Unification of the nuclear collective and single particle models

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The unification of the nuclear collective and single particle models with the help of a transformation, first published by the author, is presented. The Schrödinger equation with the new coordinates exhibits all relevant features of the so-called unified nuclear model, but it is no longer an artificial combination of the continuum, used in the collective model, and the conventional shell model. As a first application a sum rule for the quadrupole moments of mirror nuclei is derived. Estimates are given for the deformations of the charge and mass distributions of 17 F and 17 O. The approximation of strong coupling of the nucleon motions to a symmetry axis gives good results, while the weak coupling approximation does not work at all.

NUCLEAR STRUCTURE Genuine definition of single particle and collective states from A nucleon Schrödinger equation. Sum rule for q of mirror nuclei.

I. INTRODUCTION

The unified nuclear model is a combination of the original model for collective nuclear motions¹ and the shell model, but is unsatisfactory, insofar as the different features of this model are not really derived from the Schrödinger equation of A nucleons. This author was the first to publish a transformation² which brings the Schrödinger equation to a suitable form which, when including the spin orbit coupling, brings about the genuine unification of the collective and single particle models. Other authors reviewed the same transformation, some with a different mathematical formalism.³⁻⁵ The idea which led to the transformation was the following: Any collective motion in the nucleus means at the same time rotations and vibrations of the inertia ellipsoid. Single particle motions refer to the body-fixed axes defined by the principal axes and are left unchanged in collective excitations. The single particle and collective degrees of freedom defined in this way are applicable for all A, though the clean separation of collective and single particle excitations will hardly be possible for small A.

In this author's notation the transformation from the space vectors of the nucleons in the center of mass system, \vec{r}_n , to the new coordinates is defined in the following way:

$$\vec{\mathbf{r}}_{n} = s_{n1} \vec{\mathbf{y}}_{1} + s_{n2} \vec{\mathbf{y}}_{2} + s_{n3} \vec{\mathbf{y}}_{3} , \qquad (1)$$

with

$$\vec{\mathbf{y}}_i \cdot \vec{\mathbf{y}}_k = y_i y_k \delta_{ik} , \qquad (2)$$

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 $\sum_{n=1}^{A} s_{nk} = 0 , \qquad (3)$

$$\sum_{n=1}^{A} s_{nj} s_{nk} = \delta_{jk} \quad . \tag{4}$$

It is easy to show that the principal moments of inertia are

$$J_1 = m(y_2^2 + y_3^2) , (5)$$

etc. The coordinates s_{nj} are the new single particle coordinates, which are no longer independent, but connected by (3) and (4). There are six collective coordinates, namely, y_1 , y_2 , y_3 and three Euler angles defining the directions of \vec{y}_1 , \vec{y}_2 , \vec{y}_3 . These six collective coordinates are unaffected by the antisymmetrization. The Schrödinger equation in the new coordinates was given in Ref. 2. Here only the approximate form will be given, which follows for small deviations from spherical symmetry (which here always refers to the inertia ellipsoid) and by defining β and γ (Ref. 6) to get the connection to Ref. 1:

$$y_{1} = (\frac{1}{3})^{1/2} y [\cos\beta + \sqrt{2} \sin\beta \cos\gamma] ,$$

$$y_{2} = (\frac{1}{3})^{1/2} y [\cos\beta + \sqrt{2} \sin\beta \cos(\gamma - \frac{2}{3}\pi)] , \quad (6)$$

$$y_{3} = (\frac{1}{3})^{1/2} y [\cos\beta + \sqrt{2} \sin\beta \cos(\gamma - \frac{4}{3}\pi)] .$$

 β and γ in Ref. 1 refer to a nucleus which has the form of an ellipsoid. Here they refer to the inertia ellipsoid. $\beta = 0$ means spherical symmetry, that is, the three moments of inertia defined by (5) are equal. The magnitude of β is a measure for the de-

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viation from spherical symmetry. For $\gamma = n\pi/3$, with *n* an integer, one has rotational symmetry (two moments of inertia are equal). The deviation from these special values of γ is a measure for the devia-

tion from rotational symmetry.

For close to spherical nuclei (small values of β) one has for the kinetic energy of the A nucleons (ignoring all terms that are at least linear in sin β):

$$\begin{split} \sum_{i=1}^{A} \Delta_{n} \approx \frac{\partial^{2}}{\partial y^{2}} + \frac{3A-4}{y} \frac{\partial}{\partial y} + \frac{1}{y^{2}} \left\{ -\frac{3}{8} (\vec{L}_{e} - \vec{L}_{i})^{2} + \frac{\partial^{2}}{\partial \beta^{2}} + 4 \frac{\cos\beta}{\sin\beta} \frac{\partial}{\partial\beta} + \frac{1}{\sin^{2}\beta} \left[\frac{\partial^{2}}{\partial\gamma^{2}} + 3 \frac{\cos3\gamma}{\sin3\gamma} \frac{\partial}{\partial\gamma} \right] \right. \\ \left. - \frac{1}{4\sin^{2}\beta} \left[\frac{(L_{e1} + L_{i1})^{2}}{\sin^{2}\gamma} + \frac{(L_{e2} + L_{i2})^{2}}{\sin^{2}(\gamma - 2\pi/3)} + \frac{(L_{e3} + L_{i3})^{2}}{\sin^{2}(\gamma - 4\pi/3)} \right] \right. \\ \left. + 3 \left[\sum_{n} \sum_{n'} (\delta_{nn'} - \frac{1}{A} - \vec{s}_{n'} \cdot \vec{s}_{n'}) \vec{\nabla}_{n'} \cdot \vec{\nabla}_{n'} - (A-4) \sum_{n} \vec{s}_{n} \cdot \vec{\nabla}_{n} \right] \right] \end{split}$$

+(kinetic energy of the center of mass).

Here \vec{L}_e is the operator for the total orbital angular momentum. The components in the center of mass system are L_{ex} , L_{ey} , and L_{ez} :

$$L_{ex} = -i\hbar \sum_{n} \left[y_n \frac{\partial}{\partial z_n} - z_n \frac{\partial}{\partial y_n} \right] , \qquad (8)$$

etc., with

$$\vec{\mathbf{r}}_n = (x_n, y_n, z_n)$$

With respect to the body-fixed axes the components of \dot{L}_e are L_{e1} , L_{e2} , and L_{e3} . These are, in terms of the Euler angles,⁷

$$\begin{split} L_{e1} \pm i L_{e2} &= i \hbar e^{\mp i \psi} \left[\frac{1}{\sin \vartheta} \frac{\partial}{\partial \varphi} - \cot \vartheta \frac{\partial}{\partial \psi} \mp i \frac{\partial}{\partial \vartheta} \right] , \\ L_{e3} &= -i \hbar \frac{\partial}{\partial \psi} , \end{split}$$
(9)

 \vec{L}_i is defined in the following way (components for the body-fixed system):

$$L_{i1} = -i\hbar \sum_{n} \left[s_{n2} \frac{\partial}{\partial s_{n3}} - s_{n3} \frac{\partial}{\partial s_{n2}} \right], \qquad (10)$$

etc., so in terms of \vec{s}_n , the new single particle vectors, \vec{L}_i has the same form with respect to the body-fixed axes as \vec{L}_e has in terms of \vec{r}_n with respect to the center of mass axes. This is the reason for choosing the following indices: *e* stands for "external," *i* for "internal."

