

Doublet Splitting in the $1p$ Shell due to Tensor Interaction*

PAUL GOLDHAMMER

Department of Physics, University of Nebraska, Lincoln, Nebraska

(Received August 25, 1961)

The separation of $p_{1/2}$ and $p_{3/2}$ orbitals in N^{15} due to the tensor force has been estimated using second-order perturbation theory. The estimated splitting of 5.6 Mev is to be compared with an experimental separation of 6.3 Mev. General relationships needed in computing the doublet splitting due to tensor interaction in nuclei with a closed shell plus or minus one nucleon are developed.

1. INTRODUCTION

NUMEROUS authors¹⁻¹² have attempted to correlate the observed doublet separation in nuclei with the second-order effects of the tensor interaction operator

$$S_{ij} = \sigma_i \cdot \mathbf{n}_{ij} \sigma_j \cdot \mathbf{n}_{ij} - \frac{1}{3} \sigma_i \cdot \sigma_j, \quad (1.1)$$

which is known to be present¹³ in the nucleon-nucleon interaction.

It is easy to demonstrate that the basic effect of the tensor operator is to produce spin-orbit splitting. From two Pauli spin operators for particles i and j construct a tensor of rank 2:

$$S_{2m}(ij) = \sum_{\mu+\mu'=m} C_{\mu\mu'm}^{112} \sigma_{\mu}^i \sigma_{\mu'}^j. \quad (1.2)$$

Likewise we construct a tensor of rank two from the unit vector $\mathbf{n}_{ij} = \mathbf{n}$:

$$R_{2m}(ij) = \sum_{\mu+\mu'=m} C_{\mu\mu'm}^{112} n_{\mu} n_{\mu'}. \quad (1.3)$$

The tensor operator of Eq. (1.1) may then be expressed as the dot product of R_{2m} and S_{2m} :

$$S_{ij} = S_2(ij) \cdot R_2(ij) = \sum_m (-1)^m S_{2m}(ij) R_{2-m}(ij) \\ = (5)^{\frac{1}{2}} \sum_m C_{m-m0}^{220} S_{2m}(ij) R_{2-m}(ij). \quad (1.4)$$

Second-order terms will involve the product $S_{ij} S_{kl}$ which can be expanded making use of the $9j$ coefficient¹⁴:

$$S_{ij} S_{kl} = 5 \sum_{K=0}^4 (2K+1) \left\{ \begin{matrix} 2 & 2 & K \\ 0 & 0 & 0 \end{matrix} \right\} \sum_{M=-K}^{+K} C_{M-M0}^{KK0} \\ \times S_{KM}(ijkl) R_{K-M}(ijkl), \quad (1.5)$$

where

$$S_{KM}(ijkl) = \sum_{\mu+\mu'=M} C_{\mu\mu'M}^{22K} S_{2\mu}(ij) S_{2\mu'}(kl), \quad (1.5a)$$

and

$$R_{KM}(ijkl) = \sum_{\mu+\mu'=M} C_{\mu\mu'M}^{22K} R_{2\mu}(ij) R_{2\mu'}(kl). \quad (1.5b)$$

A $9j$ coefficient with three zeros is easily evaluated:

$$\left\{ \begin{matrix} 2 & 2 & K \\ 0 & 0 & 0 \end{matrix} \right\} = \frac{1}{5(2K+1)^{\frac{1}{2}}}, \quad (1.6)$$

and so Eq. (1.5) becomes

$$S_{ij} S_{kl} = \sum_{K=0}^4 S_K(ijkl) \cdot R_K(ijkl). \quad (1.7)$$

If LS coupling holds, evaluation of Eq. (1.7) will yield matrix elements of the form:

$$(SLJM | S_K \cdot R_K | SLJM) = (-1)^K W(JLSK; SL) \\ \times (S || S_K || S) (L || R_K || L), \quad (1.8)$$

where $W(JLSK; SL)$ is a Racah function,

$$(S || S_K || S) C_{S0S}^{SKS} = (2S+1)^{\frac{1}{2}} (SS | S_{K0} | SS), \quad (1.8a)$$

and

$$(L || R_K || L) C_{L0L}^{LKL} = (2L+1)^{\frac{1}{2}} (LL | R_{K0} | LL). \quad (1.8b)$$

Obviously this matrix element vanishes unless $S \geq K/2$ and $L \geq K/2$. Consequently for a closed shell only the term with $K=0$ in Eq. (1.7) is nonvanishing.

