# Nuclear Vibrations, Rotations, and the Shell Model. I

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The relationship between the shell model and the rotation-vibration model of nuclear structure is discussed. A method for reformulating the shell-model problem in terms of a vibrational-rotational Schrödinger equation is given. The two- and four-body problem in the sd shell is discussed in detail.

# I. INTRODUCTION

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m standing \ the \ rotational \ collective \ modes \ of \ nuclear}$ motions from the point of view of the shell model. Using a shell-model representation based on quantum numbers derived from the group  $SU_3$ , Elliott<sup>1</sup> has shown how shell-model states can be constructed which have the properties of collective rotational motion. Explicit calculations in the sd shell have been carried out using this representation for  $\mathrm{Ne}^{20}$  and  $\mathrm{Mg}^{24,2,3}$ 

Nuclear vibrational modes of motion have been treated by Griffin and Wheeler<sup>4</sup> and by Moszkowski.<sup>5</sup> Their main physical assumption is that the wave function can be expressed in terms of a "Hill-Wheeler"6 integral, which is a plausible form for a vibrating system. The problem then becomes that of finding the Schrödinger equation for the vibrational motion after one has first chosen vibrational variables. The latter problem of finding the proper vibrational variables is not quite analogous to the case of rotations where one at least knows that the canonical momenta involved are the usual angular momentum operators. In the case of vibrations one must study the Hamiltonian to find the proper variables or make some "ansatz" such as is done when one concentrates attention on quadrupole deformations.

In the present work we wish to reformulate the shellmodel problem in terms of a vibrational-rotational model. The Schrödinger equation for this model must yield the shell model energies and eigenfunctions, though the eigenfunctions may have quite a different representation. In fact, the eigenfunctions in this model explicitly display the vibrational aspect of the motion.

## II. THE TWO-BODY CASE

In our treatment of the shell-model problem we assume that we are given a two-body force plus a one-body

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central force. The one-body force represents the effects of the lower lying closed shells on the outside particles which interact among themselves via the two-body potential. Usually the outer particles are restricted to a major shell and one must set up the matrix of the given force and diagonalize it over the space of that major shell.

A simple nontrivial case is that of two particles in the sd shell without spin. There are five space-symmetric states

$$s^{2}(0), d^{2}(0), sd(2), d^{2}(2), d^{2}(4),$$

and three spatially antisymmetric states

 $d^{2}(1), sd(2), d^{2}(3).$ 

The number in parenthesis is the value of L to which the two orbitals are coupled. The shell-model Hamiltonian, a scalar, is symmetric under particle exchange; hence it only mixes states of the same L and space symmetry. For example in the case of L=0 one must diagonalize the  $2 \times 2$  matrix of H in the  $s^2(0)$ ,  $d^2(0)$ subspace. The eigenvectors of H which are symmetric under particle exchange are of the form

$$\begin{split} \Psi^{(0,1)} &= \alpha s^2(0) + \beta d^2(0), \qquad \Psi^{(2,1)} = \mu s d(2) + \nu d^2(2), \\ \mathrm{E}^{(0,2)} &= -\beta s^2(0) + \alpha d^2(0), \quad \Psi^{(2,2)} = -\nu s d(2) + \mu d^2(2), \quad (1) \\ \Psi^{(4,1)} &= d^2(4), \end{split}$$

where

$$\alpha^2 + \beta^2 = 1, \quad \mu^2 + \nu^2 = 1,$$

and the superscripts on  $\Psi^{(L,\gamma)}$  designate the angular momentum L and differentiate between states of the same angular momentum with the index  $\gamma$ .

Consider the possibility that the states  $\Psi^{(L,\gamma)}$  can be interpreted in terms of two rotational bands  $\Psi^{(L,1)}$ (L=0, 2, 4) and  $\Psi^{(L,2)}$  (L=0, 2). We assume, in addition, that the "intrinsic motion" in each band is given by independent-particle wave functions corresponding to motion in an axially symmetric field. The possible single-particle "intrinsic" orbitals are then of the form

$$y_{s_0} + d_0, -s_0 + y d_0, d_1, d_{-1}, d_2, d_{-2},$$
 (2)

where y is a deformation sensitive parameter which gives the ratio of  $d_0$  to  $s_0$  state in the  $m_L = 0$  orbitals. Let us assume in addition that the orbital  $ys_0+d_0$  lies lowest in energy. Our intrinsic wave function would then be

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<sup>†</sup> The research reported in this document has been sponsored in part by the Aeronautical Research Laboratory, OAR through the European Office, Aerospace Research, U. S. Air Force.

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<sup>1</sup> J. P. Elliott, Proc. Roy. Soc. (London) A245, 128, 562 (1958).
<sup>2</sup> M. K. Banerjee and C. A. Levinson (to be published).
<sup>3</sup> M. K. Banerjee, C. A. Levinson, and S. Meshkov (to be published).

 <sup>&</sup>lt;sup>4</sup> J. J. Griffin and J. A. Wheeler, Phys. Rev. 108, 311 (1957).
 <sup>5</sup> S. A. Moszkowski, Phys. Rev. 110, 403 (1958).
 <sup>6</sup> D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1106 (1953).

given by

$$(y:1,2) = [ys_0(1) + d_0(1)] \times [ys_0(2) + d_0(2)] / (1+y^2). \quad (3)$$

An intrinsic state  $\Phi$  rotating with angular momentum L can be represented<sup>7,8</sup> by the wave function

$$P^L\Phi(y:1,2),$$

where  $P^L$  projects angular momentum L out of  $\Phi$ . The assumption of a rotational band  $\Psi^{(L,1)}$  is equivalent to assuming that some  $y = y_1$  exists such that

$$\Psi^{(L,1)}(1,2) = N_L P^L \Phi(\gamma_1; 1,2), \tag{4}$$

where  $N_L$  is a normalizing constant.