II. GENERAL PROPERTIES OF THE KINETIC ENERGY OPERATOR

Equation (7) contains the well-known terms of Ref. 1 describing rotations, vibrations, and their

coupling, namely, the terms with L_{e1}^2 , etc., and with derivatives with respect to β and γ . In addition, there are terms with derivatives with respect to y describing density vibrations. They are coupled via the factor $1/y^2$ before the braces to all the other motions. Single particle motions are described by L_{i1}^2 , etc., and all the terms in the last line of Eq. (7). The Coriolis-type terms $L_{e1}L_{i1}$, etc., give a coupling between the single particle motion and the total orbital angular momentum. There is further coupling between the different kinds of motions via the coordinate dependent factors before the various derivatives. There will of course be further coupling by the potential energy.

III. ANTISYMMETRIZATION

The six collective coordinates y, φ , ϑ , ψ , β , and γ are symmetric with respect to exchange of the nucleons. So the antisymmetrization of wave functions affects the single particle vectors \vec{s}_n only, and that antisymmetrization would indeed be an almost hopeless task, just as in the ordinary shell model, when using Jacobi coordinates instead of single particle vectors. On the basis of these difficulties almost all shell model calculations are done with single particle vectors with the resulting risk of creating spurious states (that is, excitations of the center of mass motions). The additional constraints (4) further enhance the difficulties of antisymmetrization. So to make calculations manageable it is probably best to treat the \vec{s}_n vectors as approximately independent, requiring the constraints (3) and (4) for the expectation values only. In that case the sums over n and n' in Eqs. (7) and (10) run from 1 to A. [If one would take (3) and (4) into account rigorously, the sums would include independent terms of the

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 \vec{s}_n vectors only.²] The terms $(\vec{s}_n \cdot \vec{s}_{n'})(\vec{\nabla}_n \vec{\nabla}_{n'})$ are taken into account as a perturbation only.

It is obvious that this approximation will be poor for small particle numbers. For four particles, for example, one has nine degrees of freedom. Treating the \vec{s}_n vectors as independent, one would have 18. Furthermore, the single particle terms containing Δ_n and $\Delta_{n'}$ in Eq. (7) disappear when taking (3) and (4) into account for four particles.⁸ This and some general properties of the single particle vectors \vec{s}_n , with Eqs. (3) and (4) rigorously taken into account, are discussed in the Appendix. These properties are important when dealing with a small number of particles, e.g., four or five.

IV. DEFINITION OF SINGLE PARTICLE AND COLLECTIVE STATES

The discussion in the following will be restricted to a simple case to make it more transparent: a single nucleon outside closed shells. The dependence of the wave function on the \vec{s}_A vector of this last nucleon is taken into consideration alone in addition to the dependence on the collective coordinates. No antisymmetrization is done.

The polar coordinates of \vec{s}_A in the body-fixed system are defined in the usual way:

$$s_{A1} = s_A \sin \vartheta_A \cos \varphi_A ,$$

$$s_{A2} = s_A \sin \vartheta \sin \varphi_A ,$$

$$s_{A3} = s_A \cos \vartheta_A .$$
(11)

Pure collective excitations in the sense of Ref. 1 are obtained when

$$\vec{\mathbf{L}}_i \Psi = 0 \ . \tag{12}$$

The wave function Ψ here depends on the six collective coordinates and on \vec{s}_A .

Equation (12) would mean that the last nucleon is in an s state or, in the more general case of several nucleons outside closed shells, their orbital angular momenta couple to zero. With Eq. (12) valid, the Coriolis-type terms $L_{e1}L_{i1}$, etc., in the kinetic energy operator (7) vanish. The only coupling between collective and single particle degrees of freedom then comes from the factor $1/y^2$ before the brace. If one excludes density vibrations, $1/y^2$ is replaced by its expectation value and there is no longer any coupling between collective and single particle motion. The collective part of the Hamiltonian is the same as in Ref. 1 and is dealt with in numerous papers. The more complicated case of nonvanishing internal angular momentum requires a new definition of single particle states. For simplicity it is assumed here that the potential does not depend on the polar angles ϑ_A and φ_A . That is wrong in general, but near spherical symmetry and with central interactions (but without spin orbit coupling) it would be a good approximation: Let

$$V[(\vec{\mathbf{r}}_A - \vec{\mathbf{r}}_1)^2]$$

be the potential of such an interaction between nucleons 1 and A. It is

$$V[(\vec{r}_{A} - \vec{r}_{1})^{2}] = V[(s_{A1} - s_{11})^{2}y_{1}^{2} + (s_{A2} - s_{12})^{2}y_{2}^{2} + (s_{A3} - s_{13})^{2}y_{3}^{2}].$$
(13)

When

$$y_1^2 = y_2^2 = y_3^2 \text{ (spherical symmetry) ,}$$

$$V[(\vec{r}_A - \vec{r}_1)^2] = V[(\vec{s}_A - \vec{s}_1)^2 y_1^2] .$$
(14)

This V depends on the angle between \vec{s}_A and \vec{s}_1 , but not on the orientation of \vec{s}_A . One would have

$$\vec{\mathbf{L}}_i^2 \Psi = \hbar^2 l_i (l_i + 1) \Psi . \tag{15}$$

Spin orbit coupling will cause a mixture of different l_i values, but for now this mixing will be ignored. With potentials of the form (14) the solutions of the Schrödinger equation are called $\Psi_{l_e l_i}^{l_s}$ in the following, for which one has, in addition to (15),

$$\begin{split} \vec{\mathbf{L}}_{e}^{2} \Psi_{l_{e}l_{i}}^{l_{s}} &= \hbar^{2} l_{e} (l_{e} + 1) \Psi_{l_{e}l_{i}}^{l_{s}} , \\ L_{ez} \Psi_{l_{e}l_{i}}^{l_{s}} &= \hbar M_{e} \Psi_{l_{e}l_{i}}^{l_{s}} , \\ (\vec{\mathbf{L}}_{e} + \vec{\mathbf{L}}_{i})^{2} \Psi_{l_{e}l_{i}}^{l_{s}} &= \hbar^{2} l_{s} (l_{s} + 1) \Psi_{l_{e}l_{i}}^{l_{s}} . \end{split}$$
(16)

 $\Psi_{l_e l_i}^{l_s}$ was not indexed with M_e , as this quantum number is of less importance.

