

this kind of mixing indicates that the intensity of the  $p_{1/2}^2 p_{3/2} f_{5/2}$  state is slightly larger than 72%.

### V. SUMMARY

The  $E2$  transition rate in  $Pb^{207}$  gives a value for the surface tension parameter,  $C=1100$  Mev. The  $E2$  transition rate in  $Pb^{206}$  gives  $C=520$  Mev. The quadrupole moment of  $Bi^{209}$  is consistent with  $C \approx 1000$  Mev. The discrepancy between the results of  $Pb^{207}$  and  $Pb^{206}$  appears to be real and cannot be resolved at this time.

The good agreement between the predicted energy levels and the experimentally determined energy levels of  $Pb^{204}$  show that short-range two-body forces describe the interaction between the external nucleons fairly well. Also the splitting of the levels for the first two

Mev are due for the most part to these external nucleons and do not seem to be affected by the collective motion of the core. Even the large values of the surface tension deduced in this article are not sufficient to account for the very long lifetime of the  $4+$  to  $2+$  transition in  $Pb^{204}$ . A further partial explanation of this long lifetime is suggested by the shell model calculation—that the dominant configurations in the  $2+$  and  $4+$  states differ in the quantum numbers of two particles.

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## Perturbation Procedure for Bound States of Nuclei\*

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The model of nucleons moving in a fixed harmonic oscillator well provides a convenient starting point for calculations on the structure of light nuclei. One complication, the nondiagonal energy operator associated with the motion of the center of mass, can be eliminated simply by adding the harmonic potential operator of the center-of-mass motion to the correct Hamiltonian operator of the system.

Following the construction of the correct zeroth-order linear combinations (in case of degeneracy) and the evaluation of the first-order energy matrix, the further development of the theory, in the direction of an exhaustive investigation of the consequences of assumed interaction operators, requires the evaluation of second- and higher order contributions to the energy. A simple, accurate, and powerful procedure for evaluating the second-order energy and other second-order quantities in closed form is described and explicit formulas are given for the application to the ground states of the deuteron, the triton, and the alpha particle. Numerical results for the deuteron, where a comparison with exact calculations is possible, are surprisingly good. The extension of these calculations to the first  $p$ -shell and beyond with the aid of the technique of fractional parentage coefficients appears feasible.

### I. INTRODUCTION

NUMEROUS attempts have been made to correlate the observed properties of light nuclei with assumptions about the nuclear forces.<sup>1-4</sup> The nonvanishing quadrupole moment of the deuteron requires a tensor component in the correct combination of nuclear forces. Calculations with tensor forces are difficult and have been worked out to a satisfactory degree of accuracy only for two- and three-particle problems. Rarita

and Schwinger,<sup>5</sup> using a combination of central and tensor forces, succeeded in fitting the binding energy and quadrupole moment of the deuteron and also the low-energy  $p-n$  scattering data (which essentially determines the position of the first excited state (virtual) of the deuteron). Pease and Feshbach<sup>6</sup> extended the theory to the three-particle problem using a variational technique to compute the binding energy of the triton. All the experimental data can be fitted except the Coulomb energy of  ${}^2_2He_1$ .

Feingold<sup>7,8</sup> has extended the study of the tensor force to four-, five-, six-, and seven-particle systems. This study indicates that some of the effects usually ascribed to a spin-orbit force may arise, in part at least, from a

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<sup>1</sup> E. P. Wigner and E. Feenberg, Repts. Progr. Phys. **8**, 274 (1941).

<sup>2</sup> L. Rosenfeld, *Nuclear Forces* (Interscience Publishers, Inc., New York, 1948).

<sup>3</sup> J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952).

<sup>4</sup> D. R. Inglis, Revs. Modern Phys. **25**, 390 (1953).

<sup>5</sup> W. Rarita and J. Schwinger, Phys. Rev. **59**, 436 (1941), and **59**, 556 (1941).

<sup>6</sup> R. L. Pease and H. Feshbach, Phys. Rev. **88**, 945 (1952).

<sup>7</sup> A. M. Feingold, Ph.D. thesis, Princeton University, 1952 (unpublished).

<sup>8</sup> D. H. Lyons and A. M. Feingold, Phys. Rev. **95**, 606 (1954).

tensor force. General arguments yielding the same tentative conclusion have been developed independently by Wigner<sup>9</sup> and Keilson.<sup>10</sup> Recently the ground-configuration matrix of the tensor interaction in the  $p$ -shell has been computed<sup>11</sup> and a research group in England is reportedly calculating interaction matrices which include other than ground configurations.

The labor involved in the last-named calculation is clearly tremendous. This paper is the result of an attempt to include the effects of configuration interaction in nuclear energy calculations without computing a prohibitive number of matrix elements. Results obtained for the  $1s$  shell indicate that the extension of the method described here to the  $1p$  shell is feasible and that this application should involve less labor than the computation of the interaction matrix.

The method described here is closely related to that used by Feingold although in detail there is little resemblance. Both methods include contributions from all configurations in second order, but neglect higher-order contributions. The present method is somewhat more elegant and has the advantage of giving exact results in the limit of weak nuclear forces. Related techniques have also been employed in early studies of exchange force models.<sup>12,13</sup>

## II. PERTURBATION TECHNIQUE

In zero order, the nuclear system is treated as a collection of single-particle harmonic oscillators with the Hamiltonian

$$H_0' = \frac{1}{2}\hbar\omega \sum (p_i^2 + q_i^2) \quad (1)$$

in which

$$\begin{aligned} p_i &= (\hbar/m\omega)^{1/2} \nabla_i, \\ q_i &= (m\omega/\hbar)^{1/2} \mathbf{r}_i. \end{aligned} \quad (2)$$

The actual physical system is governed by the Hamiltonian

$$H' = H_0' + \left[ \sum_{i<j} V_{ij} - \frac{1}{2}\hbar\omega \sum q_i^2 \right] \quad (3)$$

under the assumption that two-particle operators, denoted by  $V_{ij}$ , provide the major part of the nuclear potential energy (note, however, that the specialized form of the nuclear interaction operator does not enter into the general formulation of the perturbation method).