When Eq. (4) no longer holds we must seek a more general description of the wave functions  $\Psi^{(L,\gamma)}$ . In order to describe vibrations we can assume that the proper "intrinsic" state is not simply  $\Phi(y: 1,2)$  but a packet of such states with different deformation parameters y. We then have the more general assumption

$$\Psi^{(L,\gamma)}(1,2) = P^L \int \phi^{(L,\gamma)}(y) \Phi(y;1,2) dy.$$
 (5)

If  $\phi^{(L,\gamma)}(y)$  is peaked about some value of  $y = y_0$  we can speak of vibrations about an equilibrium position  $y_0$ . Rather than discuss  $\phi^{(L,\gamma)}(y)$  directly it is more convenient to introduce the functions  $\psi^{(L,\gamma)}(y)$ , where

$$\psi^{(L,\gamma)}(y) \equiv \int \Psi^{(L,\gamma)*}(1,2) \Phi(y:1,2) d\tau_1 d\tau_2.$$
 (6)

From the definition of  $\Phi(y: 1, 2)$  we see that  $\psi^{(L, \gamma)}(y)$  is of the form

$$\psi^{(L,\gamma)}(y) = (A + By + Cy^2)/(1 + y^2), \qquad (7)$$

where *A*, *B*, and *C* are constants. The  $\psi^{(L,\gamma)}(y)$  functions are the expansion coefficients of  $\Phi(y: 1,2)$  in terms of  $\Psi^{(L,\gamma)}(1,2)$ . Hence

$$\Phi(y:1,2) = \sum_{L,\gamma} \psi^{(L,\gamma)}(y) \Psi^{(L,\gamma)}(1,2).$$
(8)

In order to derive the equations satisfied by  $\Psi^{(L,\gamma)}(y)$  we now consider the effect of operating on  $\Phi(y:1,2)$  with *H*. In the shell-model space in which we are working, the vector

$$H\Phi(y:1,2) \tag{9}$$

can be expanded as a linear combination of the five wave functions

$$\frac{s_0(1)s_0(2)}{\sqrt{2}}, \quad \frac{d_1(1)d_{-1}(2)+d_{-1}(1)d_1(2)}{\sqrt{2}}, \quad d_0(1)d_0(2), \\ \frac{s_0(1)d_0(2)+d_0(1)s_0(2)}{\sqrt{2}}, \quad \frac{d_2(1)d_{-2}(2)+d_{-2}(1)d_2(2)}{\sqrt{2}}, \quad (10)$$

or any other five linearly independent combinations of these five functions. For convenience we choose the

<sup>8</sup> R. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957).

following five wave functions which are in general linearly independent:

$$\Phi(y; 1,2), \quad \mathbf{L}^{2}\Phi(y; 1,2), \quad \mathbf{L}^{4}\Phi(y; 1,2),$$
$$\frac{d}{dy}\Phi(y; 1,2), \quad \frac{d^{2}}{dy^{2}}\Phi(y; 1,2). \quad (11)$$

The expansion of  $H\Phi$  now can be written

$$H\Phi(y:1,2) = [-P_{2a}(y) - P_{2b}(y)\mathbf{L}^2 - P_{2c}(y)\mathbf{L}^4 - P_1(y) \\ \times (d/dy) - P_2(y)(d^2/dy^2)]\Phi(y:1,2), \quad (12)$$

where the expansion coefficients are  $-P_{2a}$ ,  $-P_{2b}$ ,  $-P_{2c}$ ,  $-P_{1}$ , and  $-P_{2}$ .

Introducing the expansion (8) for  $\Phi(y: 1, 2)$  into Eq. (12) and using the fact that

$$H\Psi^{(L,\gamma)}(1,2) = E^{(L,\gamma)}\Psi^{(L,\gamma)}(1,2),$$

$$L^{2}\Psi^{(L,\gamma)}(1,2) = L(L+1)\Psi^{(L,\gamma)}(1,2),$$
(13)

we find

$$\sum_{L,\gamma} E^{(L,\gamma)} \psi^{(L,\gamma)}(y) \Psi^{(L,\gamma)}(1,2)$$

$$= \sum_{L,\gamma} \left[ P_{2a}(y) + P_{2b}(y) L(L+1) + P_{2c}(y) L^2(L+1)^2 + P_1(y) (d/dy) + P_0(y) (d^2/dy^2) \right] \psi^{(L,\gamma)}(y) \Psi^{(L,\gamma)}(1,2).$$
(14)

Equating coefficients of  $\Psi^{(L,\gamma)}(1,2)$  on both sides of the above equation we finally have our vibrational equation:

$$[P_{2a}(y) + P_{2b}(y)L(L+1) + P_{2c}(y)L^{2}(L+1)^{2} + P_{1}(y)(d/dy) + P_{0}(y)(d^{2}/dy^{2})] \psi^{(L,\gamma)}(y) = -E^{(L,\gamma)}\psi^{(L,\gamma)}(y).$$
(15)

The solutions of this equation which are of the form of Eq. (7) will yield the shell-model eigenvalues  $E^{(L,\gamma)}$ . The functions  $\psi^{(L,\gamma)}(y)$  have no simple orthonormality or completeness relations since they are not solutions of a self-adjoint equation. In order to put the vibrational equation into a more physically transparent form we must transform to new independent *and* dependent variables.

Equation (15) is of the form:

$$[P_0(y)(d^2/dy^2) + P_1(y)(d/dy) + P_2(y)] \psi(y)$$
  
=  $-E\psi(y). (16)$ 

Multiplying by  $[1/P_0(y)] \exp \int {}^{y} [P_1(y')/P_0(y')] dy'$  we get the standard Sturm-Liouville form:

$$(d/dy) \left\{ \left[ \exp \int^{y} (P_{1}/P_{0}) \right] (d/dy) \psi(y) \right\} \\ + \left[ P_{2}(y)/P_{0}(y) \right] \left[ \exp \int^{y} (P_{1}/P_{0}) \right] \psi(y) \\ + E \left\{ \exp \left[ \int^{y} (P_{1}/P_{0}) \right] / P_{0}(y) \right\} \psi(y) = 0. \quad (17)$$

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<sup>&</sup>lt;sup>7</sup> See discussion of  $P^L \Phi$  in reference 2.