The wave function can now be expanded in terms of $\Psi_{l_el_i}^{l_s\kappa}$, which in addition to \vec{L}_e^2 , L_{ez} , \vec{L}_i^2 , and $(\vec{L}_e + \vec{L}_i)^2$, is an eigenfunction of $L_{e3} + L_{i3}$:

$$\Psi_{l_e l_i}^{l_s \kappa} = \sum_{K_i} \begin{pmatrix} l_i & l_e & l_s \\ K_i & \kappa - K_e & \kappa \end{pmatrix} D_{M_e, \kappa - K_i}^{l_e}(\varphi \vartheta \psi) \times Y_{l_i K_i}(\vartheta_A \varphi_A) .$$
(17)

There are $2l_s + 1$ different functions (17) and they are the complete system in the five-dimensional space of φ , ϑ , ψ , ϑ_A , and φ_A for fixed values of l_e , l_i , l_s , and M_e . The solution of the Schrödinger equation $\Psi_{l_i l_e}^{l_s}$ can be expanded in these functions with the expansion coefficients depending on the collective coordinates and on s_A :

$$\Psi_{l_e l_i}^{l_s} = \sum_{\kappa} f_{\kappa}(y, \beta, \gamma, s_A) \Psi_{l_e l_i}^{l_s \kappa} .$$
(18)

A word should be said here about Eq. (17): The right-hand side looks like an addition of two orbital angular momenta to give a total orbital angular momentum quantum number l_s . This interpretation is of course incorrect. The total orbital angular momentum is \vec{L}_e with quantum number l_e . The total angular momentum will be obtained by adding the spin angular momentum to \vec{L}_e , which was left out so far and will be discussed below. \vec{L}_i refers to the motion in the body-fixed system and cannot be added to \vec{L}_e to give another orbital angular momentum. So the addition is a formal one and l_s is just a quantum number which occurs because

$$\vec{\mathbf{L}}_{s}^{2} = (\vec{\mathbf{L}}_{e} + \vec{\mathbf{L}}_{i})^{2}$$

commutes with the total Hamiltonian. The magnitude of the quantum number l_s contains a statement about the magnitude of the nuclear deformation. Looking at the kinetic energy operator, Eq. (7), one sees that the terms with $(L_{ej} + L_{ij})^2$ have singularities at $\beta = 0$, that is, for spherical symmetry. So when $l_s \neq 0$ and, as a consequence, the expectation values of $(L_{ej} + L_{ij})^2$ do not vanish, the wave function must be zero at $\beta = 0$. So all states with $l_s \neq 0$ are nonspherical. The deviation from spherical symmetry will in general increase with increasing l_s . States with $l_s = 0$ may be spherically symmetric.

To make these statements more transparent, here is a simple example in which rotational symmetry with $y_1 = y_2$ is assumed, that is, $\gamma = \pi/3$ or $\gamma = 4\pi/3$. Furthermore, the potential is assumed not to depend on β . Then the ground state with $l_s = 0$ does not depend on β . For the excited states with $l_s \neq 0$ one has a positive potential proportional to

$$\frac{1}{\sin^2\beta}l_s(l_s+1), \qquad (19)$$

which has its origin in the term

$$\frac{1}{\sin^2\beta} \left[(L_{e1} + L_{i1})^2 + (L_{e2} + L_{i2})^2 \right].$$
 (20)

Equation (19) is a positive potential that increases in strength with increasing l_s . So the expectation value of β will increase with l_s . If one has a potential energy with a strong maximum at $\beta = 0$ and no γ dependence, the ground state of the nucleus will have $l_s = 0$ and $l_e = l_i$. These states are the closest analog to the ordinary single particle states and will be called single particle states henceforth. Their definition is

$$\Psi_{\rm sp} = f_0(y,\beta,s_A) \sum_{K_i} \begin{pmatrix} l_i & l_i & 0\\ K_i & -K_i & 0 \end{pmatrix} D^{l_i}_{M,-K_i}(\varphi,\vartheta,\psi) Y_{l_iK_i}(\vartheta_A\varphi_A) .$$
⁽²¹⁾

The single particle coordinates of one nucleon and the collective degrees appear in Eq. (21) as assumed above. Then the last line of (7) reduces to

$$\left[1-\frac{1}{A}-s_A^2\right]\Delta_A-(A-4)s_A\frac{\partial}{\partial s_A}.$$
 (22)

To further simplify the problem, a simple s_A dependence of the potential is assumed, such that the total potential has the form

$$V = V_{y}(y) + \frac{1}{y^{2}} \{ V_{\beta}(\beta) + V_{s_{A}}(s_{A}) \} .$$
 (23)

Equation (23) includes the ordinary shell model with an oscillator potential, which has no s_A dependence at all and also no β dependence, because

$$\sum_{n=1}^{A} r_n^2 = y^2 \tag{24}$$

as a consequence of the constraints (4). The very important difference in comparison to the ordinary shell model is the strong β dependence of the poten-

tial assumed here.

Placing (21) into the Schrödinger equation, multiplying with the complex conjugate (c.c.) of the sum in Eq. (21), and integrating over φ , ϑ , ψ , ϑ_A , and φ_A , one obtains an equation for f_0 the solution of which, with the lowest energy eigenvalue, is just f_0 . Now there may be different kinds of excitations, as will be discussed below.

A. Single particle excitations

(1). Excitations of the internal angular momentum, that is, l_i in the excited state is different from the ground state; but still $l_s = 0$. So the form (21) of the wave function is retained.

(2). Excitations in the s_A space. With the simple form (23) of the potential one has

$$f_0 = g_0(y,\beta) h_0(s_A) , \qquad (25)$$

so there may be separate excitations of the s_A dependence.

B. Collective excitations

(1). Vibrational states: pure excitatons in y, β , and γ space. In this case there is a function g in (25) which is different from the ground state.

(2). Rotational states: $l_s \neq 0$; l_i unchanged; the y, β , and γ dependence also change in this case.

There may of course be excitations which include all the different kinds.

Strictly speaking there is never a pure single particle excitation, even with the potential of the form (23), because the y dependence of the wave function in an excited state will always be different from the ground state. But $V_y(y)$ must have a very strong maximum for a special value of y leading to a constant nuclear density, almost equal in all states. That means that the y dependence is almost the same in all states, except of course for vibrations in y space (density or monopole vibrations), which seem to be rare in nuclei.

Support for the new definition of (21) as genuine single particle states comes from looking at the ordinary shell model states. Transforming them with (1)to the new coordinates one will probably find in all cases that the largest percentage of the wave function has the form (21). As an example, the transformation was performed for a single case only, namely, a *d* nucleon in an oscillator potential, and all other nucleons in *s* states. In that case the fraction, which the genuine single particle state (21) contributes to the wave function, is

$$(3A-1)/(3A+3);$$

it is close to 1. The rest will be of a collective nature. This result is quite satisfactory and shows that the old problem of a genuine unification of the single particle and collective models may really be solved via the transformation (1): In the body-fixed system one has a clear distinction between collective and single particle states, while the ordinary shell model states always contain a small fraction of collective excitation when looked at from the new standpoint. This fact explains that one needs quite a number of ordinary shell model states to describe a collective excitation.