In Eq. (3) one cannot proceed immediately to treat the term in square brackets as a perturbing potential. The difficulty is that the bracketed expression depends

on the coordinates of the center of mass and would, therefore, mix states having different energies associated with the motion of the center of mass. The relation

$$\begin{aligned} \sum q_i^2 &= \frac{1}{A} \sum_{i<j} (\mathbf{q}_i - \mathbf{q}_j)^2 + A\mathbf{Q}^2, \\ \mathbf{Q} &= \sum \mathbf{q}_i/A, \end{aligned} \quad (4)$$

makes the difficulty explicit and at the same time indicates how it may be eliminated. The center-of-mass potential energy  $\frac{1}{2}\hbar\omega A\mathbf{Q}^2$  is added to  $H'$ , resulting in the following modified Hamiltonian:

$$\begin{aligned} H &= H' + \frac{1}{2}\hbar\omega A\mathbf{Q}^2 \\ &= H_0' + \left[ \sum_{i<j} V_{ij} - \frac{1}{2}\hbar\omega \sum (q_i^2 - Q^2) \right]. \end{aligned} \quad (5)$$

Now  $H$  contains the Hamiltonian operator for the harmonic motion of the center of mass as an additive term; consequently the eigenstates of  $H$  are also eigenstates of the center-of-mass Hamiltonian.

In many problems the determinantal wave functions generated by the set of low (or ground) configurations contain the coordinates of the center of mass only in a common factor which describes the zero-point motion of the center of mass with the energy  $\frac{3}{2}\hbar\omega$ . This statement applies when, for each of the four spin and isobaric spin states, all oscillator shells below the topmost shell are fully occupied. Under the stated condition the replacement of  $\mathbf{q}_i$  by  $\mathbf{q}_i - \mathbf{Q}$  in a determinant changes each column into a linear combination of the original column and of other columns; the additional terms may be dropped because a determinant with two equal columns vanishes.

One other adjustment is desirable. In order to fit the potential energy in  $H'$  as nearly as possible to the average potential due to the nuclear forces, it is convenient to add a term  $\sum U(\mathbf{q}_i - \mathbf{Q})$  where  $U$  is a wide well with a flat bottom. The radius of  $U$  is made large enough so that it has no effect on the wave functions of low radial quantum number. Edge effects can be neglected, if, as seems reasonable, orbitals of very high radial quantum number are present in the perturbed wave function only with very small amplitudes; in the evaluation of matrix elements it is then permissible to replace  $U$  by a constant. Now we write

$$\begin{aligned} H_0 &= H_0' + \sum U(\mathbf{q}_i - \mathbf{Q}) \\ &= \frac{1}{2}\hbar\omega \sum (p_i^2 + q_i^2) + \sum U(\mathbf{q}_i - \mathbf{Q}), \\ H &= H_0 + \left[ \sum_{i<j} V_{ij} \right. \\ &\quad \left. - \frac{1}{2}\hbar\omega \sum (q_i^2 - Q^2) - \sum U(\mathbf{q}_i - \mathbf{Q}) \right], \end{aligned} \quad (6)$$

<sup>9</sup> E. P. Wigner, Proceedings of the Conference at Rio de Janeiro and Sao Paulo, Brazil (July 15-30, 1952) (unpublished).

<sup>10</sup> J. Keilson, Phys. Rev. **82**, 759 (1951).

<sup>11</sup> J. P. Elliott, Proc. Roy. Soc. (London) **A218**, 345 (1953).

<sup>12</sup> G. Horvay, Phys. Rev. **55**, 70 (1939).

<sup>13</sup> B. O. Grönblom, Z. Physik **110**, 37 (1938).

and denote the operator in square brackets by  $W$ . The notation  $\psi_n$  and  $E_n$  is used for the eigenfunctions and eigenvalues of  $H_0$ .

We use a modified first-order wave function in the form<sup>14,15</sup>

$$\psi = \frac{1}{N} \left[ \psi_0 + \sum \frac{W_{n0}}{E - E_n} \psi_n \right], \tag{7}$$

$$N^2 = 1 + \sum \frac{|W_{n0}|^2}{(E - E_n)^2}.$$

For convenience, the depth of  $U$  is chosen so that  $W_{00} = 0$ . This means that the first-order energy correction vanishes for one low state and is small for other low states generated by the same configuration. If degeneracy exists in the zeroth-order formulation of the problem  $\psi_0$  must be written as a suitable linear combination of normalized orthogonal functions in the subspace defined by  $E_n = E_0$ . Terms with  $E_n = E_0$  may then be omitted from the sums in Eq. (7). A procedure for determining the correct linear combination is developed in Appendix C.

The energy formula,  $E = (\psi | H | \psi)$ , can be expressed in the form

$$E - E_0 = \sum \frac{|W_{0n}|^2}{E - E_n} + \sum_{n,m} \frac{W_{0n} W_{nm} W_{m0}}{(E - E_n)(E - E_m)}. \tag{8}$$

All contributions from the second-order sum in Eq. (8) have the same sign (if  $E_0 \leq E_n$ ). The third-order energy correction contains both positive and negative terms (from the fluctuating signs of  $W_{0n}$  and  $W_{nm}$ ) so that internal cancellation assists in reducing the magnitude of the sum. We omit the third-order energy correction in the following discussion. Verification of the relation  $N^2 - 1 \ll 1$  supplies a partial justification for this omission.

The abbreviations

$$M = \frac{1}{2} \hbar \omega \sum (q_i^2 - Q^2),$$

$$V = \sum_{i < j} V_{ij}, \tag{9}$$

$$U = \sum U(\mathbf{q}_i - \mathbf{Q}),$$

and the relations

$$W_{n0} = V_{n0} - M_{n0} - U_{00} \delta_{n0}$$

$$= 0 \quad \text{for } n=0, \tag{10}$$

$$U_{nm} = (V_{00} - M_{00}) \delta_{nm} = (E_0 - E_0') \delta_{nm},$$

<sup>14</sup> E. P. Wigner, *Math. u. Naturwiss. Anzeig. d. Ungar. Akad. Wiss.* L III, 475 (1935).

<sup>15</sup> P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Chap. 9.

enable us to write

$$\sum \frac{|W_{n0}|^2}{E - E_n} = \sum' \frac{|(V - M)_{n0}|^2}{E - E_n}$$

$$= \sum \frac{|V_{n0}|^2}{E - E_n} - \frac{1}{E - E_0} \sum_{(0)} |V_{n0}|^2$$

$$+ \frac{1}{E - E_0 - 2\hbar\omega} \{ \sum [ |M_{n0}|^2 - V_{0n} M_{n0} - V_{n0} M_{0n} ]$$

$$- \sum_{(0)} [ |M_{n0}|^2 - V_{0n} M_{n0} - V_{n0} M_{0n} ] \}. \tag{11}$$

The primed summation signifies that terms with  $E_n = E_0$  are omitted, while (0) signifies that the summation is limited to states with  $E_n = E_0$ . Since  $M$  contains the coordinates only to the second power,  $M_{n0}$  fails to vanish only if state  $n$  differs from state 0 by zero or two units of excitation, i.e.,  $E_n = E_0$  or  $E_n = E_0 + 2\hbar\omega$ . Equation (11) may be simplified by introducing the relations

$$\sum [ |M_{n0}|^2 - V_{0n} M_{n0} - V_{n0} M_{0n} ]$$

$$= (M^2)_{00} - (VM)_{00} - (MV)_{00}, \tag{12}$$

$$\sum_{(0)} [ |M_{n0}|^2 - V_{0n} M_{n0} - V_{n0} M_{0n} ]$$

$$= (V_{00} - M_{00})^2 - \sum_{(0)} |V_{n0}|^2 + \sum_{(0)} |W_{n0}|^2, \tag{13}$$

the first a consequence of closure and the second following from Eq. (10).