The principal effect of the term $S_K \cdot R_K$ ($K \neq 0$) is to produce a spin-orbit splitting. To illustrate this consider the case where $K=1$, which produces the doublet splitting. When $S=\frac{1}{2}$, one can have $J=L \pm \frac{1}{2}$ and the splitting of these two terms may be characterized by the ratio of two Racah coefficients:

$$\frac{W([J=L-\frac{1}{2}] L \frac{1}{2} K; \frac{1}{2} L)}{W([J=L+\frac{1}{2}] L \frac{1}{2} K; \frac{1}{2} L)} = -\frac{L+1}{L}, \quad (1.9)$$

the reduced matrix elements in Eq. (1.8) retaining the

* Supported in part by a grant from the National Science Foundation.

¹ S. Dancoff, Phys. Rev. **58**, 326 (1940).

² A. M. Feingold, Phys. Rev. **101**, 258 (1956).

³ A. M. Feingold, Phys. Rev. **105**, 944 (1957).

⁴ A. M. Feingold, Phys. Rev. **114**, 540 (1959).

⁵ L. S. Kisslinger, Phys. Rev. **104**, 1077 (1956).

⁶ B. P. Nigam and M. K. Sundaresan, Can. J. Phys. **36**, 571 (1958).

⁷ A. Sugie, P. E. Hodgson, and H. H. Robertson, Proc. Phys. Soc. (London) **A70**, 1 (1959).

⁸ S. Nagata, T. Sasakawa, T. Sawada, and R. Tamagaki, Progr. Theoret. Phys. (Kyoto) **22**, 274 (1959).

⁹ T. Teresawa, Progr. Theoret. Phys. (Kyoto) **23**, 87 (1960).

¹⁰ A. Arima and T. Teresawa, Progr. Theoret. Phys. (Kyoto) **23**, 115 (1960).

¹¹ A. Arima, Nuclear Phys. **18**, 196 (1960).

¹² P. Goldhammer, Phys. Rev. **122**, 207 (1961).

¹³ W. Rarita and J. Schwinger, Phys. Rev. **59**, 436 (1941) and **59**, 556 (1941).

¹⁴ A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

same values for both terms. In a like manner the term with $K=2$ splits triplets, $K=3$ quartets, and so on.

The vector term:

$$S_{1M}(ijkl) = (1/40)^{1/2} \{ \sigma^i \cdot (\sigma^j \times \sigma^k)_M \sigma^l + \sigma^i \cdot (\sigma^j \times \sigma^k)_M \sigma^l + \sigma^i \cdot (\sigma^j \times \sigma^l)_M \sigma^k + \sigma^i \cdot (\sigma^j \times \sigma^l)_M \sigma^k \}, \quad (1.10a)$$

$$R_{1M}(ijkl) = (2/5)^{1/2} \mathbf{n}_{ij} \cdot \mathbf{n}_{kl} (\mathbf{n}_{ij} \times \mathbf{n}_{kl})_M, \quad (1.10b)$$

defined in Eqs. (1.5), has been the object of considerable attention in the literature.¹⁻¹² A term of this type is required to explain the energy levels of nuclei in the nuclear shell model,^{15,16} and the problem of whether or not the second-order tensor term provides a doublet splitting adequately large and consistently in the right direction is an old one.¹ Another possible source of the doublet splitting is that a two-body spin-orbit operator is actually present in the nucleon-nucleon interaction.^{17,18}

The first p shell ($5 \leq A \leq 16$) would seem to provide a natural testing ground for a theory of the doublet splitting since it is in this shell that this effect is first required. Furthermore the doublet splitting builds up in the first p shell, the $p_{3/2}$ – $p_{1/2}$ separation being only about 2.6 Mev for the extra nucleon in He^5 , and 6.3 Mev in N^{15} at the end of the shell.¹⁹ In this paper we shall attempt to correlate this building up of the doublet separation with the second-order effect of the tensor operator.