V. SPIN ORBIT COUPLING

The spin orbit coupling is introduced as a phenomenologic interaction to obtain the magic numbers in the ordinary shell model. If one transforms the inner product $\vec{\sigma}_n \cdot \vec{l}_n$, which occurs in the spin orbit coupling, with (1) to the body-fixed system, one obtains a sum of two terms; the first is proportional to $\vec{\sigma}_n \cdot \vec{L}_e$, where \vec{L}_e is the total orbital angular momentum, Eq. (9). The second term is

proportional to

 $\vec{\sigma}_n \cdot \vec{l}_{ni}$, where

$$\vec{1}_{ni} = -i \not n \left[s_{n2} \frac{\partial}{\partial s_{n3}} - s_{n3} \frac{\partial}{\partial s_{n2}}, \dots, \dots \right]$$
(27)

is the orbital angular momentum operator for the *n*th nucleon defined with the single particle coordinates s_n and occurring in Eq. (10) already. The index *i* stands for "internal" as before.

The factors multiplying these two terms are rather complicated functions of all the coordinates. As a consequence, this transformed spin orbit coupling would complicate the mathematical treatment of all the problems. For this reason the spin orbit coupling is redefined. The first term is ignored completely; only the term (26) is taken into account. For the factor multiplying (26) one will take simple functions of s_n , possibly of the same form as in the ordinary shell model, with r_n now replaced by s_n .

With such a spin orbit interaction the quantity

$$\vec{j}^{2} = \left[\vec{L}_{i} + \frac{1}{2}\sum_{n}\vec{\sigma}_{n}\right]^{2}$$
(28)

will play the role which the total angular momentum plays in the ordinary shell model. The solution of the Schrödinger equation will be an eigenfunction of \vec{j}^2 . It must of course be an eigenfunction of the total angular momentum square

$$\vec{\mathbf{J}}^{2} = \left[\vec{\mathbf{L}}_{e} + \frac{1}{2}\sum_{n}\vec{\sigma}_{n}\right]^{2}.$$
(29)

It is not so obvious that it really is, because (26) contains the Euler angles: If one refers the components of the two vectors in (26) to the center of mass system, then \vec{L}_{ni} depends on the Euler angles. One can see this from the form (27) of the vector operator \vec{L}_{ni} , which refers to the body-fixed axes and does not depend on the Euler angles. This dependence is brought in through the rotation to the center of mass system. If, on the other hand, one chooses the body-fixed system as the frame of reference, the components of the vector operator $\vec{\sigma}_n$ depend on the Euler angles.

As (29) depends on the Euler angles too, a check on the commutation relations seemed necessary. It revealed that \vec{J}^2 and the spin orbit coupling commute. \vec{j}^2 , Eq. (28) also depends on the Euler angles via the term $\vec{L}_i \cdot \vec{\sigma}_n$. One finds that \vec{j}^2 and \vec{J}^2 also commute. \vec{L}_e^2 does not commute with the spin orbit coupling; hence different values of l_e will appear in the wave function.

(26)

VI. THE CASES OF STRONG AND WEAK COUPLING

One can now construct eigenfunctions which correspond to the cases of the so-called strong and weak coupling in the Nilsson model. The operators and their eigenvalues are as follows:

OperatorEigenvalue
$$\vec{J}^2$$
 $\hbar^2 J (J+1)$ J_{z} $\hbar M$ \vec{J}^2 $\hbar^2 j (j+1)$ j_3 $\hbar m_j$ $(\vec{L}_e + \vec{L}_i)^2$ $\hbar^2 l_s (l_s+1)$ $L_{e^3} + L_{i3}$ $\hbar \kappa$ \vec{L}_e^2 $\hbar^2 l_e (l_e+1).$

The case of the so-called strong coupling can only occur when the nucleus is deformed; for example, when $y_1 = y_2 \neq y_3$. One has a potential which depends strongly on ϑ_A and hence couples the particle motion to the nuclear symmetry axis. In this case one will use eigenfunctions of the five commutable operators \vec{J}^2 , J_z , \vec{j}^2 , j_3 , and $L_{e3} + L_{i3}$, though the solution will not be an eigenfunction of \vec{j}^2 ; it will be a mixture of functions with different j. But in many cases it may be sufficient to take into account a single j value; that will be done here. The eigenfunctions of \vec{J}^2 , J_z , and $L_{e3} + L_{i3}$ can be written immediately and have the form

$$\sum_{m_e} \begin{pmatrix} l_e & \frac{1}{2} & J \\ m_e & M - m_e & M \end{pmatrix} D^l_{m_e,\kappa - K_i}(\varphi, \vartheta, \psi) Y_{lK_i}(\vartheta_A, \varphi_A) s_{M - m_e} .$$
(30)

In addition, (30) is an eigenfunction of \vec{L}_e^2 , \vec{L}_i^2 , and L_{i3} . In general the solution of the Schrödinger equation will be a linear combination of eigenfunctions with different eigenvalues of these three latter operators. s_{M-m_e} are the spinfunctions α and β of the nucleon.

In our case one has to construct from (30) eigenfunctions of \vec{j}^2 and j_3 . They will be linear combinations of (30): ſ ٦

$$\Psi_{jm_{j\kappa}}^{JM} = \sum_{l_{e}} \sum_{K_{i}} \sum_{m_{e}} a_{l_{e}K_{i}} \begin{bmatrix} l_{e} & \frac{1}{2} & J \\ m_{e} & M - m_{e} & M \end{bmatrix} D_{m_{e},\kappa-K_{i}}^{l_{e}} Y_{lK_{i}} S_{M-m_{e}} .$$
(31)

Here only a single l value has been taken into account as mentioned above. $a_{L_eK_i}$ are determined in the following way: Applying

$$j_3 = L_{i3} + \frac{1}{2}\sigma_3 \tag{32}$$

[where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the spin operator of the single nucleon referred to the body-fixed system] to (31) one has to use

$$L_{i3}Y_{IK_i} = \hbar K_i Y_{IK_i} .$$

 σ_3 cannot be applied to s_{M-m_p} directly, because this spinfunction refers to the center of mass system. One has to relate it with the functions $D_{\mu\mu'}^{1/2}(\varphi \vartheta \psi)$ to the $s'_{\mu'}$ in the body-fixed system. Having done that, σ_3 can be applied to $s'_{\mu'}$ and the requirement that (31) is an eigenfunction of j_3 yields relations between the coefficients $a_{l_e K_i}$. Other relations are found when requiring that (31) is an eigenfunction of \vec{j}^2 . It is already an eigenfunction of \vec{L}_i^2 and of $\vec{\sigma}^2$ occurring in \vec{j}^2 , but not of $\vec{L}_i \cdot \vec{\sigma}$. Again the components of \vec{L}_i and of $\vec{\sigma}$ are referred to the body-fixed system:

$$\dot{\mathbf{L}}_i \cdot \vec{\sigma} = L_{i1}\sigma_1 + L_{i2}\sigma_2 + L_{i3}\sigma_3 . \tag{34}$$

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Again one has to use the form of (31) in which the s_{M-m_e} are transformed to the body-fixed system.

