intrinsic Hamiltonian would be to include terms which result from vibrational and rotational-vibrational interactions. For an axial quadrupole vibrating about an equilibrium value  $q_0$ , the collective potential energy would be proportional to  $(Q_2^0 - q_0)^2$ . The lowest order non-constant term in this expression is  $\propto Q_2^0$ , the one-body mass-quadrupole operator. This suggests that we use a constrained Hamiltonian

$$H_1 = H - 0.27J^2 - \lambda Q_2^0. \quad (35)$$

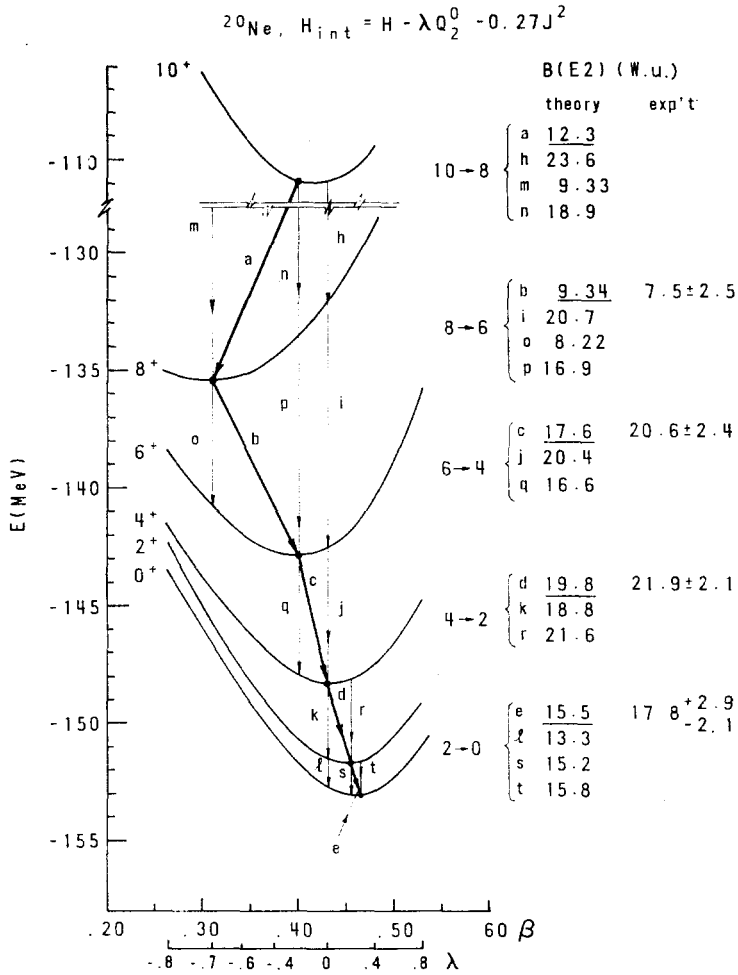


Fig. 3. Projected energies of the ground band of  $^{20}\text{Ne}$ , versus the mass quadrupole cranking parameter  $\lambda$ , used in the intrinsic Hamiltonian  $H_1 = H - 0.27J^2 - \lambda Q_2^0$ . The abscissa is linear in  $\beta$ , the mass quadrupole deformation parameter<sup>2)</sup>. We also give  $B(E2)$  values in Weisskopf units (1 W.u. =  $3.23 e^2 \cdot \text{fm}^4$ ) for the transitions indicated by lettered arrows. The agreement with experiment is good for the transitions b, c, d, e, which occur between states at the energy minima.

This was done for  $^{20}\text{Ne}$  and the results are shown in fig. 3, where the binding energies are plotted against  $\beta$  (as well as against  $\lambda$ ), the quadrupole deformation parameter, defined in ref. <sup>2)</sup>. Compared to energies obtained using  $H_1 = H - 0.27J^2$  ( $\lambda = 0$  in fig. 3) only 350 keV is gained in the ground state, but 3.79 MeV is gained in the  $8^+$  state. Thus, the predicted level spacing has improved, as seen in the fourth column of table 2. However the excitation energy of the  $8^+$  state is still 5.8 MeV too high<sup>22)</sup>.

It is interesting to observe, in fig. 3, that the deformation decreases with increasing spin from the  $0^+$  to the  $8^+$  state. (The  $10^+$  state has components mainly outside of the

TABLE 2  
Properties of the ground state rotational band of  $^{20}\text{Ne}$

| $J^\pi$ | $\lambda^a)$ | $E$ (MeV)       |       | $\langle Q_2 \rangle$      |        | $\langle Q_4 \rangle$      |        | $\langle r^2 \rangle^{\frac{1}{2}}_{\text{proton}}$ |       | $B(E2; J \rightarrow J-2)$ |                                 |
|---------|--------------|-----------------|-------|----------------------------|--------|----------------------------|--------|-----------------------------------------------------|-------|----------------------------|---------------------------------|
|         |              |                 |       | $(e \cdot \text{fm}^2)^c)$ |        | $(e \cdot \text{fm}^4)^c)$ |        |                                                     |       | $(\text{W.u.})^d)$         |                                 |
|         |              | VPHF exp. $^b)$ |       | int.                       | static | int.                       | static | c.m.                                                | lab   | VPHF                       | exp. $^e)$                      |
| $0^+$   | 0.25         | 0               | 0     | 23.7                       | 0      | 164                        | 0      | 2.678                                               | 2.718 |                            |                                 |
| $2^+$   | 0.20         | 1.41            | 1.63  | 23.3                       | - 7.71 | 161                        | 9.72   | 2.673                                               | 2.713 | 15.5                       | $17.8 \pm \overset{+2.9}{-2.1}$ |
| $4^+$   | 0            | 4.75            | 4.25  | 21.6                       | - 8.49 | 149                        | 23.9   | 2.655                                               | 2.695 | 19.8                       | $21.9 \pm 2.1$                  |
| $6^+$   | -0.30        | 10.3            | 8.78  | 19.6                       | - 8.60 | 135                        | 30.1   | 2.635                                               | 2.675 | 17.6                       | $20.6 \pm 2.4$                  |
| $8^+$   | -0.70        | 17.7            | 11.95 | 14.9                       | - 7.49 | 114                        | 26.5   | 2.606                                               | 2.646 | 9.34                       | $7.5 \pm 2.5$                   |
| $10^+$  | -0.30        | 42.1            |       | 19.6                       | -10.1  | 135                        | 43.8   | 2.674                                               | 2.714 | 12.3                       |                                 |

$^a)$  This is used in  $H_1 = H - 0.27 J^2 - \lambda Q_2^0$ .

$^b)$  Ref.  $^{21})$ .

$^c)$   $Q_\lambda^\mu = [4\pi/(2\lambda+1)]^{1/2} \sum_{i=\text{proton}} r_i^\lambda Y_\lambda^\mu(\theta_i, \phi_i)$ ,  $\langle Q_2^0 \rangle_{\text{int}} = \langle \chi_1 | Q_2^0 | \chi_1 \rangle$ .

$^d)$  1 W.u. =  $3.23 e^2 \cdot \text{fm}^4$ .

$^e)$  Ref.  $^{29})$ .

TABLE 3  
Some constrained HF results for  $^{20}\text{Ne}$ , with  $H_1 = H - \lambda Q_2^0 - \mu J^2$

| $(\lambda, \mu)$                           | (0, 0)  | (0, 0.27) | (0.25, 0.27) |
|--------------------------------------------|---------|-----------|--------------|
| $\langle J^2 \rangle_1$                    | 19.54   | 21.49     | 22.48        |
| $\langle Q_2^0 \rangle_1$ (fm $^2$ ) $^a)$ | 42.00   | 42.15     | 47.06        |
| $\langle H \rangle_1$ (MeV)                | -147.63 | -147.37   | -146.78      |
| $E_{0+}$ (MeV)                             | -152.22 | -152.73   | -153.08      |
| $E_{0+} - \langle H \rangle_1$ (MeV)       | -4.59   | -5.36     | -6.30        |

$^a)$  Intrinsic mass quadrupole moment.

s-d shell and is not expected to behave the same as the rest of the band.) This phenomenon has an important effect on the predicted  $B(E2)$  values, which will be discussed in detail in a later section. We only mention here that due to the decreased deformation, the high spin states are expected to be more sensitive to vibrational correlations; these in turn should decrease the high spin energies relative to the lower one.

We conclude our discussion of the energetics of  $^{20}\text{Ne}$ , in table 3, by showing the variation of the expectation values  $\langle J^2 \rangle_1$ ,  $\langle Q_2^0 \rangle_1$  and  $\langle H \rangle_1$ , and the ground state energy  $E_{0+}$ , with the constraint parameters  $\lambda$  and  $\mu$  in  $H_1 = H - \mu J^2 - \lambda Q_2^0$ . We notice that  $\langle J^2 \rangle \approx 20$ , a rather small value. This is part of the reason why the projected spectrum is not quite rotational. We also note that although the intrinsic energy has its minimum at  $(\lambda, \mu) = (0, 0)$ , the energy gain upon projection,  $\langle H \rangle_1 - E_{0+}$ , increases from 4.59 MeV at (0, 0) to 6.30 MeV at (0.25, 0.27), so that the loss of 0.85 MeV of intrinsic binding energy is overcome and a net slight gain of 0.86 MeV in projected energy is actually achieved. Since, however, this gain is minimal we prefer

to think that it is the improved theoretical level spacings and  $B(E2)$  values which make the effort of going to non-zero  $(\lambda, \mu)$  worthwhile.