2. GENERAL RELATIONS FOR A SINGLE NUCLEON OR HOLE ADDED TO A CLOSED SHELL

In a preceding paper²⁰ we have formulated a procedure for applying the second-order perturbation method of Bolsterli and Feenberg²¹ to nuclei with doubly closed shells, and later¹² extended this to include nuclei with closed shells plus a single nucleon. A simple modification extends the procedure to nuclei with one hole in a doubly closed shell.

The derivation is contingent on our being able to write a zero-order wave function as a single determinant of particle orbitals:

$$\psi_0 = (A!)^{-1/2} |u_1 u_2 \cdots u_A|. \quad (2.1)$$

One can then express the matrix elements of any two-body operator O_{12} in terms of the density matrices

$$(a|\rho|b) = \sum_{l=1}^A u_l^*(a) u_l(b) \quad (2.2)$$

as follows:

¹⁵ M. G. Mayer, Phys. Rev. **75**, 1969 (1949).
¹⁶ O. Haxel, J. H. D. Jensen, and H. E. Suess, Ergeb. exakt. Naturw. **26**, 244 (1952).

¹⁷ J. L. Gammel and R. M. Thaler, Phys. Rev. **107**, 1337 (1957).

¹⁸ P. S. Signell and R. E. Marshak, Phys. Rev. **106**, 832 (1957).

¹⁹ D. R. Inglis, Revs. Modern Phys. **25**, 390 (1953).

²⁰ P. Goldhammer, Phys. Rev. **116**, 676 (1959).

²¹ M. Bolsterli and E. Feenberg, Phys. Rev. **101**, 1349 (1956).

$$\frac{1}{2} A(A-1)(O_{12}O_{12})_{00}$$

$$= \frac{1}{2} \int \cdots \int [(1,2|\rho^2 O_{12} O_{12}|1,2) - (1,2|\rho^2 O_{12} O_{12}|2,1)] d\mathbf{r}_1 d\mathbf{r}_2, \quad (2.3a)$$

$$A(A-1)(A-2)(O_{12}O_{13})_{00}$$

$$= \int \cdots \int \sum_{\nu} (-1)^{\nu} P_{\nu}(abc) \times (1,2,3|\rho^3 O_{12} O_{13}|a,b,c) d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3, \quad (2.3b)$$

$$\frac{1}{4} A(A-1)(A-2)(A-3)(O_{12}O_{34})_{00}$$

$$= \frac{1}{4} \sum_{\nu} (-1)^{\nu} P_{\nu}(abcd) \times \int \cdots \int (1,2,3,4|\rho^4 O_{12} O_{34}|a,b,c,d) \times d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4, \quad (2.3c)$$

where $P_{\nu}(abc)$ simply permutes a, b, c over 1, 2, 3.

If ψ_0 represents a closed shell plus one nucleon (or hole), the density matrix can be written

$$(a|\rho|b) = \sum_{\text{closed shell}} u_l^*(a) u_l(b) \pm u_n^*(a) u_n(b), \quad (2.4)$$

where the positive sign is taken for the additional nucleon and the negative sign for a hole (if we are dealing with a hole there is naturally a term with $l=n$ in our sum). The density matrices in Eqs. (2.3) may then be expanded in the following manner:

$$(1,2|\rho^2 O_{12} O_{12}|1,2) = \sum_{\text{closed shell}} u_l^*(1) u_l^*(2) O_{12} O_{12} u_l(1) u_l(2) \pm 2 u_n^*(1) \{ \sum_{\text{closed shell}} u_l^*(2) O_{12} O_{12} u_l(2) \} u_n(1). \quad (2.5)$$

In Eq. (2.5) we omit the self-energy term:

$$u_n^*(1) u_n^*(2) O_{12} O_{12} u_n(1) u_n(2), \quad (2.5a)$$

since the same term appears in $(1,2|\rho^2 O_{12} O_{12}|2,1)$ with opposite sign. Owing to the fact that spurious terms of this sort properly cancel out of the final expression, we suppress them from the start.