The final result one finds this way is

$$\Psi_{jm_{j\kappa}}^{JM} = (8\pi^{2})^{-1/2} \sum_{l_{e}} \sum_{m_{e}} \sum_{K_{i}} (-)^{l_{e}} (2l_{e}+1)^{1/2} \begin{pmatrix} l_{e} & \frac{1}{2} & J \\ m_{e} & M-m_{e} & M \end{pmatrix} \\ \times \begin{pmatrix} J & \frac{1}{2} & l_{e} \\ \kappa-m_{j} & m_{j}-K_{i} & \kappa-K_{i} \end{pmatrix} \begin{pmatrix} l & \frac{1}{2} & j \\ K_{i} & m_{j}-K_{i} & m_{j} \end{pmatrix} D_{m_{e},\kappa-K_{i}}^{l_{e}} Y_{lK_{i}} S_{M-m_{e}} .$$
(35)

 $y_1 = y_2$ owing to the term

In the strong coupling case one has a ϑ_A -dependent potential and the general solution of the Schrödinger equation, assuming a nucleus of rotational symmetry, will be a linear combination of functions (35) belonging to different eigenvalues *j*. Furthermore, κ must be zero in the case of rotational symmetry with

$$\frac{1}{\sin^2(\gamma - 4\pi/3)} (L_{e3} + L_{i3})^2 \tag{36}$$

in the kinetic energy, which is singular when $y_1 = y_2$. The spectra of nuclei with strong coupling consist of $|m_j|$ bands (usually called K bands; the symbol m_j is used here because the definition of j is different from the ordinary unified model), see e.g., Ref. 9. The Coriolis term is treated as a perturbation in that case. The corresponding term here is the one which is proportional to

$$L_{e_1}L_{i_1} + L_{e_2}L_{i_2} . (37)$$

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The expectation value of (37) using (35) with $\kappa = 0$ as the wave function is found to be proportional to

$$(-)^{J}(J+\frac{1}{2})\delta_{|m_{j}|,1/2},$$
 (38)

with a very small correction proportional to

$$(J + \frac{1}{2})\delta_{|m_i|, 1/2}$$
, (39)

that is, without the factor $(-)^J$ of Eq. (38). So the characteristics of the $|m_j| = \frac{1}{2}$ band are reproduced in the genuine unified nuclear model. In the case of weak coupling one has no potential which couples the single particle motion to the axes \vec{y}_1, \vec{y}_2 , and \vec{y}_3 . So l and l_s are good quantum numbers, but m_j is not. The solution of the Schrödinger equation is again taken as a linear combination of (30):

$$\Psi_{jl_{s\kappa}}^{JM} = \sum_{l_{e}} \sum_{K_{i}} \sum_{m_{e}} b_{l_{e}K_{i}} \begin{pmatrix} l_{e} & \frac{1}{2} & J \\ m_{e} & M - m_{e} & M \end{pmatrix} D_{m_{e},\kappa-K_{i}}^{l_{e}} Y_{lK_{i}} S_{M-m_{e}} .$$
(40)

The expansion coefficients $b_{l_eK_i}$ are determined in the same way as the $a_{l_eK_i}$ of Eq. (31), the only difference being that (40) must be an eigenfunction of $(\vec{L}_e + \vec{L}_i)^2$ instead of j_3 . The result is the following:

$$\Psi_{jl_{s\kappa}}^{JM} = (8\pi^{2})^{-1/2} \sum_{l_{e}} \sum_{m_{e}} \sum_{K_{i}} (2j+1)^{1/2} (2l_{e}+1) \begin{cases} l & l_{e} & l_{s} \\ J & j & \frac{1}{2} \end{cases}$$

$$\times \begin{bmatrix} l_{e} & \frac{1}{2} & J \\ m_{e} & M - m_{e} & M \end{bmatrix} \begin{bmatrix} l & l_{e} & l_{s} \\ K_{i} & \kappa - K_{i} & \kappa \end{bmatrix} D_{m_{e},\kappa - K_{i}}^{l_{e}} Y_{lK_{i}} S_{M-m_{e}} .$$
(41)

For spherical symmetry ($\beta = 0$) one has $l_s = 0$, which follows from the singular behavior of the kinetic energy operator. From the properties of the 6*j* symbol in (41) one obtains J=j. So the spins of nuclei near closed shells, like those of ¹⁷O and ¹⁷F, are reproduced.

VII. FIRST APPLICATION: QUADRUPOLE MOMENTS OF MIRROR NUCLEI

The relation between deformations and charge distributions on one hand and the quadrupole moments of mirror nuclei on the other hand are examples of the usefulness of the genuine unified nuclear model. The quadrupole moment operator of a single proton has approximately the following form [(43)], when transformed to the new coordinates;

$$Q_n = 3z_n^2 - r_n^2 \tag{42}$$

$$\approx [8\pi (10\pi)^{1/2}/15] s_n^2 y^2 [\sqrt{2}\chi_{20}^{20}\beta \cos(\gamma - 4\pi/3) + \chi_{22}^{00}], \qquad (43)$$

where

$$\chi_{l_{e}l_{i}}^{l_{g}\kappa} = [(2l_{e}+1)/8\pi^{2}]^{1/2} \sum_{K} \begin{pmatrix} l_{e} & l_{i} & l_{g} \\ K & \kappa - K & \kappa \end{pmatrix} D_{0K}^{l_{e}}(\varphi, \vartheta, \psi) Y_{l_{i},\kappa - K}(\vartheta_{A}, \varphi_{A}) .$$
(44)

There are additional terms in Q which contain all the functions (44) with $l_e = l_i = 2$. They were dropped in Eq. (43) because they are linear in β (those with $l_g = 2$) or quadratic (those with $l_g = 4$; odd values of l_g do not occur) and their contributions are small compared to those of the two terms in Eq. (43). For rotational symmetry with $y_1 = y_2$ one has either $\gamma = 4\pi/3$ (prolate nuclei) or $\gamma = \pi/3$ (oblate nuclei).