We now turn to our  $^{24}\text{Mg}$  results. Here again, the dependence of the results on the  $J^2$  term is weak, as in the case of  $^{20}\text{Ne}$ , and so will not be shown. The nucleus  $^{24}\text{Mg}$ , however, has an axially asymmetric  $|\chi\rangle$  and therefore we use the following constrained intrinsic Hamiltonian:

$$H_I = H - 0.27J^2 - \lambda Q_2^0 - \mu Q_2^2. \quad (36)$$

Since the calculation of projected energy is in practice very time consuming for a non-axial nucleus, the two parameters in (36) are varied one at a time, while keeping the other at zero. The non-axial  $|\chi\rangle$  of  $^{24}\text{Mg}$  obtained with  $H_I = H$  typically has four  $K$ -bands, with  $K = 0, 2, 4$ , and  $6$ , in our large basis. The probabilities ( $n_K^2$  in eq. (18)) for these bands are 0.3888, 0.4920, 0.1147 and 0.0044 respectively. The sum of the remaining weights for components with  $|K| > 6$  is less than  $10^{-4}$ . This represents the upper error limit of our projection scheme. According to table 1 (case 2) 128 Euler angles are needed to perform the projection. This may be compared with eight angles needed for  $^{20}\text{Ne}$ . If an accuracy of 0.5 % only were required for  $^{24}\text{Mg}$ , the  $|K| = 6$  components could be ignored and only 72 angles would then be needed for the three-band projection. For the present four-band calculation, some of the  $K$ -mixing coefficients are given in table 4. There the  $|K| = 6$  coefficients are very small and have been omitted for compactness although the numerical work was done with their effect taken into account. The VPHF results are shown in fig. 4. The largest value achieved here for the binding energy,  $E_b$ , is 183.6 MeV. Compared to an intrinsic HF energy of 176.5 MeV for  $^{24}\text{Mg}$  reported in ref. <sup>2)</sup>, this represents a gain of 7.1 MeV due to projection and variation. However the theoretical  $E_b$  still has a

TABLE 4  
Non-orthogonal, normalised  $K$ -band mixing coefficients  $x_K^{J\sigma} = X_K^{J\sigma} \sqrt{N_{KK}^{-1}}$ , for  $^{24}\text{Mg}$

| $J_\sigma$ <sup>b)</sup> | $x_K^{J\sigma}$ <sup>a)</sup> |           |           |
|--------------------------|-------------------------------|-----------|-----------|
|                          | $ K  = 0$                     | $ K  = 2$ | $ K  = 3$ |
| 0                        | 1                             | 0         | 0         |
| 2 <sub>1</sub>           | 0.992                         | 0.099     | 0         |
| 2 <sub>2</sub>           | -0.133                        | 0.995     | 0         |
| 3 <sub>1</sub>           | 0                             | 1         | 0         |
| 4 <sub>1</sub>           | 0.882                         | 0.369     | -0.011    |
| 4 <sub>2</sub>           | -0.491                        | 0.940     | -0.024    |
| 5 <sub>1</sub>           | 0                             | 1.003     | -0.046    |
| 6 <sub>1</sub>           | 0.708                         | 0.531     | -0.041    |
| 4 <sub>3</sub>           | 0.001                         | -0.014    | 1.000     |
| 6 <sub>2</sub>           | -0.771                        | 0.908     | -0.026    |
| 5 <sub>2</sub>           | 0                             | -0.036    | 1.002     |

<sup>a)</sup> Note that  $\sum_K (x_K^{J\sigma})^2 \neq 1$  due to non-orthogonality effects (eq. (29)).

<sup>b)</sup> See fig. 5 for energies.

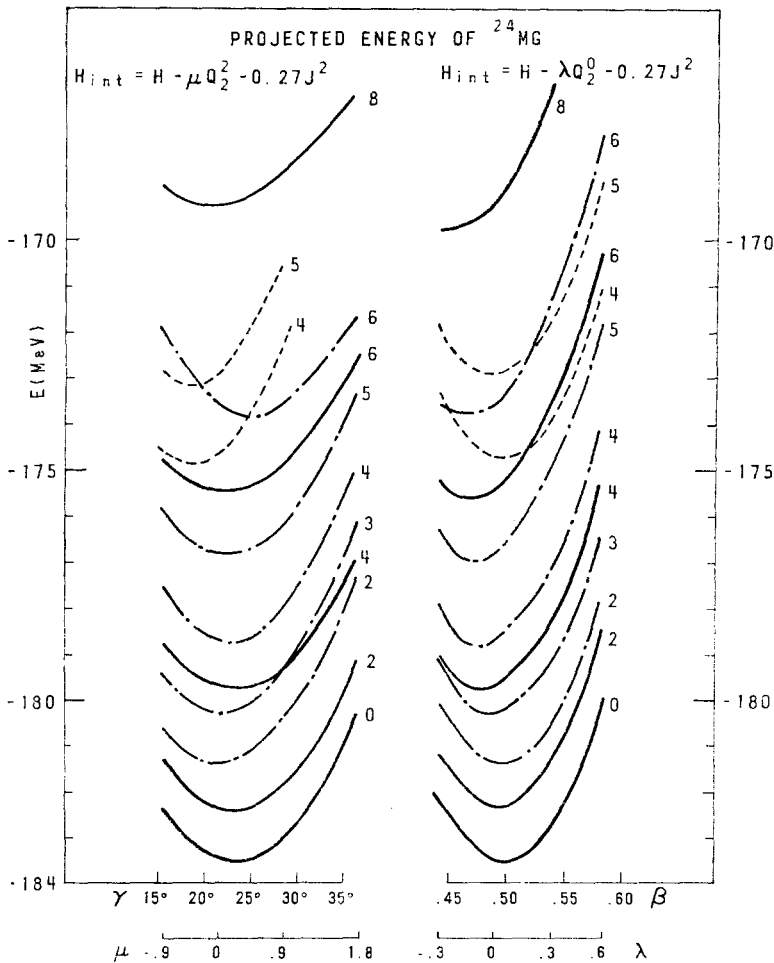


Fig. 4. Projected energies of the level in the non-axial ground band of  $^{24}\text{Mg}$  versus  $\lambda$  and  $\mu$ , the cranking parameters in  $H_1 = H - 0.27J^2 - \lambda Q_2^0 - \mu Q_2^2$ . The parameters  $\beta$  and  $\gamma$  are the quadrupole deformation and axial asymmetry parameters, respectively <sup>2</sup>).

deficiency of 14.7 MeV when compared to the experimental  $E_b$  of 198.3 MeV. Similarly the deficiency in  $E_b$  for  $^{20}\text{Ne}$  is 7.4 MeV.

We note the following features in fig. 4: (a) the three bandheads shown ( $0_1^+$ ,  $2_2^+$ ,  $4_3^+$ ) all have deformations corresponding to  $\beta \sim 0.5$ , and for each band  $\beta$  decreases with increasing spin; (b) the non-axiality parameter,  $\gamma$ , for the  $0^+$  state is  $\approx 24^\circ$  and essentially does not change throughout the ground band; (c) the  $\gamma$  for the  $K = 2$  band-head ( $2_2^+$ ) is  $\approx 21^\circ$  and increases with increasing spin; (d) the excitation energy of the  $2_2^+$  state *does not* increase with decreasing  $\gamma$ .

The final VPHF spectrum is shown in fig. 5, where all states are taken at their respective variational minimum in fig. 4. These states can be analyzed into approxi-

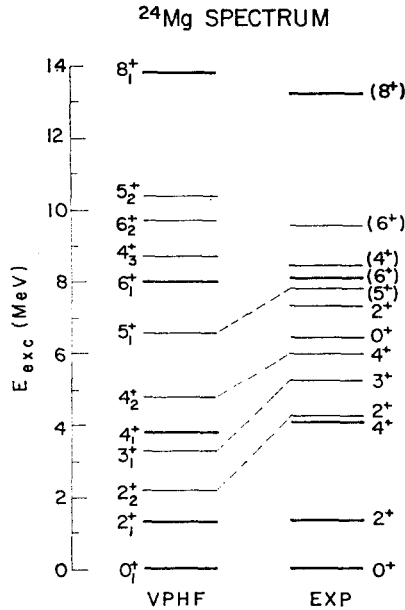


Fig. 5. Energy levels of  $^{24}\text{Mg}$ . The heavy lines indicate the  $K \approx 0$  ground band. The  $2_2^+$ ,  $3_1^+$ ,  $4_2^+$ ,  $5_1^+$  and  $6_2^+$  levels belong to the  $K \approx 2$  band, while the  $4_3^+$ ,  $5_2^+$  states belong to the  $K \approx 4$  band.

mate  $K$ -bands. Thus the  $0_1^+$ ,  $2_1^+$ ,  $4_1^+$ ,  $6_1^+$  and  $8_1^+$  belong to the  $K \approx 0$  band, although starting at  $J = 4$  there is a substantial amount of  $K$ -mixing. The level spacings within this band are well matched with the observed spacings. The  $2_2^+$ ,  $3_1^+$ ,  $4_2^+$ ,  $5_1^+$ ,  $6_2^+$  states belong to the  $K \approx 2$  band. This band is depressed by 1.3 to 1.9 MeV compared to experiment<sup>23)</sup>. This defect was first noticed by Elliot and Harvey<sup>24)</sup> in their pioneering work on the application of SU(3) group to nuclear structural problems. It was also noted recently in the SU(3) based, shell model calculation of Strottman<sup>25)</sup>. In the  $j$ - $j$  coupled shell model calculations of McGrory and Wildenthal<sup>26)</sup> the position of the  $K \approx 2$  band was correctly predicted. Since both shell model calculations use the same  $G$ -matrix elements, the difference in the results must come from the different methods used to truncate the bases. Strottman<sup>25)</sup> speculates that the difference might be due to the fact that in the  $j$ - $j$  model no more than two particles were allowed in the  $0d_{3/2}$  orbit.