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We now introduce a new independent variable, z,

$$z = \int^{y} (1/P_0)^{1/2} dy'.$$
 (18)

In problems with realistic nuclear forces  $P_0(y)$  will generally be positive. If not, then the transformations can be modified so that z is real. We also introduce a new dependent variable u.

$$u = \left\{ \exp\left[ \int^{u} (P_{1}/P_{0}) dy' \right] \middle/ P_{0}^{1/4} \right\} \psi.$$
 (19)

In terms of u and z, the vibrational equation becomes

$$-\left[d^2u(z)/dz^2\right]+V(z)u(z)=Eu(z),$$

where

$$V = -P_{2} + \left(2\frac{dP_{1}}{dy} - \frac{d^{2}P_{0}}{dy^{2}}\right) / 4 + \left(\frac{dP_{0}}{dy} - 2P_{1}\right) \left(3\frac{dP_{0}}{dy} - 2P_{1}\right) / 16P_{0}.$$
 (20)

Sturm-Liouville theory<sup>9</sup> gives us the orthogonality properties of  $\psi(y)$ . We introduce the weight function

$$W(y) = 1/P_0 \exp \int^y (P_1/P_0) dy'.$$
 (21)

Assume that  $\exp \int {}^{y}(P_{1}/P_{0})dy'$  has two zeros which we designate a and b, where a < b. In the interval between a and b we assume  $P_{0}$  has no zeros and that  $W \ge 0$ . It then follows that for any solutions  $\psi_{1}, \psi_{2}$  of Eq. (17) corresponding to different eigenvalues  $E_{1}$  and  $E_{2}$ 

$$\int_{a}^{b} \psi_{1}(y)\psi_{2}(y)W(y)dy = 0.$$
 (22)

It is convenient to normalize  $\psi_i(y)$  so that

$$\int_{a}^{b} \psi_{i}(y)\psi_{j}(y)W(y)dy = \delta_{ij}.$$
(23)

Returning to Eq. (8), which gives the expansion for  $\Phi(y; 1,2)$ , we multiply both sides by  $\psi^{(L,\gamma)}(y)W(y)$  and integrate to give

$$\int_{a}^{b} \psi^{(L,\gamma)}(y) W(y) \Phi(y; 1, 2) dy$$
  
=  $\sum_{L',\gamma'} \int_{a}^{b} \psi^{(L,\gamma)}(y) W(y)$   
 $\times \psi^{(L',\gamma')}(y) \Psi^{(L',\gamma')}(1, 2) dy.$  (24)

<sup>9</sup> Cf. for example H. Margenau and G. M. Murphy, *The Mathematics of Physics and Chemistry* (D. Van Nostrand Company, Inc., Princeton, New Jersey, 1947), Sec. 8.5, p. 253. For L=L', we use Eq. (23) (assume  $E^{(L,1)} \neq E^{(L,2)}$ ) giving

$$\int_{a}^{b} \psi^{(L,\gamma)}(y)W(y)\Phi(y;1,2)dy$$
  
=  $\Psi^{(L,\gamma)}(1,2) + \sum_{\substack{L',\gamma'\\L'\neq L}} \int_{a}^{b} \psi^{(L,\gamma)}(y)W(y)$   
 $\times \psi^{(L',\gamma')}(y)\Psi^{(L',\gamma')}(1,2)dy.$  (25)

For  $L \neq L'$ , we have no orthogonality relations since  $\psi^{(L,\gamma)}$ ,  $\psi^{(L',\gamma')}$  obey different differential equations. Finally, we project angular momentum L from both sides of Eq. (25) and obtain

$$\int_{a}^{b} \psi^{(L,\gamma)}(y) W(y) P^{L} \Phi(y; 1,2) dy = \Psi^{(L,\gamma)}(1,2).$$
(26)

Thus, we have recovered the form of Eq. (5) where we can identify

$$\phi^{(L,\gamma)}(y) = \psi^{(L,\gamma)}(y)W(y). \tag{27}$$

If we introduce the rotation operator

$$\hat{\mathcal{R}}(\Omega) = \exp(-i\alpha L_z) \exp(-i\beta L_y) \exp(-i\gamma L_z),$$
  

$$\Omega = (\alpha, \beta, \gamma),$$
(28)

and define the rotated wave function

$$\hat{R}(\Omega)\Phi(y;1,2) \equiv \Phi(\Omega,y;1,2), \tag{29}$$

we can express  $P^L \Phi(y: 1, 2)$  as

$$P^{L}\Phi(y;1,2) = \int \frac{D_{0,0}^{L*}(\alpha,\beta,\gamma)}{8\pi^{2}/(2L+1)} \times \Phi(\Omega,y;1,2)d\gamma \sin\beta d\beta d\alpha, \quad (30)$$

where  $D_{mk}{}^{L}(\alpha,\beta,\gamma)$  is the standard rotation matrix. Thus we can write  $\Psi^{(L,\gamma)}(1,2)$  in the form

$$\Psi^{(L,\gamma)}(1,2) = \int_{a}^{b} W(y) dy \int d\Omega \psi^{(L,\gamma)}(y) \\ \times \frac{D_{0,0}^{L*}(\alpha,\beta,\gamma)}{(8\pi^{2})/(2L+1)} \Phi(\Omega,y;1,2). \quad (31)$$

This is the Hill-Wheeler<sup>6</sup> form in terms of a vibrational wave function  $W(y)\psi^{(L,\gamma)}(y)$  and a rotational wave function  $D_{0,0}^{L^*}(\alpha,\beta,\gamma)/[8\pi^2/(2L+1)]$ .

### **III. MANY-PARTICLE SYSTEMS**

We have obtained a vibrational-rotational description which is equivalent to the shell model. For more than two particles, it is impossible to express  $H\Phi$  in terms of functions like

$$\mathbf{L}^{2}\Phi$$
,  $\mathbf{L}^{4}\Phi$ ,  $(d/dy)\Phi$ ,  $\mathbf{L}^{2}(d/dy)\Phi$ ,  $\cdots$ .

Hence, an exact equivalence to the shell model cannot be obtained. Nevertheless, we wish to examine to what extent the exact two-body treatment can be generalized.

Consider, for example, an intrinsic state  $\Phi(y:1,2,\dots,A)$  which depends on some deformation parameter y. We then define the function

$$\psi^{(L,\gamma)}(y) \equiv \int \Psi^{(L,\gamma)*}(1,\cdots A) \times \Phi(y;1,\cdots A) d\tau_1 \cdots d\tau_A, \quad (32)$$

and try to find a differential equation satisfied by  $\psi^{(L,\gamma)}(y)$ . In order to determine an approximate vibrational equation, we can project the vector  $H\Phi(y:1,\cdots A)$  on the space defined by the vectors

$$\Phi$$
,  $\mathbf{L}^{2}\Phi$ ,  $\mathbf{L}^{4}\Phi$ ,  $(d/dy)\Phi$ ,  $(d^{2}/dy^{2})\Phi$ .