There is a certain justification for calling the first term in (43), which is proportional to χ^{20}_{20} , the contribution of the *n*th proton to the collective part of the quadrupole moment. The second term, which is proportional to χ^{00}_{22} , is the single particle quadrupole moment. Justification for this terminology is as follows: The function χ_{20}^{20} does not depend on the angles ϑ_A and φ_A . So even with the proton A in the 1s state this term will give a contribution to the quadrupole moment. An example would be a wave function with $l_e = 2$, which in addition to the dependence on φ , ϑ , and ψ , depends only on y_1 , y_2 , and y_3 and not on \vec{s}_n (for example, a rotational state of a system of particles which are all in the 1s state). The quadrupole moment then comes from the deformation of the charge distribution (which for $\beta = 0$ is spherically symmetric).

The second term in (43) also contributes when there is no deformation ($\beta = 0$). It does not contribute for single particle states of spherical symmetry (l=0). This dependence on the angular distribution of the single particle justifies the designation of this term as a single particle quadrupole moment.

In the following the author will attempt to explain the quadrupole moments of the two mirror nu-

$$\Psi = \left(\frac{5}{8}\pi^{-2}\right)^{1/2} \sum_{K} \begin{bmatrix} 2 & 2 & 0 \\ K & -K & 0 \end{bmatrix} D_{2K}^{2}(\varphi, \vartheta, \psi) f_{2, -K}$$

(which is for M = 2, as needed to compute the quadrupole moment). The functions $f_{2,k}$ contain the spin functions, the single particle coordinates \vec{s}_n , and the collective coordinates y_1, y_2 , and y_3 . They are eigenfunctions of \vec{L}_i^2 and L_{i3} with eigenvalues 2 and k, respectively, just as for the ordinary antisymmetrized shell model wave function with one nucleon in the $d\frac{5}{2}$ shell. The expectation value of χ^{20}_{20} , the first term in (43) is found to be zero. This follows after integration over φ , ϑ , and ψ using the fact that the functions $f_{2,K}$ are normalized:

$$\langle f_{2,K} | f_{2,K} \rangle = 1$$
 (48)

In (48) integrations are performed over all spatial coordinates except φ , ϑ , and ψ , and summations over all spin coordinates. The matrix element of χ^{20}_{20}

clei ¹⁷O and ¹⁷F, which have approximately the following values¹⁰:

¹⁷O:
$$q \approx -26 \text{ mb}$$
, (45)
¹⁷F: $q \approx 100 \text{ mb}$.

One might think that the difference in the Coulomb interactions between these two nuclei could be responsible for making ¹⁷F a prolate nucleus in contrast to the seemingly oblate ¹⁷O. For completeness such a calculation was attempted. It turned out that such an explanation is out of the question. It would require a very large nonspherical part of the Coulomb interaction of the *d* nucleon with the rest of the nucleus, that is, of the form

$$f(y_1, y_2, y_3, s_A) Y_{2m}(\vartheta_A, \varphi_A) .$$

$$(46)$$

The magnitude of (46), required to explain the quadrupole moments, would be such that the energy spectra of the two mirror nuclei would be completely different. The conclusion is that the effect of the Coulomb interaction on the quadrupole moments is negligible. In the following a completely antisymmetrized wave function is assumed. For the orbital angular momentum only the contribution of $l_e = 2$ is carried along, although $l_e = 3$ will give some contribution for a $d\frac{5}{2}$ state, as can be seen from Eq. (35).

The case of weak coupling, corresponding to Eq. (40), will be discussed first. For small deformations, which one expects for ¹⁷O and ¹⁷F, one may drop the contributions of $l_s \neq 0$. Then the wave function has the following form:

is then proportional to

$$\sum_{K} \begin{bmatrix} 2 & 2 & 2 \\ K & 0 & K \end{bmatrix},$$
(49)

which is zero.

The second term in Eq. (43) contains the matrix element of χ_{22}^{00} and gives a nonzero contribution to the quadrupole moment. In the following, Q_n [Eq. (43)] will be written as

$$Q_n = Q_n^c + Q_n^s , \qquad (50)$$

where c and s stand for "collective" and "single" particle, respectively. Statements about the quadrupole moments of mirror nuclei can now be derived from the contraints (4), which are equivalent to the

following six constraints, as can be shown easily:

$$\sum_{n=1}^{A} s_n^2 Y_{2m}(\vartheta_n, \varphi_n) = 0 , \qquad (51a)$$

$$\sum_{n=1}^{A} s_n^2 = 3 . (51b)$$

The same spherical harmonics as in (51a) are present in χ^{00}_{22} .

One has

$$\sum_{n=1}^{A} \chi_{22}^{00}(n) s_n^2 = 0$$
(52)

or

$$\sum_{n=1}^{A} Q_n^s = 0 . (53)$$

The sum in (53) includes the neutrons, while in the quadrupole moment only the protons enter:

$$Q = \sum_{\text{protons}} (Q_n^c + Q_n^s) .$$
 (54)

For the expectation values it was already shown that in the case of weak coupling there is no contribution from Q_n^c , so

$$q = \langle Q \rangle = \sum_{\text{protons}} \langle Q_n^s \rangle .$$
 (55)

As the wave function is completely antisymmetrized, the contributions of all the protons are equal:

$$\langle Q_n^s \rangle = \langle Q^s \rangle_{\text{proton}}$$
 (56)

Here the index *n* was simply dropped and $\langle Q^s \rangle_{\text{proton}}$ is the contribution of a single proton to the quadrupole moment. Then (55) is

$$q = Z \langle Q^s \rangle_{\text{proton}} .$$
⁽⁵⁷⁾

The constraints (53) can be written (taking the less stringent form for the expectation values now)

$$Z\langle Q^s \rangle_{\text{proton}} + N \langle Q^s \rangle_{\text{neutron}} = 0.$$
 (58)

In mirror nuclei the roles of protons and neutrons are exchanged. This means for the example of 17 F and 17 O (ignoring the effect of the Coulomb interaction; see the above discussion):

$$\langle Q^s \rangle_{\text{proton}}^{17_{\text{F}}} = \langle Q^s \rangle_{\text{neutron}}^{17_{\text{O}}}$$
 (59)

and for the quadrupole moments:

$$q(^{17}O) = 8 \langle Q^s \rangle_{\text{proton}}^{17},$$

$$q(^{17}F) = 9 \langle Q^s \rangle_{\text{proton}}^{17},$$

$$= 9 \langle Q^s \rangle_{\text{neutron}}^{17O},$$

$$= -8 \langle Q^s \rangle_{\text{proton}}^{17O},$$
(60)

as a consequence of (58) and (59).

So the quadrupole moments of the two mirror nuclei should be of opposite sign and equal in magnitude when using the weak coupling approximation, that is there is no coupling of the nucleon motion to one of the axes \vec{y}_1 , \vec{y}_2 , or \vec{y}_3 . This statement is correct for any deformation β , and apart from the weak coupling approximation the derivation is rigorous.