The results of the spin sums on $S_{10}(ijkl)$ needed in evaluating the density matrices are displayed in Table I. In the Appendix we shall discuss a modified form of the Bolsterli-Feenberg perturbation procedure.

3. APPLICATION TO N^{15}

In estimating the spin-orbit splitting in N^{15} we shall use the tensor interaction operator:

$$\frac{1}{4} (1 - \tau_1 \cdot \tau_2) S_{12} J_s(r_{12}/r_0)^2 \exp(-r_{12}^2/r_0^2), \quad (3.1)$$

where $J_s = -107.29$ Mev, $r_0 = 1.54 \times 10^{-13}$ cm, and τ_1 and τ_2 are isobaric spin operators. This is the tensor

TABLE I. Density matrix elements of $S_{10}(ijkl)$ needed in the applications. Absent permutations either vanish or are equivalent to one present by simply symmetry considerations.

		a	b			α	β	$\chi_{\frac{1}{2}}(a)(\sigma_b \rho S_{10}(1212) \sigma_\beta) \chi_{\frac{1}{2}}(\alpha)$		
		1	2			1	2	$(5/2)^{\frac{1}{2}}$		
		1	2			2	1	$(5/2)^{\frac{1}{2}}$		
		a	b	c			α	β	γ	$\chi_{\frac{1}{2}}(a)(\sigma_b, \sigma_c \rho^2 S_{10}(1213) \sigma_\beta, \sigma_\gamma) \chi_{\frac{1}{2}}(\alpha)$
		1	2	3			1	3	2	$(5/2)^{\frac{1}{2}}$
		2	1	3			3	1	2	$(5/2)^{\frac{1}{2}}$
		3	1	2			2	1	3	$-(5/2)^{\frac{1}{2}}$
		3	1	2			2	3	1	$-(5/2)^{\frac{1}{2}}$
		1	2	3			3	1	2	$(5/2)^{\frac{1}{2}}$
		2	1	3			1	3	2	$(5/2)^{\frac{1}{2}}$
		a	b	c	d	α	β	γ	δ	$\chi_{\frac{1}{2}}(a)(\sigma_b, \sigma_c, \sigma_d \rho^3 S_{10}(1234) \sigma_\beta, \sigma_\gamma, \sigma_\delta) \chi_{\frac{1}{2}}(\alpha)$
		1	2	3	4	4	3	2	1	$(5/2)^{\frac{1}{2}}$
		2	1	3	4	3	4	2	1	$(5/2)^{\frac{1}{2}}$
		3	1	2	4	2	4	3	1	$-(5/2)^{\frac{1}{2}}$
		4	1	2	3	1	4	3	2	$-(5/2)^{\frac{1}{2}}$
		1	2	3	4	4	3	1	2	$(5/2)^{\frac{1}{2}}$
		2	1	3	4	3	4	1	2	$(5/2)^{\frac{1}{2}}$
		3	1	2	4	1	4	3	2	$-(5/2)^{\frac{1}{2}}$
		4	1	2	3	2	4	3	1	$-(5/2)^{\frac{1}{2}}$

part of a two-body Serber interaction (with repulsive core) which has been fitted²⁰ to the binding energies of H^2 , H^3 , and He^4 , the electric quadrupole moment of H^2 , the rms radii of H^2 and He^4 , and the H^3 - He^3 Coulomb energy difference. This interaction was employed²⁰ in a calculation on O^{16} using second-order perturbation theory which yielded a total binding energy about 8% short of the experimental value, and an rms radius about 7% too small.