For higher accuracy one could add higher powers of  $L^2$  and even consider terms like

$$\mathbf{L}^2(d/dy)\Phi$$
,  $\mathbf{L}^2(d^2/dy^2)\Phi$ .

The general problem of projecting  $H\Phi$  on a set of functions  $\hat{O}_i\Phi$ , where  $\hat{O}_i$  are some set of operators, is equivalent to finding a set of functions  $a_i(y)$  such that

$$H\Phi = \sum_{i} a_{i}(y)\bar{O}_{i}\Phi + \chi, \qquad (33)$$

where  $\chi$  is a vector orthogonal to all  $\hat{O}_i \Phi$ , that is

$$\chi | \hat{O}_i \Phi \rangle = 0. \tag{34}$$

Using this relation we can take the scalar product of Eq. (33) with the set of vectors  $\hat{O}_{j}\Phi$  and obtain the set of equations for  $a_{i}(y)$ 

$$(\Phi | \hat{O}_{j}H | \Phi) = \sum_{i} a_{i}(y) (\Phi | \hat{O}_{j}\hat{O}_{i} | \Phi).$$
(35)

Once the expansion coefficients  $a_i(y)$  are found, the problem is continued exactly as in the two-body case. This method is not exact; one must therefore inquire about the conditions for which the approximation of projecting  $H\Phi$  on a limited subspace is accurate. Since the method leads rather directly to a model of a vibrating system, we shall see that if one assumes that the final wave function has a vibrational form, then, indeed the method of projecting will be accurate.

We therefore assume that to a good approximation  $\Psi^{(L,\gamma)}(\mathbf{1},\cdots A)$  can be written in the form

$$\Psi^{(L,\gamma)}(1,\cdots A) = P^L \int \phi^{(L,\gamma)}(y) \Phi(y;1,\cdots A) dy, \quad (36)$$

with the assumption that  $\phi^{(L,\gamma)}(y)$  is peaked about some  $y=y_0$  as shown in Fig. 1.

Hence  $\Psi^{(L,\gamma)}(1, \dots A)$  is made up of a packet of states  $P^L \Phi(y; 1, \dots A)$  weighted by  $\phi^{(L,\gamma)}(y)$ . The Hamiltonian must have the property that it does not strongly admix states  $P^L \phi(y; 1 \dots A)$  inside the packet with those outside the packet. Otherwise  $\phi^{(L,\gamma)}(y)$  would not be peaked. It is therefore possible for y, in the neighborhood



of  $y_0$ , to expand  $HP^L\phi(y: 1 \cdots A)$  in a series:

$$HP^{L}\Phi(y:1,\cdots A) \doteqdot [a_{L}(y)+b_{L}(y)(d/dy) + c_{L}(y)(d^{2}/dy^{2})]P^{L}\Phi(y:1,\cdots A).$$
(37)

To prove this result we note that our assumption of weak admixture of distant states can be written as

$$HP^{L}\Phi(y:1,\cdots A) \doteqdot \int f_{L}(y,y')P^{L}\Phi(y':1,\cdots A)dy',$$
(38)

where  $f_L(y,y')$  is large only for  $y' \sim y$  and we only consider values of y in the neighborhood of  $y_0$ . Since  $f_L(y,y')$  is only large for  $y' \sim y$  we can expand  $P^L \Phi(y', 1 \cdots A)$  inside the integral to give

$$P^{L}\Phi(y') \sim P^{L}\Phi(y) + (y'-y)(d/dy)P^{L}\Phi(y) + \frac{1}{2}(y'-y)^{2}(d^{2}/dy^{2})P^{L}\Phi(y).$$
(39)

Substituting this into Eq. (38) we arrive at the form of Eq. (37), where the coefficients  $a_L(y)$ ,  $b_L(y)$ , and  $c_L(y)$  are

$$a_{L}(y) = \int f_{L}(y,y')dy',$$
  

$$b_{L}(y) = \int f_{L}(y,y')(y'-y)dy',$$
 (40)  

$$c_{L}(y) = \int f_{L}(y,y')\frac{(y'-y)^{2}}{2}dy'.$$

We next define operators  $a(y,\mathbf{L}^2)$ ,  $b(y,\mathbf{L}^2)$ ,  $c(y,\mathbf{L}^2)$  such that

$$a_L(y)P^L\Phi(y:1,\cdots A) = a(y,\mathbf{L}^2)P^L\Phi(y:1,\cdots A),$$
 etc. (41)

In fact we see that  $a_L(y) = a(y, L(L+1))$ , etc. Finally we have

$$HP^{L}\Phi(y:1,\cdots A) \doteqdot [a(y,\mathbf{L}^{2})+b(y,\mathbf{L}^{2})(d/dy) + c(y,\mathbf{L}^{2})(d^{2}/dy^{2})]P^{L}\Phi(y:1,\cdots A). \quad (42)$$

We can sum both sides on the index L and using the fact that

$$\sum_{L} P^{L} = 1, \tag{43}$$

we finally obtain

$$H\Phi(y:1,\cdots A) \doteqdot [a(y,\mathbf{L}^2)+b(y,\mathbf{L}^2)(d/dy) + c(y,\mathbf{L}^2)(d^2/dy^2)]\Phi(y:1,\cdots A), \quad (44)$$

from which it follows as before that

$$\begin{array}{l} \underline{[}a(y,L(L+1))+b(y,L(L+1))(d/dy) \\ +c(y,L(L+1))(d^2/dy^2)]\underline{\psi}^{(L,\gamma)}(y) \\ & \div E^{(L,\gamma)}\underline{\psi}^{(L,\gamma)}(y), \quad (45) \end{array}$$

where  $\psi^{(L,\gamma)}(y)$  is defined in Eq. (6) and  $E^{(L,\gamma)}$  is an eigenvalue of H. The L<sup>2</sup> dependence of  $a(y, L^2)$ ,  $b(y, L^2)$ and  $(cy, L^2)$  may be quite complicated in general. In practice one must assume some simple form such as

$$a(y, \mathbf{L}^2) = a_0(y) + a_1(y)\mathbf{L}^2 + a_2(y)\mathbf{L}^4$$

and similarly for  $b(y, \mathbf{L}^2)$  and  $c(y, \mathbf{L}^2)$ .