The experimental values for q are opposite in sign, but very different in magnitude. Moreover, when using a simple shell model version for f_{2K} one obtains a quadrupole moment between 20 and 30 mb for ¹⁷O, and correspondingly, between -20 and -30 mb for ¹⁷F (this latter value is about the same as in the ordinary shell model). So the quadrupole moments in the weak coupling approximation are also wrong in sign.

The uncertainty in the values comes from different choices of y^2 , which was defined in Eq. (6), y_1^2 , y_2^2 , and y_3^2 are related to the moments of inertia by Eq. (5). Taking an almost spherical nucleus, which is justified here (see below), one has approximately:

$$y_1^2 \approx y_2^2 \approx y_3^2 \approx y^2/3 ,$$

$$J_1 \approx J_2 \approx J_3 \approx 2my^2/3 .$$
(61)

Assuming constant density inside the nucleus and zero density outside, one has

$$2my^2/3 \approx (\frac{2}{5})mA^{5/3}r_0^2 .$$
 (62)

There is quite an uncertainty in y^2 as the assumption of constant density is not correct and as r_0 may be somewhere between 1 and 1.4 fm.

The assumption of weak coupling has to be abandoned in the present case. Satisfactory results are found in the strong coupling approximation. Before deriving the quadrupole moments in this approximation a general formula will be given here, which is valid in any approximation, including the weak coupling. For simplicity only wave functions are considered which are eigenfunctions of \vec{L}_e^2 with quantum numbers L_e :

$$\Psi = [(2l_e+1)/8\pi^2]^{1/2} \sum_{K} D_{l_eK}^{l_e}(\varphi, \vartheta, \psi) g_K .$$
(63)

The restriction of the weak coupling approximation, that the functions g_K are eigenfunctions of \vec{L}_i^2 and L_{i3} , is dropped. Applying the relation (58) (which is rigorous) to a certain nucleus ZN [this is added as an upper index in Eq. (58) now] and replacing

$$N\langle Q^s \rangle_{\text{neutron}}^{ZN}$$
 (64)

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one obtains

$$Z\langle Q^s \rangle_{\text{proton}}^{ZN} + N\langle Q^s \rangle_{\text{proton}}^{NZ} = 0.$$
 (66)

As N is the proton number in the nucleus NZ, the relation (66) means that the sum of the single particle contributions to the quadrupole moments of mirror nuclei is zero. As a consequence, the sum of the quadrupole moments of mirror nuclei is different from zero only when $\beta \neq 0$:

$$q^{ZN} + q^{NZ} \propto \beta . \tag{67}$$

No approximation has been made to obtain Eq. (67). It also remains valid when more than one l_e value is included in Eq. (63).

To get some qualitative results a simple wave function in the strong coupling approximation is applied now to ¹⁷F and ¹⁷O (with 1s and 1p shells filled and one nucleon in the 2d shell): For the spatial part of the wave function of the nucleons in the s and p shells,

$$f_{lm}(s_n)Y_{lm}(\vartheta_m,\varphi_n) \tag{68a}$$

is used. The wave function of the nucleon in the *d* shell together with the dependence on the Euler angles is (with $y_1 = y_2 \neq y_3$):

$$f_{22}(s_n)(\frac{5}{16}\pi^{-2})^{1/2}[Y_{22}(\vartheta_n,\varphi_n)D_{2,-2}^{-2}(\varphi,\vartheta,\psi) + Y_{2,-2}(\vartheta_n,\varphi_n)D_{22}^{-2}(\varphi\vartheta\psi)].$$
(68b)

The functions f_{lm} must be seen as the unknown functions, which are to be determined eventually by a variational calculation. Below it is found that the f_{lm} are different in the substates $m = \pm 1$ and m = 0. The wave function will have a factor depending on y and β which multiplies the Slater determinant. The quadrupole moments of the two mirror nuclei will be given below in terms of the expectation values of s_n^2 , y^2 , and β . Owing to the charge independence of the nuclear forces (the roles of neutrons and protons are exchanged in mirror nuclei) all the quantities of ¹⁷O can be expressed by those of ¹⁷F. The following abbreviations will be used:

$$x_1 = \sum_{\text{protons}} \langle s_n^2 \rangle , \qquad (69a)$$

$$x_2 = \sum_{\text{neutrons}} \langle s_n^2 \rangle , \qquad (69b)$$

$$x_{3} = \left(\frac{2}{5}\right) \left\{ \left\langle s_{n}^{2} \right\rangle_{l=1,m=0}^{\text{proton}} - \left\langle s_{n}^{2} \right\rangle_{l=1,|m|=1}^{\text{proton}} \right\} - \left(\frac{1}{7}\right) \left\langle s_{n}^{2} \right\rangle_{l=2,|m|=2}^{\text{proton}}, \quad (69c)$$

$$x_4 = \left(\frac{2}{5}\right) \left\{ \left\langle s_n^2 \right\rangle_{l=1,m=0}^{\text{neutron}} - \left\langle s_n^2 \right\rangle_{l=1,|m|=1}^{\text{neutron}} \right\}, \quad (69d)$$

$$P_1 = \pm \langle \beta \rangle \langle y^2 \rangle 2^{5/2} / 21 , \qquad (69e)$$

$$P_2 = \langle y^2 \rangle_{\frac{8}{21}}^{\frac{8}{21}} , \qquad (69f)$$

where all the quantities refer to ${}^{17}F$ and $\langle s_n{}^2 \rangle_{l=1,m=0}^{proton}$ is the expectation value of $s_n{}^2$ for a proton in a 1p state with m=0, etc.

The two quadrupole moments, for which the approximate experimental values 100 mb and -26 mb are taken, and the constraints (51a) and (51b) which connect the expectation values of the different s_n^2 are now [using (68)]:

$$p_1 x_1 + p_2 x_3 = 100 \text{ mb}$$
, (70a)

$$p_1 x_2 + p_2 x_4 = -26 \text{ mb}$$
, (70b)

$$x_1 + x_2 = 3$$
, (70c)

$$x_3 + x_4 = 0$$
. (70d)

Adding (70a) and (70b) one finds, with (70c) and (70d),

$$p_1 = (\frac{74}{3}) \text{ mb}$$
 (71)

So there are three equations left for the five quantities x_1 , x_2 , x_3 , x_4 , and p_2 . From the size of the nuclear radius one knows [see Eq. (62)], that y^2 is probably within the following range:

$$1000 \text{ mb} \le \langle y^2 \rangle \le 1500 \text{ mb} , \qquad (72a)$$

so

$$381 \text{ mb} \le p_2 \le 571 \text{ mb}$$
. (72b)

Assuming that the average value of $\langle s_n^2 \rangle$ for protons is equal to the average of $\langle s_n^2 \rangle$ for neutrons, one has

$$x_1 = \frac{27}{17}, \ x_2 = \frac{24}{17},$$
 (73)

and hence

$$p_2 x_3 = -p_2 x_4 \approx 61 \text{ mb}$$
. (74)

with (72b) one has

$$-0.16 \le x_4 \le -0.1 \tag{75}$$

and with (69d)

$$0.25 \le \langle s_n^2 \rangle_{l=1, |m|=1}^{\text{neutrons}} - \langle s_n^2 \rangle_{l=1, m=0}^{\text{neutrons}} \le 0.4 .$$
(76)

In the ordinary shell model this quantity would be zero. This quantity not being zero means a considerable deformation of the 1*p* shell. Owing to (76) the neutron 1*p* shell is oblate: The average distance from the center of mass of the neutrons with l=1, |m|=1 is considerably larger than that for l=1, m=0. The |m|=1 neutrons have a density distri-

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bution which is proportional to $\sin^2 \vartheta_n$. It has its maximum in the $\vec{y}_1 - \vec{y}_2$ plane. Owing to (76) its radius is increased, while the radius of the m = 0 distribution, which has its maximum on the \vec{y}_3 axis, is diminished.