The $p_{\frac{3}{2}}$ - $p_{\frac{1}{2}}$ splitting in N^{15} is estimated by computing the separation of two such holes in O^{16} . One must note that this differs from doing a proper calculation on N^{15} . The oscillator well depth, which serves as the size parameter, is taken to be the one which minimizes the binding energy of O^{16} ($\hbar\omega=17.25$ Mev), instead of properly deriving the two well depths appropriate to the $p_{\frac{3}{2}}$ and $p_{\frac{1}{2}}$ states of N^{15} . In view of the approximation that is made by terminating the perturbation series at second-order the distinction between the spin-orbit splitting in O^{16} orbitals and actual N^{15} states is probably not a critical one.

The $p_{\frac{3}{2}}$ - $p_{\frac{1}{2}}$ separation is given by the expression:

$$\Delta = \alpha^4 (3J_s^2/\hbar\omega) \{ 5(A_{-2\ 7/2} - 2A_{0\ 7/2} + A_{2\ 7/2}) + 35(A_{0\ 9/2} - A_{2\ 9/2}) - 10(B_{-2\ 7/2} - B_{0\ 7/2} + B_{2\ 7/2}) - 35(1+\alpha^4)B_{0\ 9/2} + 35(1+\alpha^2)B_{2\ 9/2} + (315/2)\alpha^4(1+4\alpha^2+2\alpha^4)B_{2\ 11/2} + (315/2)\alpha^8 B_{4\ 11/2} + 5(C_{-2\ 7/2} - C_{2\ 7/2}) \}, \quad (3.2)$$

where $\alpha^2 = (\hbar/M\omega r_0^2)$,

$$A_{ln} = \int_0^1 t^{l+\delta-1} [(1+2\alpha^2)^2 - 4\alpha^4 t^2]^{-n} dt, \quad (3.2a)$$

$$B_{ln} = \int_0^1 t^{l+\delta-1} [(1+2\alpha^2)^2 - \alpha^4 t^2]^{-n} dt, \quad (3.2b)$$

and

$$C_{ln} = \int_0^1 t^{l+\delta-1} (1+2\alpha^2)^{-2n} dt = (1+2\alpha^2)^{-2n} / (\delta+l). \quad (3.2c)$$

The second-order energy shift δ ($-\hbar\omega\delta = E - E_0$) is taken to be zero, which means that we are calculating the second-order energy shift in the Rayleigh-Schrödinger perturbation expansion, not the Brillouin-Wigner. Our computed separation is 5.6 Mev to be compared with the experimental value of 6.3 Mev.

4. CONCLUSIONS

A similar calculation for the doublet splitting in He^5 was reported in a previous paper.¹² The separation derived for that case was considerably too large (3.4 Mev compared to 2.6 Mev by experiment). Since unrealistic assumptions were made concerning the size parameter (He^5 is unbound) which would favor a large splitting, this result is not in too poor agreement with the observed value. At least two authors^{7,8} have attempted more realistic phase shift calculations on the He^5 system. Strong temptation exists in doing the phase-shift calculation to consider the scattering of a neutron from an undistorted α particle. Such a restriction will yield a low estimate of the doublet splitting. The presence of a neutron in the p shell restricts the configuration mixing in the α -particle core due to the Pauli exclusion principle, and this restriction plays a decisive role in the spin-orbit splitting.⁹ Nagata *et al.*⁸ have pointed out that after such effects are included in the phase-shift calculations, the tensor interaction is capable of accounting for a major portion of the doublet splitting in He^5 .

The estimation of the doublet splitting in N^{15} de-

scribed in the preceding section is about 11% short of the observed value, a strong indication that a substantial part of this splitting may be due to the tensor-even interaction. This calculation does not clear up the problem of whether the tensor or the two-body spin-orbit interaction is primarily responsible for the doublet splitting in complex nuclei. Instead it presents a more basic problem of whether the even or odd terms produce the observed splittings. A strong spin-orbit odd interaction is required to explain the polarization found in proton-proton scattering,^{17,18} and such a term probably makes a substantial contribution²² to the doublet separation. This difficulty has previously been encountered by Brueckner *et al.*²³ who were forced to set the spin-orbit even terms equal to zero in order not to overestimate the doublet splitting. The possibility exists that second-order terms in the spin-orbit interaction yield terms opposite in sign from the tensor force, producing some cancellation.²⁴