### IV. FOUR-NUCLEON PROBLEM WITHOUT SPIN---Ne<sup>20</sup>

# A. Shell-Model Solution

In order to test the ideas presented above, the fournucleon problem in the sd shell is chosen. A spin-independent two-body force with Serber exchange is used. It has the form

$$H_{12} = V_0 \frac{\exp(-r_{12}/a)}{(r_{12}/a)} \left(\frac{1+P^x}{2}\right), \tag{46}$$

where  $P^x$  is the space exchange operator. Following Elliott and Flowers<sup>10</sup> we set  $V_0 = -45$  MeV and a = 1.37 $\times 10^{-13}$  cm. A harmonic oscillator potential is used to determine the shell-model representation. A length parameter  $b = 1.64 \times 10^{-13}$  cm is used, where  $\hbar \omega = \hbar^2 / m b^2$ is the harmonic oscillator energy spacing and m is the nucleon mass. H is then diagonalized in a standard manner to yield the shell-model wave functions and energies. The completely space symmetric wave functions (symmetry  $\lceil 4 \rceil$ ) and their eigenvalues are given in Table I.

# **B.** Projection

We first consider the model of a rotator with a fixed deformation. For this purpose we take an "intrinsic" state

$$\Phi(y; 1, 2, 3, 4) = \frac{[ys_0(1) + d_0(1)][ys_0(2) + d_0(2)][ys_0(3) + d_0(3)][ys_0(4) + d_0(4)]]}{(1 + \nu^2)^2}.$$
(47)

We now project angular momentum L out of the function  $\Phi$  using standard vector coupling techniques. These "projected" wave functions can be expanded in terms of the shell-model wave functions and one finds

$$P^{0}\Phi = \left[ y^{4}s^{4}(0) + \left(\frac{6}{5}\right)^{1/2}y^{2}d^{2}s^{2}(0) - 2\left(\frac{2}{35}\right)^{1/2}yd^{3}s(0) + \left(\frac{3}{35}\right)^{1/2}d^{4}(0) \right] / (1+y^{2})^{2},$$

$$P^{2}\Phi = \left[ 2y^{3}s^{3}d(2) - 2\left(\frac{3}{7}\right)^{1/2}y^{2}s^{2}d^{2}(2) + 2\left(\frac{3}{7}\right)^{1/2}yd^{3}s(2) - \frac{2}{(21)^{1/2}}d_{(1)^{4}}(2) - \frac{4}{(11\times21)^{1/2}}d_{(2)^{4}}(2) \right] / (1+y^{2})^{2},$$

$$P^{4}\Phi = \left[ 6\left(\frac{3}{35}\right)^{1/2}y^{2}d^{2}s^{2}(4) - 6\left(\frac{12}{5\times7\times11}\right)^{1/2}yd^{3}s(4) + 2\left(\frac{3}{35}\right)^{1/2}d_{(1)^{4}}(4) - 2\left(\frac{6}{7\times11\times13}\right)^{1/2}d_{(2)^{4}}(4) \right] / (1+y^{2})^{2},$$

$$P^{6}\Phi = \left[ 6\left(\frac{2}{7\times11}\right)^{1/2}yd^{3}s(6) - 6\left(\frac{2}{5\times7\times11}\right)^{1/2}d^{4}(6) \right] / (1+y^{2})^{2},$$

$$P^{8}\Phi \sim d^{4}(8).$$

In cases where  $d^4$  can couple to a given L in two different ways we follow the classifications scheme of Jahn<sup>11</sup> which utilizes the group  $R_5$ . We ask if y can be fixed to give a good overlap with the shell-model wave functions for the lowest states of given L. The overlap between  $P^{L}\Phi$  and the shell-model wave function is maximized as a function of y. In Table II are given the best value of y for each L, the overlap amplitude and a comparison of the shell model energies with the "projected" energies. The "projected" energies are found by taking the expectation value of the Hamiltonian with respect to the

"projected" wave functions after normalization. The  $SU_3$  scheme<sup>1</sup> of Elliott for (80) symmetry happens to be included among the possible "projected" wave functions if we set  $y = -1/\sqrt{2}$ . The energies and overlaps for this value of y are also given in Table II.

From Table II it is clear that the Elliott  $SU_3$  representation is reasonably good for the low excited states and that one can obtain a somewhat better fit to the wave functions and energies by increasing y from the Elliott value of  $-1/\sqrt{2} = -0.707$  to a value around -0.45. The value  $y = -1/\sqrt{2}$  corresponds to the maximum value of the intrinsic quadrupole moment. Hence this value of the deformation parameter corresponds to a maximum deformation. It is interesting to note that the best values of y, i.e.,  $y_L$ , cluster about an average

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<sup>&</sup>lt;sup>10</sup> J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London)

**A229**, 536 (1955). <sup>11</sup> H. A. Jahn, Proc. Roy. Soc. (London) **A201**, 516 (1950); **A205**, 192 (1951).

TABLE I. Shell-model and rotation-vibration energies. The shell-model eigenvalues -E(S.M.) in MeV and the normalized associated shell-model functions for four particles in the *sd* shell using the interaction potential of Eq. (46) are listed. Also given is -E(R.V.), the approximate eigenvalue derived using the rotational vibrational method leading to Eq. (58). The splittings are given for each model in the last two columns.

				L=0								
$-E(\mathbf{R.V.})$	-E(S.M.)	$d^4$		$d^3s$ $d^2s^2$		\$ <sup>4</sup>	S.M.	R.V.				
34.44	34.82	0.737	0.336		0.538	0.235	0	0				
27.39	28.72	-0.605	0.105		0.492	0.617	6.10	6.94				
21.88	23.05	-0.299		0.493	0.411	-0.706	11.77	12.45				
20.79	16.67	0.045	-0.795		0.547	-0.256	18.15	13.54				
L=2												
$-E(\mathbf{R.V.})$	-E(S.M.)	$d^{4}_{(1)}$	$d^{4}_{(2)}$	$d^3s$	$d^2s^2$	$ds^3$	S.M.	R.V.				
32.79	32.73	0.514	0.199	0.679	0.335	0.351	0	0				
25.74	26.32	-0.816	0.196	0.335	0	0.429	6.41	7.05				
20.37	23.24	-0.027	0.478	0.427	-0.486	-0.594	9.49	12.42				
	19.60	-0.226	0.180	-0.010	0.807	-0.516	13.23					
17.03	17.59	0.136	0.813	-0.494	0.022	0.274	15.14	15.76				
				L=4			· · · · · · · · · · · · · · · · · · ·					
$-E(\mathbf{R.V.})$	-E(S.M.)	$d^{4}_{(1)}$	$d^{4}$	(2)	$d^3s$	$d^2s^2$	S.M.	R.V.				
29.95	30.57	-0.806	-0.087		0.408	0.419	0	0				
22.08	23.78	0.576	0.340		-0.519	-0.532	6.79	7.87				
	20.94	0.067	-0.474		-0.732	0.485	9.63					
17.08	17.17	0.116	-0.808		0.167	-0.554	13.40	12.87				
				L=6								
$-E(\mathbf{R.V.})$		-E(S.M.)	$d^{4}$		$d^3s$	S.M.	R.V.					
25.97		25.70	0.670		0.743	0	0					
18.94		18.03	0.743		-0.670	7.03	7.67					
			1	z = 8, -E =	22.79							

value -0.47, implying that the concept of a single intrinsic state with a value of y independent of L is still approximately valid.