We believe that our predicted  $K \approx 4$  band is also too low, following the pattern observed for the  $K \approx 2$  band. Thus its band head, the  $4_3^+$  state should probably not be identified with the  $4^+$  state observed at 8.64 MeV, which is believed<sup>27)</sup> to belong to a  $\beta$ -band whose first two members are the  $0^+$  (6.43 MeV) and the  $2^+$  (7.35 MeV) states. The  $6^+$  state observed at 9.54 MeV may also belong to this band. However from the measured decay scheme of this state, it is consistent to identify it rather as a member of the  $K \approx 2$  band corresponding to the predicted  $6_2^+$  state at 9.7 MeV.

### 5. Static electromagnetic properties

All static electromagnetic matrix elements for  $^{20}\text{Ne}$  are calculated using the optimum states of fig. 3 and table 2. In contrast, the matrix elements for  $^{24}\text{Mg}$  are all calculated for the one intrinsic state obtained from the unconstrained Hamiltonian. Our reason for doing this is that the time required for a complete variational calculation of  $^{24}\text{Mg}$  is not justified by the expected improvements in the results. We begin with the  $^{20}\text{Ne}$  results.

Referring to fig. 3 we see that the energy minima occur at different values of  $\beta$  for each member of the rotational band. The fact that  $\beta$  decreases with increasing  $J$  is not easy to understand. Classically we may envisage that as the nucleus spins faster the centrifugal force will stretch the nucleus leading to a *larger* deformation. This trend seems to terminate at the  $10^+$  member however. Since this state is mainly outside the s-d shell, it should be strongly influenced by the s-d to p-f shell gap. This could account for the different behaviour of  $\beta$ . The various intrinsic states can be characterized by their intrinsic quadrupole as well as hexadecapole moments given in columns 5 and 7 of table 2. These moments are seen to decrease throughout the band, excepting the  $10^+$  level. The static quadrupole and hexadecapole moments

$$\langle Q_\lambda \rangle_J = \langle JJ | Q_\lambda^0 | JJ \rangle, \quad (37)$$

where

$$Q_\lambda^\mu = \sqrt{\frac{4\pi}{2\lambda+1}} \sum_{i \text{ proton}} r_i^\lambda Y_\lambda^\mu(\theta_i, \phi_i), \quad \lambda = 2, 4, \quad (38)$$

are given in columns 6 and 8. We note that our  $\langle Q_2 \rangle_J$  is a factor of 2 smaller than is sometimes defined. The value for  $2\langle Q_2 \rangle_{2^+}$ , or the static quadrupole moment of the  $2^+$  state, predicted to be  $-14.2 e \cdot \text{fm}^2$ , is somewhat smaller in magnitude than the measured value  $^{28,29})$  of  $-23 \pm 5 e \cdot \text{fm}^2$ . The theoretical  $B(E2)$  values are listed in column 11. It is seen that the agreement between the VPHF results and the experiment data  $^{30})$  in column 12 is very good. The transition strengths from the lower state are perhaps slightly underestimated. It is interesting to note that the VPHF results are very close to being proportional to those obtained by assuming the ground band to have the symmetry of the  $(\lambda\mu) = (80)$  representation of the group  $^{31})$   $\text{SU}(3)$ . Various theoretical predictions of the  $B(E2)$  values are compared in fig. 6. In the two shell model calculations, one using the  $\text{SU}(3)$  basis  $^{20})$  and the other the  $j$ - $j$  coupling basis  $^{21})$ , a charge enhancement of  $\Delta e = 0.5e$  was assigned to the valence protons and neutrons. The results of these calculations are very similar to ours (VPHF). In the  $\alpha$ -cluster  $^{32,33})$  model, all  $B(E2)$  strengths are predicted to be about 25 % to 40 % stronger than the present results. The importance of variation after projection is clearly borne out by comparing the simple PHF results (sequence i, j, k, l in fig. 3) with the VPHF results. The former are very close to being proportional to the prediction of the rigid rotor model which hardly agrees with experiment. The additional variational procedure not only suppresses (by 55 %) the  $8 \rightarrow 6$  strength, where it is

too strong in PHF, but also enhances (by 17 %) the  $2 \rightarrow 0$  strength, where it is deficient.

Another interesting aspect of the VPHF results for  $^{20}\text{Ne}$  is that the rms radius in the ground band decreases with increasing spin. In columns 9 and 10 of table 2 the radii with respect to the center of mass (c.m.) and with respect to the laboratory, respectively, are shown. This phenomenon is *not* predicted in PHF, where the rms radius *increases* with spin. This anti-centrifugal-stretching effect<sup>34)</sup> predicted by the VPHF supports the speculation of Arima and Yoshida<sup>35)</sup>, who pointed out that such an effect could explain the anomalous difference in the  $\alpha$ -widths<sup>22)</sup> of the first  $6^+$  and  $8^+$  states in  $^{20}\text{Ne}$ . Arima and Yoshida analysed the  $\alpha$ -widths of these states in terms of the product of a spectroscopic factor and a single-particle width;

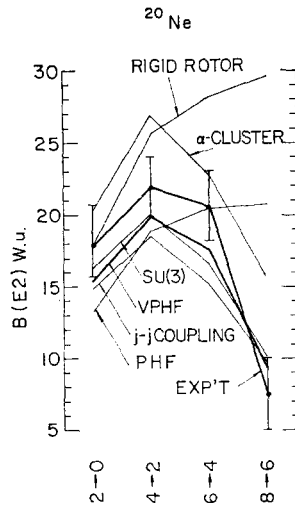


Fig. 6. The  $B(E2)$  values for transitions in the ground band of  $^{20}\text{Ne}$ . The VPHF results are represented by the transitions b, c, d, e and the PHF results by i, j, k, l in fig. 3. The "SU(3)" values come from ref. <sup>25)</sup>, the  $j$ - $j$  coupling ones are from ref. <sup>26)</sup>, and the  $\alpha$ -cluster results are from refs. <sup>32, 33)</sup>. The rigid rotor results are calculated using eq. (46) and normalized to the experimental  $B(E2; 2 \rightarrow 0)$  value.

TABLE 5  
Change in  $\rho$ , the  $\alpha$ - $^{16}\text{O}$  cluster distance in the  $^{20}\text{Ne}$  ground state band

| $J^\pi$ | $R_{\text{rms}}(^{20}\text{Ne})$ (fm) | $\rho(\alpha\text{-}^{16}\text{O})$ (fm) |                 | $\Delta\rho = \rho_0 - \rho_J$ (fm) |                 |
|---------|---------------------------------------|------------------------------------------|-----------------|-------------------------------------|-----------------|
|         |                                       | $R_{16} = 2.35$                          | $R_{16} = 2.50$ | $R_{16} = 2.35$                     | $R_{16} = 2.50$ |
| $0^+$   | 2.678                                 | 3.862                                    | 3.312           | 0                                   | 0               |
| $2^+$   | 2.673                                 | 3.840                                    | 3.287           | 0.022                               | 0.025           |
| $4^+$   | 2.655                                 | 3.761                                    | 3.194           | 0.101                               | 0.118           |
| $6^+$   | 2.635                                 | 3.672                                    | 3.089           | 0.190                               | 0.223           |
| $8^+$   | 2.606                                 | 3.540                                    | 2.931           | 0.322                               | 0.381           |
| $10^+$  | 2.674                                 | 3.844                                    | 3.292           | 0.018                               | 0.020           |

their "single particle" has reduced mass number  $\frac{1}{5}6$ , and its motion is the relative motion of the departing  $\alpha$ -particle and the residual  $^{16}\text{O}$ . Supported by their cluster model calculations for  $^{20}\text{Ne}$ , these authors believe the spectroscopic factors for the two states concerned should be substantially the same. They then proceeded to show that the difference in the single-particle widths could be explained by allowing a difference in the separation distances between the  $\alpha$  and  $^{16}\text{O}$  particles in these states. The separation distances,  $\rho$ , in the  $6^+$  and  $8^+$  states were deduced to be <sup>34, 35</sup>) 3.58 fm and 3.34 fm, respectively. From the entries in column 9 of table 2, we can calculate  $\rho$  for each state in  $^{20}\text{Ne}$ , through the equation

$$20R_{20\text{Ne}}^2 = 16R_{16\text{O}}^2 + 4R_{\alpha}^2 + \frac{1}{5}\rho^2. \quad (39)$$