The relation

$$\sum \frac{|V_{n0}|^2}{E - E_n} = - \int_0^\infty e^{\lambda E} (V e^{-\lambda H_0} V)_{00} d\lambda \tag{14}$$

is a consequence of the identity

$$\frac{1}{E - E_n} = - \int_0^\infty e^{\lambda(E - E_n)} d\lambda, \tag{15}$$

and the application of closure to the infinite summation over  $n$ . Equations (6) and (10) permit the transformation of Eq. (14) into the more explicit form

$$\sum \frac{|V_{n0}|^2}{E - E_n} = - \int_0^\infty \exp[\lambda(E - E_0 + E_0')] \times [V \exp(-\lambda H_0') V]_{00} d\lambda. \tag{16}$$

The usefulness of Eq. (16) depends entirely on the possibility of expressing the matrix element  $[V \exp(-\lambda H_0') V]_{00}$  in a form suitable for integration and numerical evaluation. A manageable form can be

attained with the help of the integral transformation

$$\exp[-\mu(p^2+q^2)]f(\mathbf{q}) = \left(\frac{k}{2\pi g}\right)^{\frac{3}{2}} \iiint d\mathbf{v} f(\mathbf{v}) \times \exp\left[-\frac{1}{2g}(q^2+v^2-2k\mathbf{q}\cdot\mathbf{v})\right] \quad (17)$$

where

$$g = \tanh 2\mu, \quad k = 1/\cosh 2\mu, \quad (18)$$

and  $f(\mathbf{q})$  is arbitrary within broad limits of continuity and integrability. A derivation is given in Appendix A. Relations equivalent to Eq. (17) are known and have been applied in the theory of metals.<sup>16</sup> We are indebted to Professor Uhlenbeck for calling our attention to the antiquity of this formula.

### III. APPLICATION TO THE 1s SHELL

The two-particle interaction operator is assumed to be a linear combination of the six charge- and velocity-independent types of nuclear potentials. This combination will be written in a way which differs from the usual one and conforms to the potentials used in nucleon-nucleon scattering as follows:

$$\begin{aligned} V_{00} &= (0|J_1|0), \\ M_{00} &= \frac{1}{4}\hbar\omega(0|q_{12}^2|0) = \frac{3}{4}\hbar\omega, \\ (M^2)_{00} &= (\frac{1}{4}\hbar\omega)^2(0|q_{12}^4|0) = 15(\frac{1}{4}\hbar\omega)^2, \\ (VM)_{00} &= \frac{1}{4}\hbar\omega(0|J_1q_{12}^2|0), \\ (VeV)_{00} &= (0|J_1eJ_1|0) + (4/9)(0|J_s\{3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}e\cdot\mathbf{n}_{12})\mathbf{n}_{12}-e\}J_s|0). \end{aligned} \quad (20)$$

$A=3$ , ground state of  ${}^1\text{H}_2$  and  ${}^2\text{He}_1$

$$\begin{aligned} V_{00} &= \frac{3}{2}(0|J_0+J_1|0), \\ M_{00} &= \frac{1}{2}\hbar\omega(0|q_{12}^2|0) = \frac{3}{2}\hbar\omega, \\ (M^2)_{00} &= \frac{1}{3}(\frac{1}{2}\hbar\omega)^2(0|q_{12}^4+2q_{12}^2q_{13}^2|0) = 3(\hbar\omega)^2, \\ (VM)_{00} &= \frac{1}{4}\hbar\omega(0|(J_0+J_1)_{12}(q_{12}^2+2q_{13}^2)|0) \\ (VeV)_{00} &= \frac{3}{2}(0|J_0(12)eJ_0(12)+J_1(12)eJ_1(12)|0) + \frac{3}{4}(0|J_0(12)eJ_0(13)+J_1(12)eJ_1(13)+6J_0(12)eJ_1(13)|0) \\ &\quad + \frac{2}{3}(0|J_s(12)\{3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}\cdot e\mathbf{n}_{12})\mathbf{n}_{12}-e\}J_s(12)|0) - \frac{2}{3}(0|J_s(12)\{3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}\cdot e\mathbf{n}_{13})\mathbf{n}_{13}-e\}J_s(13)|0) \end{aligned} \quad (21)$$

$A=4$ , ground state of  ${}^2\text{He}_2$

$$\begin{aligned} V_{00} &= 3(0|J_0+J_1|0), \\ M_{00} &= \frac{3}{4}\hbar\omega(0|q_{12}^2|0) = 9\hbar\omega/4, \\ (M^2)_{00} &= \frac{3}{2}(\frac{1}{4}\hbar\omega)^2(0|q_{12}^4+4q_{13}^2q_{12}^2+q_{12}^2q_{34}^2|0) = 11(3\hbar\omega/4)^2, \\ (VM)_{00} &= \frac{3}{8}\hbar\omega(0|(J_0+J_1)_{12}(q_{12}^2+4q_{13}^2+q_{34}^2)|0), \\ (VeV)_{00} &= 3(0|J_0(12)eJ_0(12)+J_1(12)eJ_1(12)|0) + 3(0|J_0(12)eJ_0(13)+J_1(12)eJ_1(13)+6J_0(12)eJ_1(13)|0) \\ &\quad + 3(0|J_0(12)eJ_0(34)+J_1(12)eJ_1(34)|0) + (4/3)(0|J_s(12)\{3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}\cdot e\mathbf{n}_{12})\mathbf{n}_{12}-e\}J_s(12)|0) \\ &\quad - (8/3)(0|J_s(12)\{3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}\cdot e\mathbf{n}_{13})\mathbf{n}_{13}-e\}J_s(13)|0). \end{aligned} \quad (22)$$

### IV. THE FORCE MODEL

The numerical evaluation of the integral involving  $(VeV)_{00}$  is in general extremely difficult; however, in

<sup>16</sup> A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1953), second edition, p. 163.