Similarly, it follows that the proton 1p shell is prolate. Going from the lower limit of 0.25 to the upper limit of 0.4 in (76) the deformation of the neutron 1p shell increases. For the lower limit of 0.25 the author checked that there exist reasonable values for all $\langle s_n^2 \rangle$ which solve Eq. (70). For this special example the deformation $\langle \beta \rangle$ is found from Eq. (71) with $\langle y^2 \rangle = 1500$ mb:

$$\langle \beta \rangle = 0.06 . \tag{77}$$

For comparison the deformations for the neutrons and protons will be calculated approximately.

Assuming that the proton and the neutron distributions are rotationally symmetric around the \vec{y}_3 axis, as is the mass distribution, and applying the transformation (1) to neutrons and protons separately, one obtains (again for ¹⁷F):

$$\langle \beta_p \rangle = 0.16 \text{ (prolate)}, \tag{78}$$

$$\langle \beta_n \rangle = 0.04 \text{ (oblate)}$$
. (79)

For 17 O the values of (78) and (79) have to be exchanged.

VIII. CONCLUSION

The application of the genuine unified model to the case of the two mirror nuclei 17 F and 17 O shows that the quadrupole moments of these two nuclei cannot be explained in the so-called weak coupling approximation, that is, without coupling of the nucleon motion to the symmetry axis. In that case, the sum of the two quadrupole moments would be zero and they both would be opposite in sign to the experimental values. The strong coupling approximation in which *all* the nucleons are coupled strongly to the symmetry axis (assuming that there is one) yields very good results. So it can be concluded that the truth is very close to the strong coupling approximation.

It has been demonstrated in this paper that the new concept of collective and single particle coordinates is useful for smaller nucleon numbers than the conventional collective model is. In addition, it has been shown already for a non-nuclear problem that the coordinates can be useful for very small particle numbers (in this case for four particles).¹¹

This work is dedicated to the memory of Gregory Breit, my former teacher.

APPENDIX: THE SINGLE COORDINATES

Instead of the \vec{s}_n vectors one may as well use Jacobi vectors, which are defined in terms of the \vec{s}_n (and by which the \vec{s}_n can be expressed):

$$\vec{a}_{1} = (\vec{s}_{2} - \vec{s}_{1})/\sqrt{2} ,$$

$$\vec{a}_{2} = \{\vec{s}_{3} - (\vec{s}_{1} + \vec{s}_{2})/2\}(\frac{2}{3})^{1/2} ,$$

$$\vdots$$

$$\vec{a}_{A-1} = \{\vec{s}_{A} - (\vec{s}_{1} + \cdots + \vec{s}_{A-1})/(A-1)\} \times [(A-1)/A]^{1/2} .$$
(80)

The constraints (4) also hold for these Jacobi vectors:

$$\sum_{n=1}^{A-1} a_{nj} a_{nk} = \delta_{nk} .$$
 (81)

The components of $a_{1j}, a_{2j}, \ldots, a_{A-1,j}$ can be considered the components of a unit vector. The three unit vectors with j = 1, 2, and 3 are orthogonal. So we can define them as the first three columns of an orthogonal matrix:

$$\begin{bmatrix} a_{11}, & a_{12}, & a_{13} \cdots \\ a_{21}, & a_{22}, & a_{23} \cdots \\ \vdots & \vdots & \vdots \\ a_{A-1,1}, & a_{A-1,2}, & a_{A-1,3} \cdots \end{bmatrix}.$$
 (82)

One can define the a_{nj} in terms of 3A-9 angles.

A special orthogonal matrix M would be, for example,

$$M = (M_{12} \ M_{13} \ M_{14} \cdots M_{1,A-1})$$

= $(M_{23} \ M_{24} \cdots M_{2,A-1})$
= $(M_{34} \cdots M_{3,A-1})$, (83)

where

$$\boldsymbol{M}_{12} = \begin{pmatrix} \cos\varphi_{12}, & \sin\varphi_{12}, & 0, & 0 \cdots \\ -\sin\varphi_{12}, & \cos\varphi_{12}, & 0, & 0 \cdots \\ 0, & 0, & 1, & 0 \cdots \\ 0, & 0, & 0, & 1 \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$
(84)

and M_{ik} is defined correspondingly. The first three columns of M would be just a special representation for the a_{nj} . The part of the volume element depending on the single particle coordinates, now the angles φ_{ii} , was found to be

$$(\sin\varphi_{13}\sin^{2}\varphi_{14}\sin^{3}\varphi_{15}\cdots\sin^{A-3}\varphi_{1,A-1})(d\varphi_{12}\cdots d\varphi_{1,A-1}) (\sin\varphi_{24}\sin^{2}\varphi_{25}\cdots\sin^{A-4}\varphi_{2,A-1})(d\varphi_{23}\cdots d\varphi_{2,A-1}) (\sin\varphi_{35}\cdots\sin^{A-5}\varphi_{3,A-1})(d\varphi_{34}\cdots d\varphi_{3,A-1}).$$
(85)

In the main part of this paper it was proposed to treat the \vec{s}_n vectors as independent. This can be done only when $A \gg 1$, as was already mentioned. For small particle numbers one would have to use angles as the φ_{ik} . The four particle problem has already been studied in detail.⁸ In that case the matrix (82) reduces to a three by three matrix, whose elements can be defined in terms of only three angles.

With the use of the Jacobi coordinates the double sum in the last line of Eq. (7) is replaced by

$$\sum_{n}\sum_{n'}(\delta_{nn'}-\vec{a}_n\cdot\vec{a}_{n'})\vec{\nabla}_n\cdot\vec{\nabla}_{n'}-(A-4)\sum_{n}\vec{a}_n\cdot\vec{\nabla}_n \ . \tag{86}$$

For four particles the three vectors \vec{a}_n are orthogonal unit vectors. So this whole term vanishes for A = 4.

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