**C.** Rotation-Vibration We next consider the vibrational approach. We will parametrize the orbitals in a slightly different manner.

 $\chi_0(1) = \frac{-(3x+1)s_0(1) + \sqrt{2}d_0(1)}{3(3x^2+2x+1)}.$ 

When x=0 we recover the Elliott form. This is convenient for making expansions about a deformation

which is close to correct in the static rotator model

discussed above. The two-body intrinsic state is now  $\Phi(x: 1,2) = \chi_0(1)\chi_0(2).$ 

### $\Phi(x; 1, 2) \equiv \lambda_0(1)\lambda_0(2).$

We consider a general Hamiltonian H with matrix elements given by

$$G_{1} = \langle d^{2} | V_{0} | d^{2} \rangle / 5, \qquad G_{5} = \langle s^{2} | V_{0} | d^{2} \rangle / 5^{1/2},$$

$$G_{2} = \langle d^{2} | V_{2} | d^{2} \rangle / 7, \qquad G_{6} = \langle sd | V_{2} | sd \rangle,$$

$$G_{3} = 3 \langle d^{2} | V_{4} | d^{2} \rangle / 35, \qquad G_{7} = \langle s^{2} | V_{0} | s^{2} \rangle.$$

$$G_{4} = \langle d^{2} | V_{2} | sd \rangle / (14)^{1/2},$$
(50)

The subscript on V designates the value of L to which the two orbitals are coupled. The *sd* states are symmetrized. Then, our vibrational equation reads

$$H\chi_{0}(1)\chi_{0}(2) = [a(x)+b(x)\mathbf{L}^{2}+c(x)\mathbf{L}^{4}+d(x)(d/dx) + e(x)(d^{2}/dx^{2})]\chi_{0}(1)\chi_{0}(2), \quad (51)$$

TABLE II. Comparison of energies and overlaps of the Elliott scheme and the projection method with the shell model.<sup>a</sup> The splitting is given in the last three columns.

(49)

L	$E_L$	$\langle \Phi_L ig  H ig  \Phi_L  angle$	$\langle \Phi_L^{\mathrm{E1.}}   H   \Phi_L^{\mathrm{E1.}} \rangle$	УL	$\langle \Psi_L ig  \Phi_L  angle$	$\langle \Psi_L ig  \Phi_L^{ ext{El.}}  angle$	$E_L$	$\langle \Phi_L   H   \Phi_L  angle$	$\langle \Phi_L^{\mathrm{E1.}}   H   \Phi_L^{\mathrm{E1.}}  angle$
0	34.82 32.73	34.18 32.60	33.59	-0.45	0.976	0.91	0 2 00	0	0 1 48
$\frac{2}{4}$ 6	30.57 25.70	30.23 25.70	29.10 25.48	-0.34 -0.50	0.982 1.000	0.90 0.89 0.99	4.25 9.12	3.95 8.48	4.49 8.11

\*  $\Phi_L$  is the normalized "projected" wave function;  $\Phi_L \mathbb{B}^1$  is the Elliott  $SU_3$  wave function;  $E_L$  is the shell-model energy; all energies are in units of -1 MeV;  $y_L$  is the best value of y for each L;  $\Psi_L$  is the shell-model wave function given in Table I.

Define

where

$$\rho^{2} = 3x^{2} + 2x + 1,$$

$$a(x) = \frac{4}{9\rho^{4}} \left\{ \frac{3}{4} (10G_{1} + 7G_{5} + G_{7}) + 3x(5G_{1} + 11G_{6} + 2G_{7}) + \frac{9}{2}x^{2}(5G_{1} + 21G_{5} + 4G_{7}) + 27x^{3}(5G_{5} + G_{7}) + \frac{81}{4}x^{4}(5G_{5} + G_{7}) \right\},$$

$$b(x) = \frac{1}{12} \left( -13G_{1} + 20G_{2} - 3G_{3} + 20G_{4} - \frac{13}{2}G_{5} \right) + \frac{x}{4} (20G_{4} - 13G_{5}) - \frac{39}{8}x^{2}G_{5},$$

$$c(x) = \frac{1}{24} \left\{ (G_{1} - 2G_{2} + G_{3} - 2G_{4} + \frac{1}{2}G_{5}) + 3x(-2G_{4} + G_{5}) + \frac{9}{2}x^{2}G_{5} \right\},$$

$$d(x) = \frac{1}{9\rho^{2}} \left\{ (-10G_{1} + 7G_{2} + 5G_{4} - G_{5} - G_{6} + 2G_{7}) + 3x(-30G_{1} + 49G_{2} + 44G_{4} - 21G_{5} - 7G_{6} + 6G_{7}) + 3x^{2}(-90G_{1} + 189G_{2} + 318G_{4} - 150G_{5} - 27G_{6} + 18G_{7}) \right\},$$

$$e(x) = \frac{1}{9} \left\{ (-\frac{5}{2}G_{1} + 7G_{2} + 5G_{4} - \frac{1}{4}G_{5} - G_{6} + \frac{1}{2}G_{7}) + x(-15G_{1} + 42G_{2} + 57G_{4} - 15G_{5} - 6G_{6} + 3G_{7}) + x^{2} \left( -\frac{45}{2}G_{1} + 63G_{2} + 189G_{4} - \frac{135}{2}G_{5} - 9G_{6} + \frac{9}{2}G_{7} \right) + x^{3}(189G_{4} - 135G_{5}) - x^{4}\frac{405}{4}G_{5} \right\}.$$

The two-particle vibrational problem is discussed in an accompanying paper<sup>12</sup> for potentials of varying range. As shown there, the relative importance of the rotational and vibrational modes of motion depends on the range of the two-body force. For long-range forces the nucleus only rotates; as the range of the force decreases, the vibrations become more important.