We assume the rms radii (with respect to the c.m.) of  $^{16}\text{O}$  and  $^4\text{He}$  to be known and to be independent of spin. Table 5 shows the calculated  $\rho$  assuming  $R_{\alpha} = 1.44$  [ref. <sup>2</sup>)] and two values <sup>2, 36</sup>) for  $R_{16\text{O}}$ . It is seen that the radii determined by Arima and Yoshida lie between those independently deduced here. In particular  $\rho(8^+)$  is predicted to be about 0.13–0.16 fm less than  $\rho(6^+)$ . However this difference may be slightly smaller than the difference <sup>34</sup>) required to explain the  $\alpha$ -widths. Two cautionary remarks are now in order. (a) The method for deducing  $\Delta\rho$  from the  $\alpha$ -width is somewhat crude <sup>34, 35</sup>), as it effectively involves a calculation of the mean square radius of scattering waves. Thus the error in the extracted  $\Delta\rho$  may be quite large. (b) The viewpoint adopted by Arima and Yoshida is not universally accepted. In particular Vogt <sup>37</sup>) believes there are evidences which suggest that the  $8^+$  state under concern does not belong to the ground band at all <sup>†</sup>. It is possible that each point of view represents part of the truth. In view of our difficulty in reproducing the excitation energy of the  $8^+$  state, and because the  $\Delta\rho$  we predict may not be quite as large as required, the issue of the  $\alpha$ -widths in the "ground band" of  $^{20}\text{Ne}$  should not be considered closed.

Before we turn to  $^{24}\text{Mg}$  we comment briefly on the motion of the  $^{20}\text{Ne}$  c.m.; it can be easily verified from table 2 that the rms radius of the c.m. is almost constant throughout the band, taking values between 0.458 fm and 0.464 fm. This property will be exploited when we calculate the inelastic electron scattering form factors in sect. 6.

The E2 transition strengths for  $^{24}\text{Mg}$  are given in table 6. As noted earlier these are all calculated from one intrinsic state ( $H_1 = H$ ). The SU(3)-based <sup>32</sup>) and  $j$ - $j$  coupling <sup>26</sup>) shell model result are also given. Again in the shell model charge enhancements of  $\Delta e = 0.5$  are assigned to both valence protons and neutrons. In general most theoretical results are similar, and they account for the data rather successfully. In particular we note, as mentioned in sect. 4, that it is consistent to identify the observed  $6^+$  state at 9.54 MeV with a  $6^+$  member of the  $K = 2$  band, corresponding to our  $6_2^+$  state predicted at 9.7 MeV. The more serious disagreements between PHF and data are the  $2_2^+ \rightarrow 0_1^+$  and  $2_2^+ \rightarrow 2_1^+$  E2 strengths. The inadequacy

<sup>†</sup> See, however, ref. <sup>38</sup>).

TABLE 6  
EM properties of low-lying levels in <sup>24</sup>Mg

| $J_i^\pi \rightarrow J_f^\pi$ | Branching ratio (%) |                   | $B(E2)$ (W.u.) <sup>a)</sup> |                                  |      |                    | Lifetime          |  |                    |
|-------------------------------|---------------------|-------------------|------------------------------|----------------------------------|------|--------------------|-------------------|--|--------------------|
|                               |                     |                   | shell model                  |                                  | PHF  | exp. <sup>b)</sup> | th. <sup>c)</sup> |  | exp. <sup>b)</sup> |
|                               | exp. <sup>b)</sup>  | th. <sup>c)</sup> | SU(3) <sup>d)</sup>          | $J$ - $J$ coupling <sup>e)</sup> |      |                    |                   |  |                    |
| $2_1^+ \rightarrow 0_1^+$     | 100                 | 100               | 17.4                         | 15.3                             | 19.1 | $20.8 \pm 0.8$     | 2.18 ps           |  | $2.0 \pm 0.08$ ps  |
| $4_1^+ \rightarrow 2_1^+$     | 100                 | 100               | 28.9                         | 20.0                             | 26.4 | $23 \pm 4.5$       | 50 fs             |  | $59 \pm 12$ fs     |
| $2_2^+ \rightarrow 0_1^+$     | 73                  | 32                | 1.0                          | 2.0                              | 0.41 | $1.0 \pm 0.15$     | 113 fs            |  | $128 \pm 15$ fs    |
| $\rightarrow 2_1^+$           | 23                  | 68                | 8.2                          | 1.7                              | 6.21 | $2.2 \pm 0.4$      |                   |  |                    |
| $3_1^+ \rightarrow 2_1^+$     | $\approx 100$       | 92                | 3.4                          | 2.9                              | 0.74 | $2.05 \pm 0.4$     | 289 fs            |  | $119 \pm 25$ fs    |
| $\rightarrow 4_1^+$           | $< 2$               | 3                 |                              |                                  | 10.6 | $< 20$             |                   |  |                    |
| $\rightarrow 2_2^+$           | $< 2$               | 5                 |                              | 2.67                             | 34.0 | $< 33$             |                   |  |                    |
| $4_2^+ \rightarrow 2_1^+$     | 88                  | 85                | 0.2                          | 1.9                              | 1.02 | $1.0 \pm 0.3$      | 77 fs             |  | $77 \pm 18$ fs     |
| $\rightarrow 2_2^+$           | 11                  | 11                | 9.5                          | 9.7                              | 9.0  | $16 \pm 5$         |                   |  |                    |
| $\rightarrow 4_1^+$           | 1                   | 4                 |                              |                                  | 4.4  | $\leq 7$           |                   |  |                    |
| $5_1^+ \rightarrow 4_1^+$     | 24                  | 6                 |                              |                                  | 0.86 | $\leq 2.3 \pm 0.4$ | 80 fs             |  | $35 \pm 5$ fs      |
| $\rightarrow 3_1^+$           | 68                  | 79                |                              |                                  | 17.1 | $33 \pm 5$         |                   |  |                    |
| $\rightarrow 4_2^+$           | 8                   | 15                |                              |                                  | 19.5 | $\leq 14 \pm 2$    |                   |  |                    |
| $6_1^+ \rightarrow 4_1^+$     |                     | 100               | 29.6                         | 17.5                             | 31.0 | $34 \pm 4.7$       | 6.3 fs            |  | $6 \pm 3$ fs       |
| $6_2^+ \rightarrow 4_1^+$     | $\leq 20$           | 32                | 0.5                          | 0.95                             | 0.98 | $0.7 \pm 0.4$      | 14 fs             |  | $12 \pm 5$ fs      |
| $\rightarrow 4_2^+$           | $\geq 80$           | 68                | 14.4                         | 12.2                             | 17.7 | $25 \pm 9$         |                   |  |                    |
| $8_1^+ \rightarrow 6_1^+$     |                     |                   | 23.2                         | 2.4                              | 32   | $18 \pm 3.6$       | 1.8 fs            |  | $3 \pm 2$ fs       |

<sup>a)</sup> 1 W.u. =  $4.11 e^2 \cdot \text{fm}^4$ .

<sup>b)</sup> Experimental values from refs. <sup>39-41</sup>).

<sup>c)</sup> Empirical energies are used to compute branching ratios and lifetimes.

<sup>d)</sup> Ref. <sup>25</sup>). <sup>e)</sup> Ref. <sup>26</sup>).

of the PHF in these cases is related to the theory's inability to produce large enough separation between the  $K = 2$  and the ground band. In this respect the  $j$ - $j$  coupling model is superior. In addition, there is a marked deviation between the predictions from PHF and the  $j$ - $j$  model for transitions among higher spin states. In these cases the data seem to slightly favor the PHF values; we note that the VPHF would give smaller  $B(E2)$  values for these high spin transitions. However the computing time needed for the VPHF calculation is not justified by the present status of the data. Finally, the predicted static quadrupole moment for the  $2_1^+$  (1.37 MeV) state of <sup>24</sup>Mg is  $-17.1 e \cdot \text{fm}^2$ , whereas the measured value <sup>29)</sup> is  $-21 \pm 4 e \cdot \text{fm}^2$ .

## 6. Electron scattering form factors

The measurements of elastic and inelastic electron scattering form factors samples not only the basic electric multipole moments of the nucleus but also the momentum distribution of these moments <sup>42)</sup>. However the theoretical predictions are more difficult to obtain since they require that one solve the Dirac equation and that one make some assumption about the excitation process in inelastic scattering <sup>43)</sup>. We

have only computed elastic and inelastic electron scattering form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  in the first Born approximation and we shall presently compare those with experiment.