In evaluating the right-hand side of Eq. (3.2) it is convenient to expand the integrands into a power series in l^2 , obtaining after integration an expression of the form

$$\Delta = \sum_{n=1}^{\infty} \frac{\Lambda_n}{\delta + 2n}. \quad (4.1)$$

It is important to note that spurious terms in $1/\delta$ and $1/(\delta-2)$ arise in some of the integrations, but properly cancel in the final result. Equation (4.1) is that part of the usual second-order perturbation expansion:

$$\sum' \frac{|V_{0n}|^2}{E - E_n}, \quad (4.2)$$

which contributes to the doublet splitting. Strict observance of the Pauli principle is insured by the fact that the zero-order wavefunction is properly antisymmetric, and the interaction operator ($V = \sum_{i<j} V_{ij}$) is symmetric in the coordinates of all nucleons. Spurious terms which violate the Pauli principle arise in parts of the calculation since a term of the type

$$[V_{12}(E - H_0)^{-1}V_{12}]_{00}, \quad (4.3a)$$

evaluates the contribution to the second-order energy shift from a "part" of the operator V , and this "part" is not properly symmetric. Hence in the above term one may have contributions from states where two nucleons in the $1p$ shell are demoted to the $1s$ shell. When the additional contributions from the three- and four-particle terms,

$$[V^{12}(E - H_0)^{-1}V_{13}]_{00}, \quad (4.3b)$$

$$[V^{12}(E - H_0)^{-1}V_{34}]_{00}, \quad (4.3c)$$

are included, such spurious contributions vanish identically.

When these spurious terms are deducted, it is found that the main contribution (7.6 Mev) to the doublet splitting arises from the three-body terms. The two-body terms yield 0.3 Mev, while the four-body terms give -2.3 Mev. Consequently the present calculation verifies the idea that it is the three-body terms which are of primary importance in evaluating the doublet splitting, as has long been emphasized by Feingold.²⁻⁴ The increase of the doublet splitting in N^{15} over He^5 results simply from the additional terms due to interaction of the hole with the entire $1p$ shell.

In evaluating the series in Eq. (4.1) one must take about fifteen terms in order to ensure two-place accuracy. The first term alone contributes only 2.3 Mev, which emphasizes the advantage of generating the entire series by the Bolsterli-Feenberg method. Calculations which do not include several terms in this series, or which suppress the three-body terms, must yield results much smaller than the experimental value.

In conclusion we would like to mention two obvious deficiencies in the calculation described in this paper other than the restriction of second-order perturbation theory. The radial dependence of the tensor interaction is not well established. Yukawa shapes, square wells, and straight Gaussians are often used and yield reasonable results. The form used here is fitted to the properties of nuclei in the $1s$ shell, and closely resembles the shape of the Gartenhaus²⁵ potential. Though by modifying the radial shape of the interaction one may reduce the derived doublet splitting, it is doubtful that one would reduce it so substantially that one could not conclude that the tensor interaction makes a major contribution. The size parameter used is the one derived from a calculation on O^{16} , and known to give too small a radius. Arima and Teresawa¹⁰ have pointed out that it may make sense to use an oscillator well depth parameter which yields too small a radius to a given order of perturbation theory since higher orders will yield a larger radius for the same parameter. The well parameter tends to increase through the $1p$ shell,²⁶ and the value used is probably reasonable. At any rate, it is more consistent to use a parameter derived with the force used than to simply try to fit the $N^{15}-O^{16}$ Coulomb energy difference. An additional source of error may lie in using the same size parameter in the $1s$ shell and the $1p$ shell. It is not reasonable that the $1s$ shell expands to the size indicated (about a 20% increase in rms radius) by equating these parameters, and shrinking the $1s$ shell would reinforce the doublet splitting. No attempt to include such a modification was made since little is definitely known about the proper values that one should use. However, a modified form of the Bolsterli-Feenberg perturbation procedure

²² J. W. Clark, Ann. Phys. **11**, 483 (1960).

²³ K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961).

²⁴ E. Feenberg (private communication).