$$\begin{aligned} V_{12} &= \frac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_0 \\ &\quad + \frac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_1 \\ &\quad + \frac{1}{4}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_2 \\ &\quad + \frac{1}{4}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_3 \\ &\quad + \frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)S_{12}J_s + \frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)S_{12}J_a, \end{aligned} \quad (19)$$

where each  $J$  is a function of the radial distance between the two particles. This form includes singlet-singlet, singlet-triplet, triplet-singlet, and triplet-triplet radial interactions in the spin and isobaric spin variables and independent tensor operators for symmetrical ( $s$ ) and antisymmetrical ( $a$ ) states in the space coordinator of two particles. The factor  $S_{12}$  is the tensor force operator

$$S_{12} = (\boldsymbol{\sigma}_1\cdot\mathbf{r}_{12}\boldsymbol{\sigma}_2\cdot\mathbf{r}_{12}/r_{12}^2) - \frac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2. \quad (20)$$

In the following list of matrix elements the letter  $e$  denotes the operator  $\exp(-\lambda H_0')$  and  $\mathbf{n}_{12}$  is the unit vector along  $\mathbf{r}_{12}$ . The single-particle orbitals have the form

$$\psi_{1s}(q) = \pi^{-\frac{3}{2}} \exp(-\frac{1}{2}q^2)$$

multiplied by appropriate spin and isobaric spin functions.

$A=2$ , ground state of the deuteron

the special case of Gaussian radial dependence of the potential functions, the most difficult term reduces to an easily computed one-dimensional integral. We have made calculations using the Gaussian form for  $J_0$ ,  $J_1$ , and  $J_s$ . The depth and range parameters are taken from

a calculation by Hu and Massey.<sup>17</sup> These authors determine a potential with depths and a common range parameter adjusted to fit the binding energy and quadrupole moment of the deuteron. In our notation

$$\begin{aligned} J_1(r) &= KG \exp(-r^2/r_0^2), \\ J_s(r) &= 1.77J_1(r), \\ G &= 2\hbar^2/mr_0^2 = 17.4 \text{ Mev}, \quad r_0 = 2.18 \times 10^{-13} \text{ cm}, \\ K &= -1.695. \end{aligned} \quad (23)$$

The specification of the potential is completed by setting  $J_0 = J_1$ . This is consistent with the Serber mixture of exchange forces which has been used in the interpretation of high-energy nucleon-nucleon scattering data.<sup>18</sup> One difficulty with the Serber mixture is the fact that it does not saturate. However, the more recent attempts to fit the scattering data indicate that the nuclear potential has a repulsive core.<sup>18-20</sup> Since a repulsive core strongly influences the saturation behavior,<sup>21,22</sup> the previous saturation arguments are inconclusive if the potential does actually become large and positive for small separations. It is hoped to extend the present calculations to include the effect of a repulsive core, both real (by adding a positive short-range Gaussian) and simulated (by multiplying the Gaussian by the square of the separation to make it vanish at zero range). A preliminary to these calculations will have to be an investigation of the effect of a repulsive core on the deuteron parameters.

The explicit formulas for the matrix elements involving the  $J$ 's can be expressed simply in terms of the following notation:

$$\begin{aligned} -\hbar\omega\delta &= E - E_0, \\ \hbar\omega &= G(\eta - 1) \quad \text{or} \quad r_0^2 = \frac{2\hbar}{m\omega}(\eta - 1), \\ \mu &= \frac{1}{2}\hbar\omega\lambda, \quad u = \exp(-4\mu), \\ \rho &= \frac{(\eta - 1)^2}{(\eta - u)^2}u, \quad \rho' = \frac{4(\eta - 1)^2}{(4\eta - u)^2}u, \\ F(y) &= \frac{5}{3y} \left[ 1 + \frac{3}{y}(1 - y) \left\{ (1 - y)^{\frac{1}{2}} \frac{\sin^{-1}y^{\frac{1}{2}}}{y^{\frac{1}{2}}} - 1 \right\} \right]. \end{aligned} \quad (24)$$

The results are

$$\begin{aligned} \langle 0 | J_1 | 0 \rangle / \hbar\omega &= K(\eta - 1)^{1/2} / \eta^{3/2}, \\ \langle 0 | J_1(12)q_{12}^2 | 0 \rangle / \hbar\omega &= 3K(\eta - 1)^{3/2} / \eta^{5/2}, \\ \langle 0 | J_1(12)q_{13}^2 | 0 \rangle / \hbar\omega &= \frac{3}{4}K(4\eta - 1)(\eta - 1)^{1/2} / \eta^{5/2}, \end{aligned} \quad (25)$$

<sup>17</sup> T. Hu and H. S. W. Massey, Proc. Roy. Soc. (London) **A196**, 135 (1949).

<sup>18</sup> G. Breit and M. H. Hull, Jr., Am. J. Phys. **21**, 184 (1953).

<sup>19</sup> R. Jastrow, Phys. Rev. **79**, 389 (1950); and **81**, 165 (1951).

<sup>20</sup> M. M. Levy, Phys. Rev. **88**, 725 (1952).

<sup>21</sup> K. A. Brueckner, Phys. Rev. **96**, 508 (1954).

<sup>22</sup> S. D. Drell and K. Huang, Phys. Rev. **91**, 1527 (1953).

$$\begin{aligned} &\int_0^\infty \exp[\lambda(E - E_0 + E_0')] [J_1(12)eJ_1(12)]_{00} d\lambda / \hbar\omega \\ &= K^2 \frac{\eta - 1}{\delta} \left[ \frac{1}{(\eta^2 - 1)^{3/2}} - \frac{3}{2} \int_0^1 \frac{u^{\delta/2} du}{(\eta^2 - u)^{5/2}} \right], \end{aligned} \quad (26)$$

$$\begin{aligned} &\int_0^\infty \exp[\lambda(E - E_0 + E_0')] [J_1(12)eJ_1(13)]_{00} d\lambda / \hbar\omega \\ &= 8K^2 \frac{\eta - 1}{\delta} \left[ \frac{1}{(4\eta^2 - 1)^{3/2}} - \frac{3}{2} \int_0^1 \frac{u^{\delta/2} du}{[4\eta^2 - u]^{5/2}} \right], \\ &\int_0^\infty \exp[\lambda(E - E_0 + E_0')] \\ &\quad \times [J_1(12)\{3\mathbf{n}_{12} \cdot (\mathbf{n}_{12}e \cdot \mathbf{n}_{12})\mathbf{n}_{12} - e\}J_1(12)]_{00} d\lambda / \hbar\omega \\ &= \frac{3}{5} K^2 (\eta - 1)^3 \int_0^1 \frac{u^{\delta/2} F(\rho) du}{(\eta^2 - u)^{\frac{3}{2}} (\eta - u)^2}, \end{aligned} \quad (27)$$

$$\begin{aligned} &\int_0^\infty \exp[\lambda(E - E_0 + E_0')] \\ &\quad \times [J_1(13)\{3\mathbf{n}_{13} \cdot (\mathbf{n}_{13}e \cdot \mathbf{n}_{12})\mathbf{n}_{12} - e\}J_1(12)]_{00} d\lambda / \hbar\omega \\ &= \frac{96}{5} K^2 (\eta - 1)^3 \int_0^1 \frac{u^{\delta/2} F(\rho') du}{(4\eta^2 - u)^{\frac{3}{2}} (4\eta - u)^2}. \end{aligned} \quad (28)$$

The derivation of Eqs. (27) and (28) is sketched in Appendix B.