For the four-particle case our vibrational equation is no longer exact and we consider the approximate form :

$$H\chi_{0}(1)\chi_{0}(2)\chi_{0}(3)\chi_{0}(4) = H\Phi(x:1,2,3,4) \approx [V_{1}(x) + V_{2}(x)\mathbf{L}^{2} + V_{3}(x)\mathbf{L}^{4} + V_{4}(x)(d/dx) + V_{5}(x)(d^{2}/dx^{2}) + V_{6}(x)\mathbf{L}^{2}(d/dx)]\Phi(x:1,2,3,4), \quad (53)$$

where the  $V_{i}(x)$  are functions chosen to project  $H\Phi(x; 1,2,3,4)$  on the subspace defined by the vectors

$$\Phi, \mathbf{L}^{2}\Phi, \mathbf{L}^{4}\Phi, (d/dx)\Phi, (d^{2}/dx^{2})\Phi, \mathbf{L}^{2}(d/dx)\Phi.$$
(54)

A physical interpretation of the operators in Eq. (53) is that  $L^2$  displays the rotational aspects of our system, d/dx and  $d^2/dx^2$  the vibrational.  $L^4$  and  $L^2d/dx$  embody the rotation-vibration interaction.

In terms of the two-particle matrix element combinations in Eq. (52) we can express the four-particle  $V_i$ 's as

$$V_{1}(x) = 6a + \frac{32b}{\rho^{2}} - \frac{16e}{\rho^{4}} + \frac{32(162x^{6} + 324x^{5} + 810x^{4} + 840x^{3} + 894x^{2} + 420x + 214)c}{\rho^{4}(\rho^{4} + 8\rho^{2} + 8)},$$

$$V_{2}(x) = b + \frac{16(27x^{4} + 36x^{3} + 51x^{2} + 26x + 21)c}{\rho^{4} + 8\rho^{2} + 8},$$

$$V_{3}(x) = \rho^{4}c/(\rho^{4} + 8\rho^{2} + 8),$$

$$V_{4}(x) = -4(3x + 1)b + 3d - \frac{4(3x + 1)}{\rho^{2}}e + \frac{8(1215x^{7} + 2835x^{6} + 4293x^{5} + 4005x^{4} + 1965x^{3} + 465x^{2} - 441x - 161)c}{\rho^{2}(\rho^{4} + 8\rho^{2} + 8)},$$

$$V_{5}(x) = e + \frac{16(3x + 1)^{2}(9x^{4} + 12x^{3} + 22x^{2} + 12x + 9)c}{\rho^{4} + 8\rho^{2} + 8},$$
(55)

 $V_6(x) = 8\rho^4(3x+1)c/(\rho^4+8\rho^2+8).$ 

<sup>12</sup> M. Kugler, following paper [Phys. Rev. **129**, 307 (1963)].

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We now follow the program outlined in Sec. II leading up to Eq. (45). The equation which results is

$$\begin{bmatrix} V_{1}(x) + V_{2}(x)L(L+1) + V_{3}(x)L^{2}(L+1)^{2} + V_{4}(x)(d/dx) \\ + V_{5}(x)(d^{2}/dx^{2}) + V_{6}(x)L(L+1)(d/dx) \end{bmatrix} \psi^{(L,\gamma)}(x) \doteq E^{(L,\gamma)}\psi^{(L,\gamma)}(x).$$
(56)  
From the form of  $\Phi$  we see that  
 $\psi^{(L,\gamma)}(x) = P^{(L,\gamma)}(x)/\rho^{4}(x),$ (57)

where  $P^{(L,\gamma)}(x)$  is at most a fourth degree polynomial in x. Naturally since Eq. (56) is only approximately correct we can only state that  $\psi^{(L,\gamma)}(x)$  of the above form is only an approximate solution. We are most interested in the region of  $x \sim 0$  where we found good "rotator" solutions. Hence we expand  $V_i(x)$  in a power series in x. We substitute the potential of Eq. (46) in the equations (50) for the  $G_i$ 's and obtain the following equations for the polynomials  $P^{(L,\gamma)}(x)$  to order  $x^4$ .

$$(44.102+49.222x+47.378x^{2}+16.527x^{3}+27.028x^{4})P^{(0,\gamma)}(x)$$

$$-(1.847+15.213x+27.676x^{2}+23.668x^{3}+14.594x^{4})\frac{d}{dx}P^{(0,\gamma)}(x)$$

$$+(0.158+1.000x+3.697x^{2}+4.967x^{3}+4.392x^{4})\frac{d^{2}}{dx^{2}}P^{(0,\gamma)}(x) = -E^{(0,\gamma)}P^{(0,\gamma)}(x)$$

$$\times(42.796+44.211x+38.329x^{2}+7.081x^{3}+11.585x^{4})P^{(2,\gamma)}(x)$$

$$-(1.791+14.908x+26.611x^{2}+20.528x^{3}+9.121x^{4})\frac{d}{dx}P^{(2,\gamma)}(x)$$

$$+(0.158+1.000x+3.697x^{2}+4.967x^{3}+4.392x^{4})\frac{d^{2}}{dx^{2}}P^{(2,\gamma)}(x) = -E^{(2,\gamma)}P^{(2,\gamma)}(x)$$

$$\times(37.805+33.321x+21.025x^{2}-8.073x^{3}-13.185x^{4})P^{(4,\gamma)}(x)$$

$$-(1.660+14.195x+24.125x^{2}+13.201x^{3}-3.649x^{4})\frac{d}{dx}P^{(4,\gamma)}(x)$$

$$+(0.158+1.000x+3.697x^{2}+4.967x^{3}+4.392x^{4})\frac{d^{2}}{dx^{2}}P^{(4,\gamma)}(x) = -E^{(4,\gamma)}P^{(4,\gamma)}(x)$$

$$\times(31.956+18.474x)P^{(6,\gamma)}(x)$$

$$-(1.455+13.075x)\frac{d}{dx}P^{(6,\gamma)}(x) = -E^{(6,\gamma)}P^{(6,\gamma)}(x).$$
(58)