The Coulomb form factor in the Born approximation can be written <sup>43)</sup> as

$$|F(q^2)|_{\text{s.p.}}^2 = \frac{1}{2J_i + 1} \sum_{M_i, M_f} \frac{1}{Z^2} |\langle f | \sum_{\alpha=\text{proton}}^Z e^{i\mathbf{q} \cdot \mathbf{r}_\alpha} | i \rangle|^2 = \frac{2J_f + 1}{2J_i + 1} \sum_{\lambda} |F_{\lambda; J_i \rightarrow J_f}(q^2)|_{\text{s.p.}}^2, \quad (40)$$

where  $\lambda$  is the multipolarity. The subscripts s.p. refer to the fact that s.p. wave functions, with respect to the laboratory rest frame, for *point* charges, will be used in (40). In order to compare with the data, the c.m. motion and the finite size of the proton should be accounted for <sup>43)</sup>. Thus we have

$$|F_{\lambda; J_i \rightarrow J_f}(q^2)|^2 = \frac{4\pi}{Z^2} |\langle J_f | | \sum_{\alpha=\text{proton}}^Z j_\lambda(qr_\alpha) Y_\lambda(\Omega_\alpha) | J_i \rangle|^2 F_p^2(q^2) f_{\text{c.m.}}^2(q^2), \quad (41)$$

where  $F_p^2(q^2)$  is the electric form factor for the proton which is represented here by the Stanford three-pole fit <sup>44)</sup>. We follow Lee <sup>45)</sup> and write for the center-of-mass correction factor,

$$f_{\text{c.m.}}^2(q^2) \cong 1 + \frac{1}{6}(\langle r^2 \rangle - \langle r'^2 \rangle)q^2 + \dots, \quad (42)$$

where  $\langle r^2 \rangle$  is the mean square radius with respect to the lab system and  $\langle r'^2 \rangle$  is the mean square radius with respect to the c.m. Eq. (42) will be applicable if we assume that all states concerned have the *same* c.m. motion, or, the same mean square c.m. radius, to order  $q^2$ . The calculated rms radii shown in table 2 certainly verify this assumption. The operator involved in eq. (40) is a one-body operator; this makes the task of computing  $F(q^2)$  a comparatively easy one. We have calculated the form factors for some 20 different values of  $q^2$  in the interval  $0 \leq q^2 \leq 6 \text{ fm}^{-2}$ . The smooth curves shown are interpolations between these computed values. For simplicity, all form factors are calculated using intrinsic states generated from  $H$ .

The results for the elastic form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  are shown and compared with experiment <sup>46, 47)</sup> in fig. 7. The dependence of  $F(q^2)$  on the oscillator parameter  $b$  was studied in ref. <sup>45)</sup> and found to be *weak*. The agreement with experiment for  $^{24}\text{Mg}$  is reasonable, up to the first minimum. For  $^{20}\text{Ne}$  the predicted form factor is significantly larger than the data even before the first minimum. The fit to experiment of the calculated  $F(q^2)$  can be optimized, below the first minimum, by scaling the length unit (the oscillator parameter) involved in the computation of  $F$ . This changes the predicted proton and charge rms radius with respect to the c.m. Thus, this adjustment increases the predicted proton radius of  $^{20}\text{Ne}$  by 8%, from 2.66 fm to 2.87 fm; this last figure corresponds to a charge radius <sup>48)</sup> of 2.98 fm. A similar calculation for  $^{24}\text{Mg}$  increases the predicted proton radius by  $\approx 2\%$ , from its value of 2.84 fm; this implies a new charge radius of 3.04 fm for  $^{24}\text{Mg}$ . This  $^{24}\text{Mg}$  value agrees well with the one  $3.02 \pm 0.04$  fm extracted from muonic X-rays <sup>49)</sup> and is slightly larger than the value  $2.97 \pm 0.09$  fm determined previously from fits to elec-

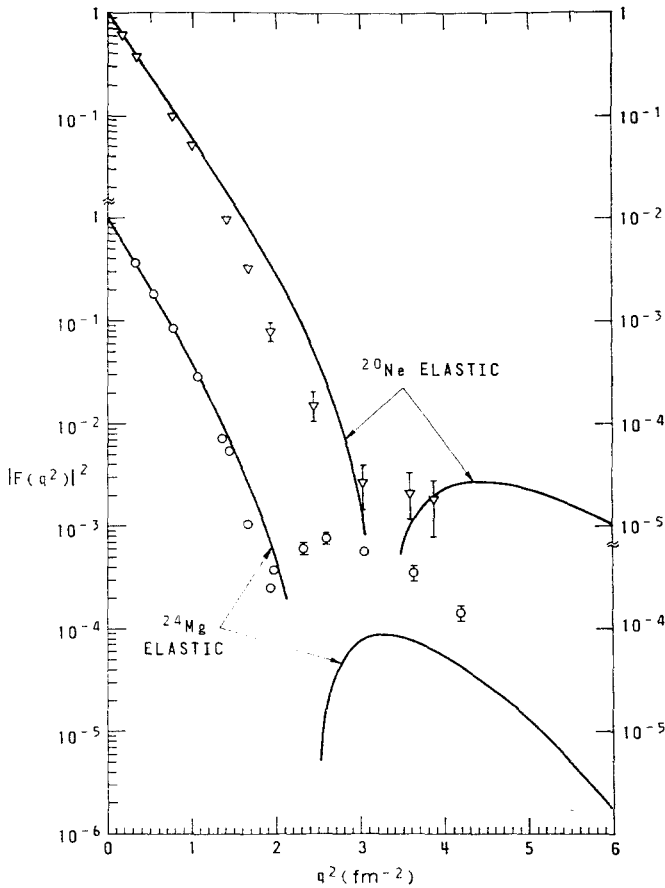


Fig. 7. Elastic Coulomb form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$ , calculated in the Born approximation. The data for  $^{20}\text{Ne}$  are from ref. <sup>46)</sup> and those for  $^{24}\text{Mg}$  come from ref. <sup>47)</sup>.

tron scattering using phenomenological charge distributions <sup>36,48)</sup>. No previous radius for  $^{20}\text{Ne}$  extracted from muonic X-rays is available, and the radius previously determined from electron scattering ranges <sup>50,51)</sup> from  $2.91 \pm 0.05$  to  $2.98 \pm 0.08$  fm. For  $^{20}\text{Ne}$  using the value  $\langle r_{\text{ch}}^2 \rangle^{\frac{1}{2}} = 2.97$  fm we can deduce the value 1.41 fm for the radius parameter  $r_0$  in the relation  $\sqrt{\frac{8}{3}} \langle r_{\text{ch}}^2 \rangle^{\frac{1}{2}} = r_0 A^{\frac{1}{3}}$ . This number is significantly larger than the corresponding one for  $^{24}\text{Mg}$  (1.35) but close to the value <sup>36)</sup>  $\approx 1.40$  extracted from  $^{16}\text{O}$ .

It is not surprising, when a density independent N-N interaction is used, that the radius predicted in a HF calculation should be too small by 2–4 %, and this effect has already been observed in ref. <sup>2)</sup>. Indeed, the discrepancy is expected to increase with mass due to the restrictions imposed on the wave functions by the finite basis. However, the present observation that the error is greater in  $^{20}\text{Ne}$ , is somewhat anomalous.

In fig. 7 (as well as in figs. 8–10), the disagreement between theory and experiment at higher momentum transfer, is partly due to the use of the Born approximation. Another contribution to the discrepancy may be that the form factor is suppressed in the region of the second maximum, when the nuclear wave function is permanently deformed <sup>45, 52</sup>). These matters can only be adequately investigated when the exact Dirac equation is solved, a project not undertaken here.

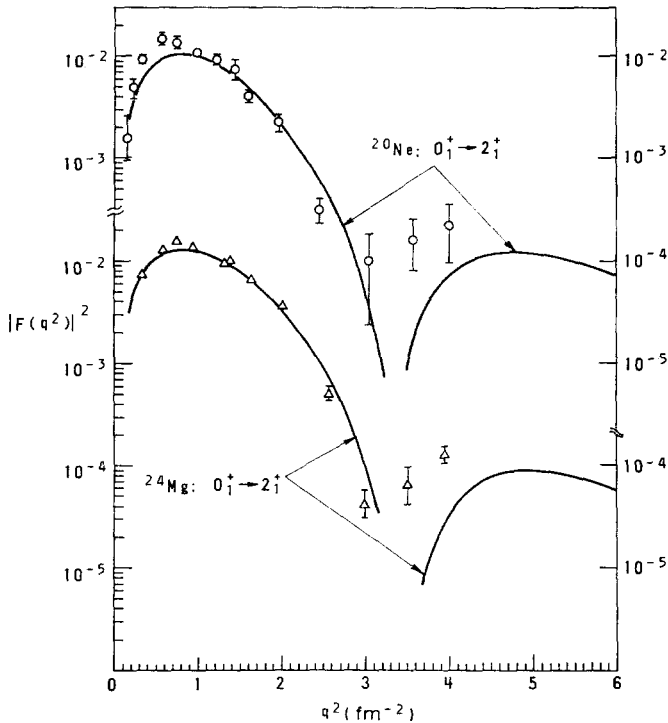


Fig. 8. Inelastic  $0_1^+ \rightarrow 2_1^+$  Coulomb form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$ . Data are from ref. <sup>47</sup>).

The inelastic form factors from the  $0_1^+$  to the  $2_1^+$  state are shown in fig. 8, and compared with experiment <sup>47</sup>). We note that the computed values for  $^{20}\text{Ne}$  at the first peak ( $q^2 \approx 0.5 \text{ fm}^{-2}$ ) would have been higher, had we used the optimum intrinsic states for the  $0^+$  and  $2^+$  states. Otherwise the agreement between theory and experiment is satisfactory, up to the first minima. We note that a somewhat improved fit would be obtained if the theoretical nuclear sizes were dilated by  $\approx 3\%$  for both nuclei. It is again probable that part of the error at higher momentum transfers comes from using the Born approximation.