These results can now be put together to yield a pair of equations for  $\delta$  and  $E - \frac{3}{2}\hbar\omega$ . The procedure is illustrated by an explicit discussion for the case of the deuteron:

$$\begin{aligned} \delta^2 &= K^2 (\eta - 1) \left[ (\eta^2 - 1)^{-3/2} - \eta^{-3} - \frac{3}{2} \int_0^1 \frac{u^{\delta/2} du}{(\eta^2 - u)^{5/2}} \right. \\ &\quad \left. + \frac{4.1772\delta}{5} (\eta - 1)^2 \int_0^1 \frac{u^{\delta/2} F du}{(\eta^2 - u)^{\frac{3}{2}} (\eta - u)^2} \right] \\ &\quad + \frac{\delta}{\delta + 2} \left[ \frac{3}{8} + \frac{3}{2} K (\eta - 1)^{1/2} / \eta^{5/2} \right], \end{aligned} \quad (29)$$

$$E - \frac{3}{2}\hbar\omega = G(\eta - 1) \left[ \frac{3}{4} - \delta(\eta) + K(\eta - 1)^{\frac{1}{2}} / \eta^{\frac{3}{2}} \right]. \quad (30)$$

From the equation expressing  $\delta$  as a function of  $\eta$  we compute the uppermost branch (maximum  $\delta$  for given  $\eta$ ) and denote it by  $\delta(\eta)$ . The minimum value of  $E - \frac{3}{2}\hbar\omega$  as a function of  $\delta(\eta)$  and  $\eta$  is the sought-for energy. The corresponding value of  $\eta$  determines the strength of the harmonic oscillator potential and the harmonic excitation energy  $\hbar\omega$ .

In Eq. (29) the terms in  $K^2$ , exclusive of the integral involving the function  $F$ , can be expanded in powers of

TABLE I. Numerical results.

A	$\eta$	$\delta$	$-E(\text{Mev})$	$\hbar\omega(\text{Mev})$	$N^2$ *
2	1.75	0.274	2.08	13.2	1.06
3	1.99	0.342	11.1	17.4	1.07
4	2.27	0.485	35.1	22.2	1.10

\* See Sec. IV.

$1/\eta^2$  and combined to give a single series with the result

$$\delta = 0.8354K^2(\eta-1)^3 \int_0^1 \frac{u^{\delta/2}F(\rho)du}{(\eta^2-u)^{\frac{3}{2}}(\eta-u)^2} + \frac{3}{8(\delta+2)} [1+2K(\eta-1)^{1/2}/\eta^{5/2}]^2 + \frac{15}{8} K^2 \frac{\eta-1}{\eta^7} \times \left[ \frac{1}{\delta+4} + \frac{7}{6\eta^2(\delta+6)} + \frac{7.9}{6.8\eta^4(\delta+8)} + \dots \right]. \quad (31)$$

In Eq. (31) the contribution from the central force resolves into a sum of contributions from the various levels of excitation as shown by the series terms in  $(\delta+2)^{-1}$ ,  $(\delta+4)^{-1}$ , ... which correspond to  $(E-E_0-2\hbar\omega)^{-1}$ ,  $(E-E_0-4\hbar\omega)^{-1}$ , ... respectively.

$$\langle \psi | 3z_1^2 - r_1^2 | \psi \rangle = -\frac{2}{3N^2} 1.77KG \int_0^\infty \exp[\lambda(E-E_0+3\hbar\omega)] [\exp(-r_{12}^2/r_0^2)(3z_{12}^2/r_{12}^2-1)e(3z_1^2-r_1^2)]_{00} d\lambda, \quad (34)$$

and finally, after replacing  $\exp(-\lambda H_0')$  by the eigenvalue  $\exp(-5\lambda\hbar\omega)$ ,

$$\begin{aligned} \langle \psi | 3z_1^2 - r_1^2 | \psi \rangle &= -\frac{2}{3N^2} 1.77KG \frac{1}{\hbar\omega} \frac{1}{M\omega} \frac{1}{\pi^3} \int_0^\infty e^{-2\mu(\delta+2)} d\mu \int \dots \int \exp\left(-q^2 - q'^2 - \frac{1}{\eta-1}q^2\right) q^2 (3\cos^2\theta-1)^2 d\mathbf{q}d\mathbf{q}' \\ &= -\frac{1.77}{5N^2} K r_0^2 \frac{(\eta-1)^{1/2}}{\eta^{5/2}} \frac{1}{\delta+2} \\ &= \frac{2.67}{N^2} \times 10^{-27} \text{ cm}^2. \end{aligned} \quad (35)$$

The evaluation of  $N^2$  is somewhat more difficult. Equation (11) may be adapted to this calculation by replacing  $E-E_n$  everywhere by  $(E-E_n)^2$ . Also Equations (12) and (13) can be used as they stand. The operation of differentiation with respect to  $E$  applied to Eq. (14) yields

$$\begin{aligned} \sum \frac{|V_{n0}|^2}{(E-E_n)^2} &= \frac{\partial}{\partial E} \int_0^\infty e^{\lambda E} (V e^{-\lambda H_0} V)_{00} d\lambda \\ &= \int_0^\infty \lambda e^{\lambda E} (V e^{-\lambda H_0} V)_{00} d\lambda. \end{aligned} \quad (36)$$

This relation can also be derived by a double application of Eq. (15) and an integration by parts. Equation (36) makes all the results of Eq. (26) available for the evaluation of  $N^2$ . In practise the integrals involving the tensor force must be evaluated by numerical integration;

The results of calculations based on the potentials and parameters of Eq. (23) are summarized in Table I.