If we set

$$P^{(L,\gamma)}(x) = \sum_{i=0}^{4} s_i^{(L,\gamma)} x^i,$$
(59)

we can equate coefficients of each power of x in Eqs. (59) and finally arrive at a set of linear equations for  $s_i^{(L,\gamma)}$ . We can put these equations in a matrix form. For example, for L=0 we find

$$\begin{pmatrix} 44.102 & -1.847 & 0.316 & 0 \\ 49.222 & 28.889 & -1.694 & 0.948 \\ 47.378 & 21.546 & 21.070 & 1.881 \\ 16.527 & 23.710 & 3.804 & 24.104 \end{pmatrix} \begin{pmatrix} s_0^{(0,\gamma)} \\ s_1^{(0,\gamma)} \\ s_2^{(0,\gamma)} \\ s_3^{(0,\gamma)} \end{pmatrix} = -E^{(0,\gamma)} \begin{pmatrix} s_0^{(0,\gamma)} \\ s_1^{(0,\gamma)} \\ s_2^{(0,\gamma)} \\ s_3^{(0,\gamma)} \end{pmatrix}.$$
(60)

In the above equation we have eliminated  $s_4^{(0,\gamma)}$  by using the condition that  $s_4^{(0,\gamma)} = \frac{3}{4}s_3^{(0,\gamma)}$  which corresponds to the condition that for L=0 there is no  $ds^3$  component. Continuing in this manner for the other L's all of the eigenvalues and eigenfunctions in the vibration rotation approach can be computed. The

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FIG. 2. Polynomials and weight factor for the case of Ne<sup>20</sup> as functions of deformation.

exact values of  $s_i^{(L,\gamma)}$  which come from the shell model can easily be found from the relation

$$\psi^{(L,\gamma)}(x) = \int \Psi^{(L,\gamma)*}(1,2,3,4) \\ \times \Phi(x;1,2,3,4) d\tau_1 d\tau_2 d\tau_3 d\tau_4.$$
(61)

The comparison between the energies obtained by the vibrational method and the exact values are given in Table I.

We see that the rotation vibration method is quite successful for the lower lying states but falls off in accuracy for the more highly excited states in Ne<sup>20</sup>. The probable explanation is that the higher excited states correspond to different vibrating intrinsic states and there is little overlap with the ground intrinsic state we assumed. The fact that there are more shell model states than vibrational-rotational states indicates that one must consider more intrinsic states.

#### V. VIBRATIONAL POTENTIAL FOR L=0

We wish to consider the transformation of Sec. II as applied to the Ne<sup>20</sup> case. We consider only L=0. For these polynomials we have an equation of the form

$$\begin{bmatrix} P_0(x) \frac{d^2}{dx^2} + P_1(x) \frac{d}{dx} + P_2(x) \end{bmatrix} P^{(0,\gamma)}(x)$$
  
=  $-E^{(0,\gamma)} P^{(0,\gamma)}(x).$  (62)

The coefficients  $P_0(x)$ ,  $P_1(x)$  derived from Eqs. (55) and



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FIG. 3. Vibrational potential V(z) for Ne<sup>20</sup> (L=0) as a function of the independent variable z.

(56) are shown in Fig. 2. The shapes of  $P_1(x)$  and  $P_0(x)$  are characteristic of a system vibrating about an equilibrium point determined by the zero of  $P_1(x)$ . This interpretation is expanded on in reference 12. The crucial factor which appears in the transformations described in Sec. II is

$$\exp\!\int_{x_0}^x (P_1/P_0) dx',$$

which occurs in the new dependent variable of Eq. (19) and in the weight function W(x) defined in Eq. (21). This factor is also plotted in Fig. 2. It has roots for large values of |x|, thus verifying our assumption that roots a and b exist. We see that the wave function u(x) can be appreciable in value only near an equilibrium point  $x \sim -0.2$  which corresponds to  $y \sim -0.57$ . This is just the neighborhood found by the projection method described above in Sec. IV B. In Fig. 3, we have plotted the potential V against the new independent variable z



FIG. 4. Comparison between shell model (----), rotation vibration (----), and the Elliott scheme  $SU_3$  (××××) eigenvalues for the Ne<sup>20</sup> case.



FIG. 5. Comparison of shell-model (S.M.) and rotation-vibration (R.V.) splittings with experimentally determined even parity levels of  $Ne^{20}$ . [See the review of experiments on  $Ne^{20}$  given by A. E. Litherland, J. A. Kuehner, H. E. Gove, M. A. Clark, and E. Almqvist, Phys. Rev. Letters 7, 98 (1961).]

defined in Eq. (18). At sphericity  $(x \sim -1/3)$  we have a small relative minimum but the vibrational potential clearly favors a prolate deformation. There is also another relative minimum in V for negative quadrupole moment deformations.

### VI. CONCLUSION

A comparison between the shell model, the vibrationrotation method, and the Elliott scheme is shown in Figs. 4 and 5, for the energy spectra of the potential of Eq. (46) for four particles. The experimental data also appear in Fig. 5. The rotation vibration method agrees quite well with the shell-model results for the lowest band and moderately well for the remaining bands. One should not expect good agreement between theory and experiment since only the [4] space symmetry was considered and no spin-orbit force or spin-dependent interaction was used. The agreement for the lowest states indicates that they are mainly dominated by the [4] symmetry which is pure spin singlet and so can be well treated by our approximations.

The interpretation of the 4-particle shell-model problem in terms of a vibrational potential has been demonstrated in detail and the spectra, wave functions, and vibrational potential exhibited. In the case studied, the low-lying states of the system had a small vibrational amplitude and could be almost as well described in terms of a nonvibrating rotator. As more particles are added to the system, it is expected that the "field producing"<sup>13</sup> part of the force will increase even more in importance until the middle of the shell is reached. Hence the model of a nonvibrating rotator is expected to be good in the *sd* shell for the low-lying states of more than three particles or holes.

# ACKNOWLEDGMENTS

We would like to thank Professor A. Kerman for several encouraging and illuminating conversations and Professor Lipkin for suggesting a fruitful approach on the four-particle vibrator problem. We would like to acknowledge the help given us by Professor S. Moszkowski whose own work on vibrators and rotators did much to stimulate us.

<sup>&</sup>lt;sup>13</sup> B. R. Mottelson, article on Nuclear Structure which appeared in *The Many-Body Problem* (Les Houches 1958 Session) (John Wiley & Sons, Inc., New York, 1959).