Fig. 9 shows the  $0_1^+ \rightarrow 2_2^+$  and the  $0_1^+ \rightarrow 4_1^+$  form factors of  $^{24}\text{Mg}$ , compared with the experimentally unresolved <sup>46</sup>) 4.23 MeV data representing the sum of the two transitions. One sees that the theoretical  $0_1^+ \rightarrow 2_2^+$  form factor above gives a reason-

able account of the data, whereas the theoretical sum would disagree markedly with the data. This indicates that there is very little E4 experimental strength between the ground state and the *first*  $4^+$  state in  $^{24}\text{Mg}$ ; this was first pointed out by Nakada *et al.* <sup>46</sup>). Thus, the large predicted form factor for  $0_1^+ \rightarrow 4_1^+$  represents a notable failure of the simple PHF, in accounting for the distribution of the E4 strengths. However, this failure does not seem to be shared by the shell model <sup>53</sup>) which exploits other degrees of freedom.

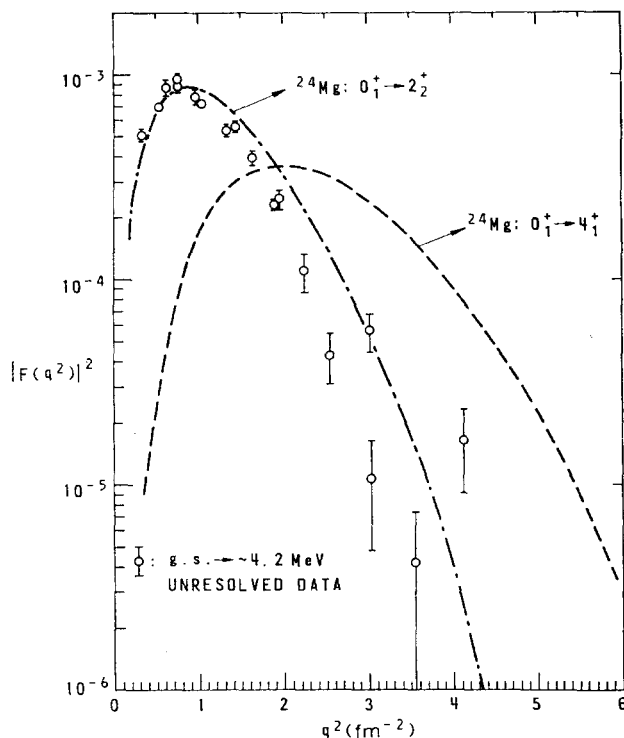


Fig. 9. Inelastic Coulomb form factors for the transitions  $0_1^+ \rightarrow 2_2^+$  and  $0_1^+ \rightarrow 4_1^+$  in  $^{24}\text{Mg}$ . The unresolved  $0 \rightarrow \approx 4.2$  MeV data are from ref. <sup>46</sup>).

The  $0_1^+ \rightarrow 4_1^+$  and  $0_1^+ \rightarrow 4_2^+$  form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  are shown and compared with the data <sup>46, 47</sup>) in fig. 10. The  $^{20}\text{Ne}$  theoretical form factor is up to 40 % too small at the peak. Thus it appears that the  $N = 2$  to  $N = 6$  hexadecapole matrix elements, which are neglected in the present calculation due to the finite basis used, do not affect the hexadecapole moments given in table 2 by more than about 20 %. In the case of  $^{24}\text{Mg}$ , the deviation is slightly more than a factor of 2 if we compare the 6.00 MeV data with the theoretical  $0_1^+ \rightarrow 4_2^+$  result alone. However the data are larger by only about 30 % than the *combined* theoretical  $0_1^+ \rightarrow 4_2^+$  and  $0_1^+ \rightarrow 4_1^+$  form factors. Thus the PHF scheme accounts for approximately the same

percentage of the observed inelastic electron scattering E4 strength in both  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  when the present basis is used. However, as mentioned earlier, the distribution of the E4 strength in  $^{24}\text{Mg}$  has not been correctly predicted.

It should be mentioned that most of the data discussed here have been fitted with relative ease <sup>46,47</sup>) by using phenomenological densities. This contrasts sharply with the PHF results, which agree poorly with data after the first minimum. Of course one expects the theoretical results to improve when the Born approximation is replaced by a better treatment. On the other hand it is not expected that such an

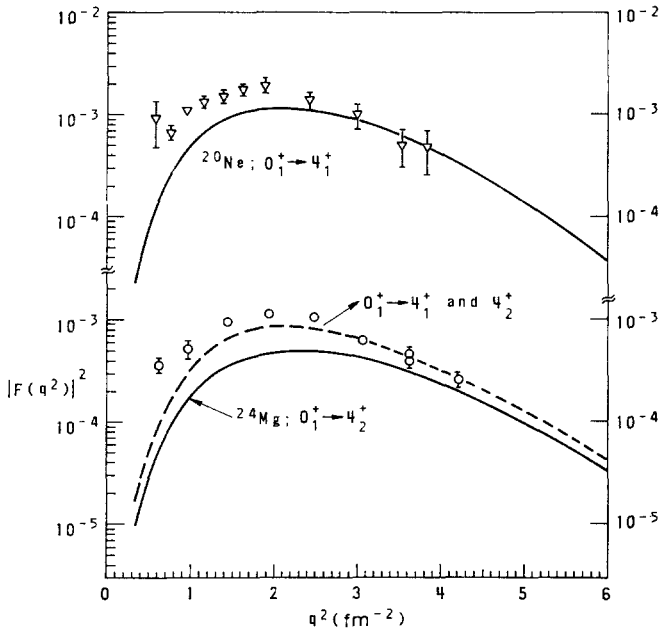


Fig. 10. Inelastic  $0_1^+ \rightarrow 4_1^+$  and  $0_1^+ \rightarrow 4_2^+$  form factors for  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  respectively. The dashed curve represents the sum of the theoretical  $0_1^+ \rightarrow 4_1^+$  and  $0_1^+ \rightarrow 4_2^+$  form factors squared in  $^{24}\text{Mg}$ . Data are from refs. <sup>46,47</sup>).

improved treatment will remove all or even most of the discrepancy between theory and the data shown here. This is because processes involving high momentum transfer are sensitive to small variations in the nuclear density whereas processes involving low momentum transfer depend only on the overall size and shape parameters of the nucleus. Since the HF theory emphasizes only the long range correlations within the nucleus we should not be surprised to find discrepancies at short distances, where the effective interaction and the single Slater determinant approximation are not expected to be accurate.

## 7. Comparison with the rotational model

The passage from the PHF scheme to the rotational model of Bohr and Mottelson<sup>54)</sup> is of considerable interest both for the gain in physical insight and for the mathematical simplifications which result in that limit. The limit is best studied<sup>55)</sup> by considering the angular overlap

$$N(\Omega) = N(\alpha, \beta, \gamma) \equiv \langle \chi_1 | \hat{R}(\alpha, \beta, \gamma) | \chi_1 \rangle, \quad (43)$$

which occurs in the projection integral discussed in sect. 3. For a highly deformed system involving a large number of particles, it suffices to rotate  $|\chi_1\rangle$  by a very small angle in order to obtain a new state which is orthogonal to the original one. Indeed it can be shown<sup>55)</sup> that for an axially symmetric  $|\chi_1\rangle$ ,

$$N(0, \beta, 0) = \exp \left\{ -\frac{1}{4}(\langle J^2 \rangle - K(K+1))\beta^2 \right\} + \mathcal{O}(\beta^4), \quad (44)$$

where  $\langle J^2 \rangle$  is the expectation value  $\langle \chi_1 | J^2 | \chi_1 \rangle$ . The rotational model assumes the limit

$$N(\Omega) \propto \delta(\Omega) = \delta(\alpha)\delta(\gamma)\delta(\beta)/\beta, \quad -\frac{1}{2}\pi \leq \beta \leq \frac{1}{2}\pi. \quad (45)$$

In this case the normalization constant  $n_{JK}$  is independent of  $K$  and is proportional to  $((2J+1)/8\pi^2)^{\frac{1}{2}}$ , and the normalized reduced matrix elements of a tensor operator  $\hat{\mathcal{O}}_\lambda$  become

$$\langle J'(K') || \mathcal{O}_\lambda || J(K) \rangle = \sqrt{\frac{2J+1}{2J'+1}} C_{K, K'-K, K'}^{J \lambda J'} \langle \chi_1 | \hat{\mathcal{O}}_\lambda^{K'-K} | \chi_1 \rangle. \quad (46)$$

The last expression is easily derived from eq. (13) and eq. (45). We note that in the limit where eq. (45) holds all the states projected from a given  $|\chi_1\rangle$  are degenerate in energy and there is no  $K$ -mixing, even when  $|\chi_1\rangle$  is axially asymmetric. Therefore one uses only eq. (46) in the rotational model to obtain reduced matrix elements between states of good  $JK$  and invokes other models to find the  $K$ -mixing coefficients; this yields

$$\langle J'(\sigma') || \mathcal{O}_\lambda || J(\sigma) \rangle = \sum_{K'K} x_{K'}^{J'\sigma'*} \langle J'(K') || \mathcal{O}_\lambda || J(K) \rangle x_K^{J\sigma}, \quad (47)$$

where the notation is that of eq. (31).