### V. QUADRUPOLE MOMENT OF THE DEUTERON

The diagonal matrix element of the quadrupole moment operator is

$$\langle \psi | 3z_1^2 - r_1^2 | \psi \rangle = \frac{2}{N^2} \sum \frac{V_{0n}(3z_1^2 - r_1^2)_{n0}}{E-E_n} + \text{third order terms.} \quad (32)$$

As in the energy calculation, the third-order terms are dropped and the second order contribution is transformed by the introduction of Eq. (15) and the application of closure with the result

$$\langle \psi | 3z_1^2 - r_1^2 | \psi \rangle = -\frac{2}{N^2} \int_0^\infty \exp[\lambda(E-E_0+3\hbar\omega)] \times (V e\{3z_1^2 - r_1^2\})_{00} d\lambda. \quad (33)$$

Only the tensor potential which contains a second-order tensor in the space coordinates contributes to the matrix element of Eq. (33). After the summation over the spin variables is carried out, the right-hand member of Eq. (33) reduces to

the integrands entering into the calculation of  $E$  and of  $N^2$  differ then merely in a factor  $\lambda = 2\mu/\hbar\omega = 1/2\hbar\omega \times \ln u$ . For the deuteron

$$\begin{aligned} \sum \frac{|W_{n0}|^2}{(E-E_n)^2} &= \frac{3}{8(\delta+2)^2} \left( 1 + 2K \frac{(\eta-1)^{1/2}}{\eta^{5/2}} \right)^2 \\ &+ \frac{15}{8} K^2 \frac{\eta-1}{\eta^7} \left[ \frac{1}{(\delta+4)^2} + \frac{7}{6\eta^2(\delta+6)^2} + \dots \right] \\ &- \frac{2}{15} K^2 (\eta-1)^3 \int_0^1 \frac{(\ln u)F(\rho)du}{(\eta-u)^2(\eta^2-u)^{\frac{3}{2}}}. \end{aligned} \quad (37)$$

Expressions similar to Eq. (37) can be derived for  $A=3$  and 4; numerical results are listed in Table I. In all these calculations the contributions from central and tensor forces are clearly separated. Since there is no

overlapping in the excited zeroth-order states mixed in by the central and the tensor forces,  $N^2-1$  can be broken down into a sum of independent terms, each one referring to a particular type of  $LS$  coupling, i.e.,

$$\begin{aligned} A=2: & \ ^3S_1, 0.01; \ ^3D_1, 0.05; \\ A=3: & \ ^2S_{\frac{1}{2}}, 0.01; \ ^4D_{\frac{3}{2}}, 0.06; \\ A=4: & \ ^1S_0, 0.01; \ ^3D_0, 0.09. \end{aligned} \quad (38)$$

Now returning to the quadrupole moment of the deuteron, insertion of  $N^2=1.06$  into Eq. (35) yields

$$\langle \psi | 3z_1^2 - r_1^2 | \psi \rangle = 2.52 \times 10^{-27} \text{ cm}^2, \quad (39)$$

which differs by 8% from the value  $2.73 \times 10^{-27} \text{ cm}^2$  used by Hu and Massey to fix the parameters of the potential operator.

## VI. DISCUSSION OF RESULTS

The computed values for the deuteron, 2.07 Mev and  $2.52 \times 10^{-27} \text{ cm}^2$ , agree remarkably well with the input values (2.19 Mev and  $2.73 \times 10^{-27} \text{ cm}^2$ ) used by Hu and Massey when the following factors are considered: (1) the zero-order approximation is worse for the deuteron than for a nucleus with a larger number of nucleons, where the competition between kinetic and potential energies in determining the binding energy is less critical (2) the oscillator potential is less suitable for the deuteron than for heavier nuclei; (3) third- and higher order terms are neglected throughout. However, it should be noted that the Gaussian potential resembles the harmonic oscillator well a good deal more than a Yukawa or repulsive core potential does, and (2) above is mitigated somewhat thereby.

The good agreement obtained for the deuteron makes the applications to the triton and the alpha particle worthwhile. The binding energies computed for these nuclides with our somewhat arbitrary potential are both larger than the experimental values by about 30%. The calculations are a bit tedious, but it is still feasible to try different potentials and make computations without the aid of elaborate computing facilities as long as Gaussian radial dependence of the potentials is assumed. Better agreement between computed and experimental energies may be expected if the range of the tensor force is somewhat greater than that of the central interaction.<sup>6,20,23</sup>

The integrals which arise for Yukawa radial dependence of the potentials appear to require a computing machine for their evaluation. In general, the calculations are of a type which could undoubtedly be set up on a machine rather easily.

A reasonably good approximation to a Yukawa potential with a repulsive core can be achieved by taking a linear combination of three Gaussian functions, one short-range and repulsive, a second attractive of intermediate range, and a third, also attractive, with somewhat greater range to fit the long-range behavior.

It is rather difficult to estimate the effect of a repulsive core. However, it seems probable that in the

deuteron, in which the nucleons tend to be rather far apart, a repulsive core of small radius should have only a small effect. The average internucleon distance is a good deal smaller in the triton and the alpha particle, so that a repulsive core may be expected to have a relatively larger effect here.

The assumption of zero range or contact interactions has been employed extensively in first-order calculations. In the present context this means replacing  $K$  by  $K'/r_0$ , where  $K'$  is a constant, and proceeding to the limit  $r_0 \rightarrow 0$ . The limiting potential then has the form of a delta function of finite strength. In terms of  $\eta$ ,  $K$  is replaced by  $K' [m\omega/2\hbar(\eta-1)]^{\frac{1}{2}}$  and the limit  $\eta \rightarrow 1$  taken. Then it is seen from Eqs. (26) and (27) that the integrals arising from the matrix elements  $(VeV)_{00}$  diverge. The divergence is sufficient to make  $\delta$  infinitely large for any value of  $\hbar\omega$ ; consequently the binding energy becomes infinite. In the deuteron problem this result could be anticipated since the delta-function well permits an infinite number of bound states. The condition for any fixed finite number of stationary states is simply  $r_0^2 \times \text{depth} \rightarrow \text{constant}$  in the limit  $r_0 \rightarrow 0$ ; the definition of a delta function requires however that  $r_0^3 \times \text{depth} \rightarrow \text{constant}$  as  $r_0$  approaches zero. In this connection it is interesting to recall that Thomas<sup>24</sup> has given a rigorous argument proving that the binding energy of a three-particle system (two neutrons and one proton) is infinite in the limit  $r_0 \rightarrow 0$  and  $r_0^2 \times \text{depth} \rightarrow \text{constant}$  if the constant is large enough to admit at least one stationary state in the neutron-proton problem.

The perturbation procedure as described is not suitable for evaluating the effect of a very strong short-range repulsive interaction. A necessary condition for the validity of the method is that the positive contribution to the energy in first order from this interaction should outweigh the negative contribution from the corresponding quadratic terms in second order. A suitable canonical transformation is required to adopt the perturbation procedure to the presence of a short-range repulsive interaction of arbitrary strength.

One of us (AMB) is undertaking to extend this type of calculation to the first  $p$ -shell using the Racah tensor formalism and the technique of fractional parentage coefficients.