²⁵ S. Gartenhaus, Phys. Rev. **100**, 900 (1955).

²⁶ R. Hofstadter, Ann. Rev. Nuclear Sci. **7**, 231 (1957).

which could incorporate this effect is presented in the Appendix.

ACKNOWLEDGMENTS

It is a pleasure to thank Professor Saul Epstein and Professor Henry Valk for interesting discussions of this work.

APPENDIX. A MODIFIED FORM OF THE BOLSTERLI-FEENBERG PERTURBATION PROCEDURE

The zero-order Hamiltonian is taken to be a sum of single-particle harmonic oscillator Hamiltonians with a uniform displacement in energy:

$$H_0 = \frac{1}{2}\hbar\omega \sum_{i=1}^A (p_i^2 + q_i^2) + U, \quad (\text{A.1})$$

with eigenfunctions and eigenvalues defined by

$$H_0\psi_n = E_n\psi_n. \quad (\text{A.2})$$

The perturbation operator is

$$W = \sum_{i < j} V_{ij} - \frac{1}{2}\hbar\omega \left(\sum_i q_i^2 - AQ^2 \right) - U, \quad (\text{A.3})$$

where V_{ij} is the nuclear interaction operator, and $Q = \sum q_i/A$. This Hamiltonian is of just the same form used by Bolsterli and Feenberg. The trial function is taken to be

$$\Psi = \frac{1}{N} \left[\varphi_0 + \sum' \frac{(\varphi_0 | W | \psi_n)}{E - E_n} \psi_n \right]. \quad (\text{A.4})$$

This prescription differs from the usual one in that φ_0 is not to be identified with ψ_0 (the oscillator ground state); rather, φ_0 may be any function of the nucleon coordinates which obeys the boundary and symmetry conditions of the problem. In particular, for O^{16} , φ_0 could be taken as a determinant of oscillator orbitals with depth parameters different from that in Eq. (A.1), and naturally different parameters for the 1s and 1p orbitals.

Substitution of (A.4) into the expression.

$$E = \int \cdots \int \Psi^* H \Psi / \int \cdots \int \Psi^* \Psi, \quad (\text{A.5})$$

yields

$$\begin{aligned} E &= (\varphi_0 | H_0 + W | \varphi_0) \\ &+ 2 \sum' \frac{(\varphi_0 | H_0 - E | \psi_n)(\psi_n | W | \varphi_0)}{E - E_n} \\ &+ \sum' \frac{|(\varphi_0 | W | \psi_n)|^2}{E - E_n} + \text{third order term.} \end{aligned} \quad (\text{A.6})$$

Equation (A.6) easily may be expressed in terms of matrix elements of zero-order functions:

$$\begin{aligned} E &= (\varphi_0 | H_0 - W | \varphi_0) \\ &- 2 \frac{(\varphi_0 | H_0 - E | \psi_0)(\psi_0 | W | \varphi_0)}{E - E_0} \\ &+ (\varphi_0 | W (E - H_0)^{-1} W | \varphi_0) \\ &- |(\varphi_0 | W | \varphi_0)|^2 (E - E_0)^{-1} \\ &+ \text{third order term.} \end{aligned} \quad (\text{A.7})$$

The energy denominator in Eq. (A.7) may be evaluated by employing the operator

$$\begin{aligned} &\exp[-\mu(p^2 + q^2)] f(\mathbf{q}) \\ &= (k/2\pi g)^{\frac{1}{2}} \int \int \int f(\mathbf{v}) \\ &\quad \times \exp \left[-\frac{1}{2g} (q^2 + v^2 - 2k\mathbf{q} \cdot \mathbf{v}) \right] d\mathbf{v}, \end{aligned} \quad (\text{A.8})$$

(where $g = \tanh 2\mu$ and $k = \cosh 2\mu$), with only minor complications due to the fact that φ_0 is not an eigenfunction of H_0 .

This modification has the advantage of additional variational flexibility since one can minimize the energy with respect to the parameters in φ_0 as well as $\hbar\omega$, and it may be useful if 1s- and 1p-shell parameters are in reality significantly different.