The accuracy of the angular orthogonalization assumed in (45) can be tested by calculating  $N(\Omega)$ . Semi-log plots of  $N(\alpha, \beta, 0)$  versus  $\beta$ , for <sup>24</sup>Mg, are shown in fig. 11 for  $\alpha = 0, 25.7, 51.4$  and  $77.1$  degrees. We note that for these values of  $\alpha$  the full width at half-maximum of  $N(\beta)$  is about  $40^\circ$ . Therefore one does not expect eq. (45) to be a very good approximation. Because of the symmetry properties given in eqs. (20a, b), the function  $N(\alpha, \beta, 0)$  is symmetric about  $\beta = 90^\circ$ . In particular the curve  $N(0, \beta, 0)$  is similar to that of the axially symmetric <sup>20</sup>Ne. Fig. 12 shows some overlap curves for <sup>24</sup>Mg, with both  $\alpha$  and  $\gamma \neq 0$ . The  $\gamma$ -dependence is seen to be similar to the  $\alpha$ -dependence.

Let us now examine the accuracy of the angular orthogonality condition assumed in the rotational model, by using the following procedure. First, we use the intrinsic matrix elements  $\langle \chi_1 | \hat{O}_2^\mu | \chi_1 \rangle$  calculated in the HF scheme. We then use eq. (46) to calculate the reduced matrix elements "predicted" by the rotational model. These are then compared with their counterparts in PHF. For  $^{24}\text{Mg}$  we calculate the rotational model matrix elements between  $K$ -mixed states, by using eqs. (46) and (49), and the  $K$ -mixing coefficients given in table 4.

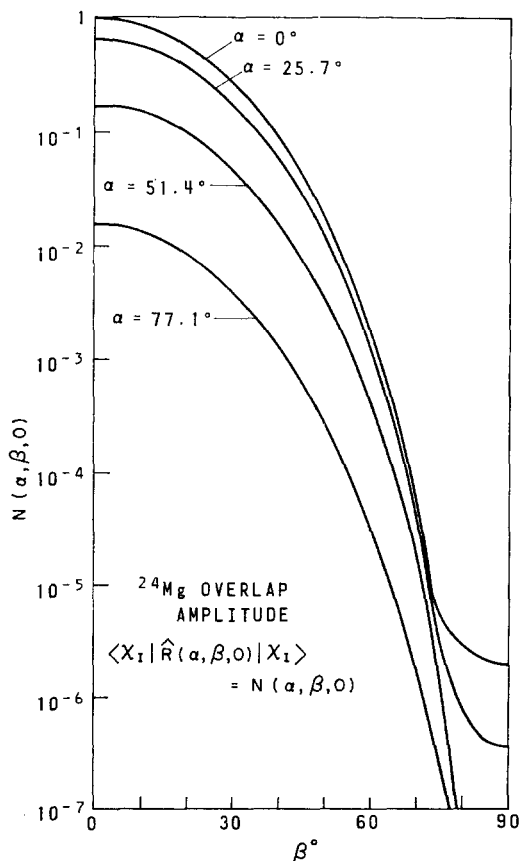


Fig. 11. Angular overlap functions  $N(\alpha, \beta, \gamma)$  of  $^{24}\text{Mg}$  versus  $\beta$ , for  $\gamma = 0$  and various values of  $\alpha$ . The function  $N(\alpha, \beta, 0)$  is symmetric about  $\beta = 90^\circ$ .

Table 7 shows the comparison between the PHF and the rotational model for the quadrupole and hexadecapole matrix elements in  $^{20}\text{Ne}$ . We note that *all* PHF matrix elements are enhanced over their rotational counterparts. We find a most interesting result, namely the enhancement can be very closely expressed by a single *constant* factor for each multipole operator. Thus for  $Q_2$  the percentage enhancement is  $\approx 7\%$  and for  $Q_4$  it is  $\approx 27\%$ . This result is furthermore general for the light

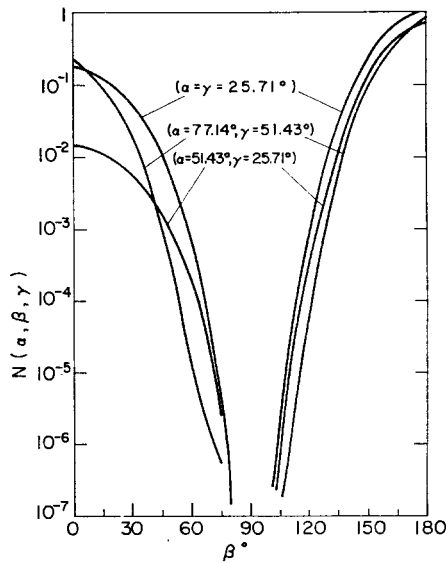


Fig. 12. The  $^{24}\text{Mg}$  angular overlap functions  $N(\alpha, \beta, \gamma)$ , for  $\alpha \neq 0$  and  $\gamma \neq 0$ .

TABLE 7  
Comparison of rotational model predictions and PHF results in  $^{20}\text{Ne}$

| $J \rightarrow J'$ | $\langle J    Q_2    J' \rangle (eb^2)^a$ |                          |                      | $\langle J    Q_4    J' \rangle (eb^4)^a$ |                          |                      |
|--------------------|-------------------------------------------|--------------------------|----------------------|-------------------------------------------|--------------------------|----------------------|
|                    | (1)<br>rot <sup>b)</sup>                  | (2)<br>PHF <sup>c)</sup> | ((2)/(1)-1) × 100(%) | (3)<br>rot <sup>b)</sup>                  | (4)<br>PHF <sup>c)</sup> | ((4)/(3)-1) × 100(%) |
| 0 → 2              | 7.81                                      | 8.39                     | 7.4                  |                                           |                          |                      |
| → 4                |                                           |                          |                      | 19.5                                      | 24.8                     | 27                   |
| 2 → 2              | -4.17                                     | -4.50                    | 7.8                  | 10.4                                      | 13.3                     | 27                   |
| → 4                | 5.60                                      | 5.99                     | 7.0                  | -9.95                                     | -12.7                    | 28                   |
| → 6                |                                           |                          |                      | 13.1                                      | 16.4                     | 25                   |
| 4 → 4              | -3.98                                     | -4.31                    | 8.2                  | 7.84                                      | 9.97                     | 27                   |
| → 6                | 5.26                                      | 5.59                     | 6.2                  | -8.76                                     | -11.0                    | 26                   |
| → 8                |                                           |                          |                      | 12.0                                      | 14.8                     | 23                   |
| 6 → 6              | -3.94                                     | -4.30                    | 9.0                  | 7.55                                      | 9.52                     | 26                   |
| → 8                | 5.12                                      | 5.45                     | 6.4                  | -8.40                                     | -10.5                    | 25                   |

<sup>a)</sup>  $b = 1.663$  fm.

<sup>b)</sup> The HF intrinsic moments  $\langle Q_2^0 \rangle = 7.81 eb^2$  and  $\langle Q_4^0 \rangle = 19.5 eb^4$  are used.

<sup>c)</sup> The HF intrinsic state corresponds to  $H_1 = H - 0.27J^2$  and is the same for all  $J$ , in this comparison.

“rotational” nuclei; in fact the enhancement is found to increase with decreasing mass number, as a consequence of the broadening of the angular overlap. For example <sup>45)</sup>, the enhancement in the  $^{12}\text{C}$  quadrupole matrix elements is  $\approx 15\%$  and  $\approx 60\%$  for the hexadecapole matrix elements.

TABLE 8  
Comparison of rotational model predictions and PHF results in  $^{24}\text{Mg}$

| $J_\sigma \rightarrow J'_\sigma$ | $\langle J_\sigma    Q_2    J'_\sigma \rangle (eb^2)^a$ |             | PHF   | $\langle J_\sigma    Q_4    J'_\sigma \rangle (eb^4)^a$ |             | PHF   |
|----------------------------------|---------------------------------------------------------|-------------|-------|---------------------------------------------------------|-------------|-------|
|                                  | rotational <sup>b)</sup>                                |             |       | rotational <sup>b)</sup>                                |             |       |
|                                  | pure $K^c$                                              | mixed $K^d$ |       | pure $K^c$                                              | mixed $K^d$ |       |
| $0_1 \rightarrow 2_1$            | 10.44                                                   | 10.54       | 11.35 |                                                         |             |       |
| $\rightarrow 2_2$                | 1.88                                                    | 0.48        | 1.67  |                                                         |             |       |
| $\rightarrow 4_1$                |                                                         |             |       | 7.23                                                    | 10.51       | 16.57 |
| $\rightarrow 4_2$                |                                                         |             |       | 11.21                                                   | 6.99        | 15.59 |
| $2_1 \rightarrow 2_1$            | -5.58                                                   | -5.51       | -5.42 | 5.18                                                    | 5.86        | 6.13  |
| $\rightarrow 2_2$                | 1.00                                                    | 2.26        | 2.89  | 3.87                                                    | 3.15        | 6.68  |
| $\rightarrow 4_1$                | 7.49                                                    | 7.10        | 8.01  | -3.68                                                   | -3.32       | -4.22 |
| $\rightarrow 4_2$                | -2.28                                                   | -0.24       | -2.22 | 0.87                                                    | -2.22       | -1.57 |
| $2_2 \rightarrow 2_2$            | 5.58                                                    | 5.16        | 5.40  | 0.64                                                    | -0.29       | -0.40 |
| $\rightarrow 4_1$                | 0.22                                                    | 1.05        | 1.58  | 6.63                                                    | 7.93        | 13.91 |
| $\rightarrow 4_2$                | 4.83                                                    | 4.78        | 4.67  | 4.28                                                    | 0.81        | -0.20 |
| $4_1 \rightarrow 4_1$            | -5.32                                                   | -3.71       | -3.73 | 2.91                                                    | 0.23        | -1.57 |
| $\rightarrow 4_2$                | 1.11                                                    | 2.28        | 2.43  | -2.75                                                   | -3.66       | -5.54 |
| $4_2 \rightarrow 4_2$            | -2.13                                                   | -4.19       | -4.25 | -1.78                                                   | 1.66        | 2.78  |

<sup>a)</sup>  $b = 1.663$  fm.