## APPENDIX A. A TRANSFORMATION FORMULA

The formula<sup>25</sup>

$$\begin{aligned} \exp[-\mu(p^2+q^2)] &= \lim_{n \rightarrow \infty} \left[ \exp\left(-\frac{\mu}{n}p^2\right) \exp\left(-\frac{\mu}{n}q^2\right) \right]^n \\ &= \lim_{n \rightarrow \infty} \left[ \exp\left(-\frac{\mu}{n}q^2\right) \exp\left(-\frac{\mu}{n}p^2\right) \right]^n \end{aligned} \quad (A1)$$

supplies the essential clue to the form of the integral transformation of Eq. (17). If  $f(q)$  is expanded by the

<sup>24</sup> L. H. Thomas, Phys. Rev. 47, 903 (1935).

<sup>25</sup> S. T. Butler and M. H. Friedman, Phys. Rev. 98, 287 (1955).

<sup>23</sup> H. Primakoff, Phys. Rev. 72, 118 (1947).

Fourier integral theorem, it is possible to show that

$$\exp\left(-\frac{\mu}{n}q^2\right)\exp\left(-\frac{\mu}{n}p^2\right)f(q) = \left(\frac{n}{4\pi\mu}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}\exp\left[-\frac{\mu}{n}q^2-\frac{n}{4\mu}u^2\right]f(q-u)du, \quad (A2)$$

and that therefore

$$\left[\exp\left(-\frac{\mu}{n}q^2\right)\exp\left(-\frac{\mu}{n}p^2\right)\right]^2f(q) = \frac{n}{4\pi\mu}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left[-\frac{\mu}{n}q^2-\frac{\mu}{n}(q-u_1)^2-\frac{n}{4\mu}(u_1^2+u_2^2)\right]\times f(q-u_1-u_2)du_1du_2, \quad (A3)$$

and so on. (A3) may be integrated once to give something of the form

$$N\int_{-\infty}^{\infty}\exp(aq^2+bqv+cv^2)f(v)dv$$

and (A2) may be rearranged to this form also, suggesting that, in general,

$$\exp[-\mu(p^2+q^2)]f(q) = N\int_{-\infty}^{\infty}\exp(aq^2+bqv+cv^2)f(v)dv. \quad (A4)$$

The following differential equation must hold:

$$\frac{\partial}{\partial\mu}\exp[-\mu(p^2+q^2)]f(q) = -(p^2+q^2)\exp[-\mu(p^2+q^2)]f(q) = \left(\frac{\partial^2}{\partial q^2}-q^2\right)\exp[-\mu(p^2+q^2)]f(q).$$

If (A4) is correct this requires

$$\int_{-\infty}^{\infty}\left[\frac{\partial N}{\partial\mu}+Nq^2\frac{\partial a}{\partial\mu}+Nqv\frac{\partial b}{\partial\mu}+Nv^2\frac{\partial c}{\partial\mu}\right]\times\exp(aq^2+bqv+cv^2)f(v)dv = N\int_{-\infty}^{\infty}(-q^2+2a+[2aq+bv]^2)\times\exp(aq^2+bqv+cv^2)f(v)dv.$$

Equating respectively terms in  $q^2$ ,  $qv$ ,  $v^2$ , and constant terms gives

$$\partial a/\partial\mu=4a^2-1, \quad (A5a)$$

$$\partial b/\partial\mu=4ab, \quad (A5b)$$

$$\partial c/\partial\mu=b^2, \quad (A5c)$$

$$\partial N/\partial\mu=2aN. \quad (A5d)$$

(A5a) is satisfied by

$$a=-\frac{1}{2}\coth 2\mu. \quad (A6a)$$

(A5b) then gives

$$b=1/\sinh 2\mu, \quad (A6b)$$

since  $\mu$  is assumed to be positive, as it will be in the applications. (A5c) now gives

$$c=-\frac{1}{2}\coth 2\mu=a, \quad (A6c)$$

and (A5d) gives

$$N^2=1/\sinh 2\mu. \quad (A6d)$$

As  $\mu$  approaches zero, the righthand side of (A4) must reduce to  $f(q)$ . By using (A6), the right side of (A4) may be written

$$N\int_{-\infty}^{\infty}\exp\left(\frac{1}{4a}q^2+au^2\right)f\left[\frac{b}{(1+b^2)^{\frac{1}{2}}}q-u\right]du.$$

For  $\mu\rightarrow 0$ , this gives,

$$\lim_{\mu\rightarrow 0}\left(\frac{2\pi}{\cosh 2\mu}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}\delta(u)f\left(\frac{q}{\cosh 2\mu}-u\right)du=(2\pi)^{\frac{1}{2}}f(q).$$

Thus, for proper normalization, a factor  $1/(2\pi)^{\frac{1}{2}}$  is needed, giving finally Eq. (17), when the transformation is extended to three dimensions.

### APPENDIX B. EVALUATION OF SECOND-ORDER TENSOR INTEGRALS

The orthogonal transformation

$$\mathbf{q}=(\mathbf{q}_1-\mathbf{q}_2)/2^{\frac{1}{2}} \quad (B1)$$

$$\mathbf{q}'=(\mathbf{q}_1+\mathbf{q}_2)/2^{\frac{1}{2}}$$

combined with a change of scale applied to the integrand of the first tensor integral in Eq. (21) yields

$$\begin{aligned} &(\exp(-r_{12}^2/r_0^2)[3\mathbf{n}_{12}\cdot(\mathbf{n}_{12}\cdot\mathbf{e}\mathbf{n}_{12})\mathbf{n}_{12}-e] \\ &\times\exp(-r_{12}^2/r_0^2))_{00} \\ &= \frac{1}{\pi^3}\left(\frac{2g\rho}{k}\right)^{\frac{3}{2}}\int\cdots\int\exp[-(v^2+q^2)](3\cos^2\theta-1) \\ &\times\exp[2\rho^{\frac{1}{2}}qv\cos\theta]d\mathbf{q}d\mathbf{v} \quad (B2) \end{aligned}$$

in which

$$\rho=\frac{(\eta-1)^2}{(\eta+u)^2}u. \quad (B3)$$

The exponential function of  $\cos\theta$  may be expanded in a power series and all indicated operations performed with the result

$$\begin{aligned} ( )_{00} &= 2\left(\frac{1-u}{u^{\frac{1}{2}}}\rho\right)^{\frac{3}{2}}\sum_0^{\infty}\frac{3\cdot 5\cdots(2l+3)}{2^l l!(2l+5)}\rho^l \\ &= 2\left[\frac{\rho}{u^{\frac{1}{2}}}\frac{1-u}{1-\rho}\right]^{\frac{3}{2}} \\ &\times\left[1+\frac{3}{\rho}(1-\rho)\left\{(1-\rho)^{\frac{1}{2}}\frac{\sin^{-1}\rho^{\frac{1}{2}}}{\rho^{\frac{1}{2}}}-1\right\}\right]. \quad (B4) \end{aligned}$$

The relation

$$\begin{aligned} &\sum_0^{\infty}\frac{3\cdot 5\cdots(2l+3)}{2^l l!(2l+5)}\rho^l \\ &= (1-\rho)^{-3/2}-\rho^{-5/2}\int_0^{\rho}x^{3/2}(1-x)^{-3/2}dx \quad (B5) \end{aligned}$$



provides the link between the first and second lines of Eq. (B4). From the definitions of  $\rho$  and the function  $F(\rho)$  [Eq. (24)]

$$1-\rho = \frac{(\eta^2-u)(1-u)}{(\eta-u)^2}, \quad (\text{B6})$$

and

$$\left( \quad \right)_{00} = \frac{6}{5}(\eta-1)^5 \frac{u^{7/4}}{(\eta^2-u)^{3/2}(\eta-u)^2} F(\rho). \quad (\text{B7})$$

A similar analysis can be applied to the second tensor integral in Eq. (21) in which  $\mathbf{n}_{13}$  replaces  $\mathbf{n}_{12}$  to the right of the operator  $e$ . The oscillator transformation substitutes  $\mathbf{v}$  for  $\mathbf{q}_1$  in the part of the integral to the right of  $e$ . The integral can then be expressed in terms of new variables

$$\begin{aligned} \mathbf{q} &= (\mathbf{v}-\mathbf{q}_3)/\sqrt{2}, \\ \mathbf{q}' &= (\mathbf{q}_1-\mathbf{q}_2)/\sqrt{2}, \\ \mathbf{q}'' &= (\mathbf{v}+\mathbf{q}_3)/\sqrt{2}, \\ \mathbf{q}''' &= (\mathbf{q}_1+\mathbf{q}_2)/\sqrt{2}, \end{aligned} \quad (\text{B8})$$

and the required operations in the  $\mathbf{q}''$  and  $\mathbf{q}'''$  spaces carried out. The remaining integrand has the form encountered in the first tensor integral except for a different numerical factor and the replacement of  $\rho$  by  $\rho'$ .

#### APPENDIX C. CONSTRUCTION OF THE CORRECT ZERO-ORDER WAVE FUNCTION

The zeroth-order wave function is written as a normalized linear combination,

$$\psi_0 = \sum_{p=1}^j C_p \psi_{0p} / \left[ \sum |C_q|^2 \right]^{1/2}, \quad (\text{C1})$$

of normalized, orthogonal eigenfunctions of  $H_0$  belonging to the eigenvalue  $E_0$ .

We need the definitions

$$\begin{aligned} X &= V - M, \\ \epsilon_{2pq} &= \sum \frac{W_{0p,n} W_{n,0q}}{E - E_n}, \\ \epsilon_{3pq} &= \sum \frac{W_{0p,m} W_{mn} W_{n,0q}}{(E - E_m)(E - E_n)}, \\ N_{pq} &= \sum \frac{W_{0p,n} W_{n,0p}}{(E - E_n)^2}, \\ P_{pq} &= \sum \frac{W_{0p,m} W_{mn} W_{n,0q}}{(E - E_m)(E - E_n)} \left[ \frac{1}{E - E_m} + \frac{1}{E - E_n} \right], \\ N &= 1 + \sum \bar{C}_p C_q N_{pq} / \sum |C_t|^2, \\ P &= \sum \bar{C}_p C_q P_{pq} / \sum |C_t|^2. \end{aligned} \quad (\text{C2})$$

Also, from Eqs. (8) and (10),

$$U_{00} = X_{00} = \sum \bar{C}_p C_q X_{0p,0q} / \sum |C_t|^2, \quad (\text{C3})$$

$$E = E_0' + \sum \bar{C}_p C_q [\epsilon_{2pq} + \epsilon_{3pq}] / \sum |C_t|^2. \quad (\text{C4})$$

For a given set of amplitudes  $C_p$ , the energy  $E - \frac{3}{2}\hbar\omega$  is the lowest root of the implicit equation (C4). The correct amplitudes are determined by minimizing this root with respect to  $\omega$  and  $C_p$ . The condition for a minimum,

$$\partial E / \partial \bar{C}_p = 0, \quad p=1,2,\dots,j, \quad (\text{C5})$$

combined with the relations

$$\begin{aligned} N_{pq} &= \partial \epsilon_{2pq} / \partial X_{00}, \\ P_{pq} &= \partial \epsilon_{3pq} / \partial X_{00}, \end{aligned} \quad (\text{C6})$$

$$\partial X_{00} / \partial \bar{C}_p = \sum C_q [X_{0p,0q} - X_{00} \delta_{pq}] / \sum |C_t|^2,$$

yields a system of nonlinear equations for the energy  $E$  and the coefficients  $C_p$ :

$$\sum_{q=1}^j C_q [X_{0p,0q} (N+P) + \epsilon_{2pq} + \epsilon_{3pq} - \{E - E_0' + (N+P-1)X_{00}\} \delta_{pq}] = 0. \quad (\text{C7})$$

We observe that (C4) can be recovered from (C7) in consequence of the relation

$$\sum \bar{C}_p \partial X_{00} / \partial \bar{C}_p = 0 \quad (\text{C8})$$

which follows from (C6) and the definition of  $X_{00}$ .

Since  $N$  and  $P$  are functions of the unknown amplitudes (C7) must be solved by a process of successive approximation. A guess at an initial set of amplitudes permits the computation of an initial value of  $N+P$ . The lowest value of  $E - E_0' + (N+P)X_{00}$  and the associated amplitudes can then be computed. The process is repeated until the assumed and computed amplitudes agree. Finally,  $X_{00}$  is computed using the correct amplitudes.

In practice, the determination of  $\psi_{0p}$  as correct zeroth-order linear combinations for the evaluation of the first-order energy may be advantageous. In this case  $X_{0p,0q} = 0$  for  $q \neq p$ , and the mixing of zeroth-order states by the nondiagonal components of the second- and third-order energy operators is seen to depend on the ratios of these components to the diagonal first-order differences  $X_{0p,0p} - X_{0q,0q}$ .

Feingold and Wigner<sup>26</sup> have stressed the possibility that degenerate or nearly degenerate zeroth-order states may be coupled strongly indirectly through remote excited states, especially in connection with the failure of  $LS$  coupling produced by a tensor interaction. The present calculation supplies a semiquantitative formulation for the argument developed in a schematic qualitative manner by Feingold and Wigner.

<sup>26</sup> A. M. Feingold and E. P. Wigner, unpublished calculations (1950); A. M. Feingold, Phys. Rev. **101**, 258 (1956).