<sup>b)</sup> The HF intrinsic moments  $\langle Q_2^0 \rangle = 10.44 eb^2$ ,  $\langle Q_2^{\pm 2} \rangle = 1.88 eb^2$ ,  $\langle Q_4^0 \rangle = 7.23 eb^4$  and  $\langle Q_4^{\pm 2} \rangle = 11.21 eb^4$  are used in the rotational model calculation.

<sup>c)</sup> Assuming pure  $K = 0$  when  $\sigma = 1$  and pure  $K = 2$  when  $\sigma = 2$ .

<sup>d)</sup> The  $K$ -mixing coefficients listed in table 4 are used, except that  $K = 4$  components are ignored.

Table 8 makes the comparison for  $^{24}\text{Mg}$ , and gives the rotational model predictions with and without  $K$ -mixing. For the former case the coefficients of table 4 are used. The pure- $K$ , mixed- $K$  and PHF result for matrix elements of  $Q_2$  are essentially in agreement, apart for some small random deviations. However, the situation is quite different for the  $Q_4$  matrix elements. There one sees a 50–100 % enhancement of the matrix elements in the PHF over those in the mixed- $K$  rotational model. Furthermore the correlation between the PHF and pure- $K$  matrix elements is very irregular, especially when the heavily  $K$ -mixed  $J = 4$  states are involved. In most of these cases the PHF and pure- $K$  results not only differ significantly in magnitude, they also have opposite signs. For any multipolarity  $\lambda$  the sensitivity of the matrix elements on  $K$ -mixing effects can be measured in terms of the ratio  $\mathcal{R}_\lambda \equiv |\langle Q_\lambda^0 \rangle| / |\langle Q_\lambda^0 \rangle|$ . For  $^{24}\text{Mg}$ ,  $\mathcal{R}_2 = 0.18$  whereas  $\mathcal{R}_4 = -1.55$ ! This explains why the deviations for  $\lambda = 4$  are so large as to make the rotational predictions unreliable.

## 8. Summary and discussion

We have seen in this paper, that the Saunier-Pearson velocity dependent interaction no. 2 gives a good representation of many low energy properties of  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$ . These results, together with those obtained for  $^{22}\text{Na}$ , a doubly odd nucleus <sup>3)</sup>,

for  $^{12}\text{C}$  [ref. <sup>45</sup>)] and for other nuclei <sup>2)</sup> with  $A \leq 40$ , indicate that this effective interaction is capable of supplying a rather detailed account of the systematics of light nuclei in the projected HF method. This method is of course at its best in the region of strong, stable deformations. Thus preliminary results <sup>10)</sup> indicate that in the region near the  $^{16}\text{O}$  closed shell, e.g.  $A = 14\text{--}18$ , it is impossible to obtain adequate wave functions using one intrinsic Slater determinant only. Similarly, for  $A > 24$ , the ground state usually belongs to a partly vibrational structure so that again one intrinsic state will not suffice. In principle such vibrations can be studied in the framework of multiconfiguration Hartree-Fock theory <sup>56)</sup>.

Apart from the limitations imposed by the PHF model, the only other limitations of the present method come from some known residual deficiencies of the Saunier-Pearson interaction. Thus the depression of the  $K = 2$  band in  $^{24}\text{Mg}$  which is probably due to an insufficient amount of two-body spin orbit coupling <sup>57-59)</sup>, leads, in  $^{56}\text{Fe}$ , to an actual inversion of the  $K = 0$  and  $K = 2$  band-head <sup>57)</sup> energies.

It was shown in sect. 3 that the replacement of the three-dimensional integration over the Euler angles by exact finite summations (eq. (14)), combined with the cross-density method of Löwdin (eqs. (21)–(25)) and the use of symmetry relations (eqs. (19) and (20)) results in a highly efficient method for angular momentum projection. Of course eq. (20) is applicable only to  $|\chi_i\rangle$  which are invariant under the four-group, but analogous relations can easily be derived for any other point group.

We have seen in sect. 4 that the method of variation after projection yields small additional energy gains and significantly improved level schemes. However the calculated  $8^+$  state, and to a lesser extent, the  $6^+$  state in  $^{20}\text{Ne}$  still occur at too high excitation energies. In  $^{24}\text{Mg}$  the  $K = 2$  band is too low by  $\approx 2$  MeV. Sect. 5 showed that the VPHF calculation can be pushed to a rather high level of refinement. In  $^{20}\text{Ne}$ , for example, the decrease in E2 transition strengths as one goes up the ground state rotational band was correlated with a decrease in  $^{16}\text{O}\text{--}\alpha$  intercluster distance which results in decreased  $\alpha$ -widths, two effects which have been independently observed. It is also worthy mentioning that the present calculation accounts for essentially all the E2 strengths in the two nuclei reported here without the help of any adjustable parameter. In view of the difficulties faced in attempting <sup>60)</sup> to calculate effective charges microscopically, it is rewarding to find that they are in fact not required in the PHF scheme. There is at present no reason to doubt similar successes can be met for most light deformed nuclei <sup>2, 3, 45)</sup>. There is still however much room for improvement, for example the predicted static quadrupole moment of the first  $2^+$  state in  $^{20}\text{Ne}$  is significantly smaller, in magnitude, at  $-14.2 e \cdot \text{fm}^2$ , than the measured value,  $-23 \pm 5 e \cdot \text{fm}^2$ .

Inelastic electron scattering processes were studied in sect. 6. They showed good agreement for the  $0^+ \rightarrow 2^+$  form factors up to the region of the first minima, as expected. More surprising however was the agreement found for the  $0^+ \rightarrow 4^+$  form factors. This led to the conclusion that the omitted  $N = 4$  terms in the wave functions contain only about 35 % of the E4 strength. In addition, the computed elastic

form factors showed that the charge radii of  $^{20}\text{Ne}$  and  $^{24}\text{Mg}$  were underestimated by some 8 % and 2 % respectively.

Our comparison with the rotational model (RM), represented by eq. (46), can be summarized as follows. For axially symmetric nuclei, multipole matrix elements calculated in PHF are enhanced over their counterparts predicted in the RM. The enhancement factor increases with decreasing mass, and with increasing multipolarity. For  $^{20}\text{Ne}$  the  $\lambda = 2$  matrix elements are enhanced by  $\approx 7\%$  and the  $\lambda = 4$  matrix elements by  $\approx 27\%$ . For nonaxial nuclei the reliability of the RM prediction is affected by the amount of  $K$ -mixing and by the ratio  $\mathcal{R}_\lambda = |\langle Q_\lambda^2 \rangle / \langle Q_\lambda^0 \rangle|$  (assuming mainly two  $K$ -bands, with  $\Delta K = 2$ ). For a given amount of  $K$ -mixing the random errors occurring in the RM increase with  $\mathcal{R}_\lambda$ . Thus for  $^{24}\text{Mg}$  and  $\lambda = 4$ , where  $\mathcal{R}_4 = 1.55$ , the RM predictions are highly unreliable. The situation for  $\lambda = 2$  is much better as  $\mathcal{R}_2$  is only 0.18.

The present work makes little mention of magnetic moment operators. For the two nuclei reported here,  $L$ - $S$  coupling prevails and since  $S \cong 0$  for all low-lying states the M1 operator is essentially proportional to the total angular momentum. However our experience has been that M1 and Gamow-Teller matrix elements<sup>57)</sup> are not always reliably predicted in the present scheme, especially for odd and doubly odd<sup>3)</sup> nuclei. This is because these operators are not spatial operators and are not too sensitive to long-range spatial correlations – the forte of HF – but rather to small and random components in the wave functions.

One of the most noticeable restrictions of the present work is that the intrinsic state  $|\chi_I\rangle$  must have good parity. This eliminates all  $1p$ - $1h$ ,  $1\hbar\omega$  correlations from the HF Slater determinants. Such correlations may be important in the lighter nuclei. For example they are known to contribute sizeably to the properties of  $^6\text{Li}$ .

Finally, we end this work by stating our belief that the present calculations show that there may exist a reasonable description of nuclei in terms of density independent and energy independent effective interactions. The advent of folded diagrams<sup>61)</sup> has shown the path for the construction of such effective interaction matrix elements from a realistic  $G$ -matrix. We believe much can be gained by using the effective interactions thus constructed in structural calculations of the kind described here.

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