Theoretical Calculation of the Binding Energy of O^{16}†

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The second-order perturbation procedure of Bolsterli and Feenberg is applied to the ground state of O^{16}. The two-body interaction operator employed has a Serber exchange character with repulsive core and tensor component, determined to give a reasonable fit to the properties of H^2, H^3, He^3, and He^4 to the accuracy of the perturbation procedure. The resulting eigenstate for O^{16} is found to have energy eigenvalue -129.2 Mev and rms radius 2.33×10^{-13} cm. Coulomb forces are neglected. Components in the wave function different from the zero-order shell-model state are found to have a statistical weight of about 18%.

1. INTRODUCTION

MANY attempts have been made to correlate the properties of light nuclei with two-body nuclear interactions.[1–5] Bolsterli and Feenberg[6] have devised a second-order perturbation procedure for such calculations which reduces mathematical labor, and is fairly accurate if the zero-order wave function is a good approximation to the actual eigenstate. We shall briefly review this procedure here, in order to define our notation.

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

$$H_0=\tfrac{1}{2}\hbar\omega\sum_{i=1}^{A}(p_i^2+q_i^2)+U=\sum_{i=1}^{A}H_{\rm osc}(i)+U. \tag{1-1}$$

The perturbation operator is

$$W=\sum_{i<j}V_{ij}-\tfrac{1}{2}\hbar\omega\Big(\sum_i q_i^2-AQ^2\Big)-U, \tag{1-2}$$

where V_{ij} is the nuclear interaction operator between particles i and j, and $\mathbf{Q}=(1/A)\sum\mathbf{q}_i$. The depth of U is adjusted so that $W_{00}=0$. The approximate eigenvalue E is implicitly given by

$$E-E_0=-\int_0^\infty e^{\lambda(E)}(Ve^{-\lambda H_0}V)_{00}d\lambda-\frac{|V_{00}|^2}{E-E_0}+\frac{1}{E-E_0-2\hbar\omega}\big[(M^2)_{00}-(M_{00})^2-2(MV)_{00}+2M_{00}V_{00}\big], \tag{1-3}$$

where

$$E_0=V_{00}-M_{00}+(H_{\rm osc})_{00}, \tag{1-4}$$

and

$$M=\tfrac{1}{2}\hbar\omega\Big(\sum_i q_i^2-AQ^2\Big)=(\hbar\omega/2A)\sum_{i<j}q_{ij}^2. \tag{1-5}$$

The operator $e^{-\lambda H_{\rm osc}}$ is transformed into manageable form by

$$\exp[-\mu(p^2+q^2)]f(\mathbf{q})=(k/2\pi g)^{\frac{3}{2}}\iiint f(\mathbf{v})\times\exp[-(\tfrac{1}{2}g)(q^2+v^2-2k\mathbf{q}\cdot\mathbf{v})]d\mathbf{v}, \tag{1-6}$$

where $g=\tanh2\mu$, $k=\text{sech}2\mu$, and $\mu=\frac{1}{2}\hbar\omega\lambda$. $\hbar\omega$ is determined to minimize the energy of the physical system $(E-\frac{3}{2}\hbar\omega)$. Mixing of configurations higher than the zero-order is given by

$$N^2-1=\sum_{n\neq0}\frac{|W_{n0}|^2}{(E-E_n)^2}, \tag{1-7}$$

where N normalizes the perturbed wave function

$$\Psi=\frac{1}{N}\Big[\psi_0+\sum_{n\neq0}\frac{W_{0n}\psi_n}{E-E_n}\Big]. \tag{1-8}$$

This procedure, which has the elegant advantage of involving only matrix elements with zero-order harmonic oscillator wave functions, was originally applied to H^2, H^3, and He^4. This method has been extended, with refinements,[7,8] to third order in H^2. In this case at least the higher orders to not appear to make a significant difference in the energy.[9]

In this paper we shall prescribe formulas for extending the method to heavier nuclei whose zero-order wave function may be taken as a closed (doubly magic) oscillator shell, and apply them to O^{16}.

2. GENERAL RELATIONS FOR DOUBLY MAGIC SHELLS

When we have a closed oscillator shell our wave function may be written as a single determinant of

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particle orbitals:

$$\psi_0=(A!)^{-\frac{1}{2}}|u_1u_2\cdots u_A| =(A!)^{-\frac{1}{2}}\sum_\nu(-1)^\nu P_\nu u_1(1)u_2(2)\cdots u_A(A), \quad (2\text{-}1)$$

where P_ν is simply a permutation operator, and we sum over all permutations of A particles in A distinct orbitals. Introducing the density matrix

$$(a|\rho|b)=\sum_{l=1}^{A}u_l^*(a)u_l(b), \quad (2\text{-}2)$$

where the sum goes over all orbitals, and likewise

$$(a,b|\rho^2|c,d)=\sum_{k,l}u_l^*(a)u_k^*(b)u_l(c)u_k(d) =(a|\rho|c)(b|\rho|d), \quad (2\text{-}3)$$

one can obtain V_{00} in a manageable form:

$$V_{00}=\tfrac{1}{2}A(A-1)\int\cdots\int\psi_0^*V_{12}\psi_0d\mathbf{r}_1d\mathbf{r}_2\cdots d\mathbf{r}_A =\tfrac{1}{2}\sum_{l,k}\int\cdots\int u_k^*(1)u_l^*(2)V_{12}[u_k(1)u_l(2)-u_k(2)u_l(1)]d\mathbf{r}_1d\mathbf{r}_2 =\tfrac{1}{2}\int\cdots\int[(1,2|\rho^2V_{12}|1,2)-(1,2|\rho^2V_{12}|2,1)]d\mathbf{r}_1d\mathbf{r}_2. \quad (2\text{-}4)$$

Likewise one may express

$$(Ve^{-\lambda H_0}V)_{00}=\tfrac{1}{2}A(A-1)(V_{12}e^{-\lambda H_0}V_{12})_{00}+A(A-1)(A-2)(V_{12}e^{-\lambda H_0}V_{13})_{00}+\tfrac{1}{4}A(A-1)(A-2)(A-3)(V_{12}e^{-\lambda H_0}V_{34})_{00} \quad (2\text{-}5)$$

in terms of density matrices:

$$\tfrac{1}{2}A(A-1)(V_{12}e^{-\lambda H_0}V_{12})_{00} =\tfrac{1}{2}e^{-\lambda E_0}\int\cdots\int\{(1,2|\rho^2V_{12}\exp[-\lambda H_{\text{osc}}(1)-\lambda H_{\text{osc}}(2)]V_{12}\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]|1,2) -(1,2|\rho^2V_{12}\exp[-\lambda H_{\text{osc}}(1)-\lambda H_{\text{osc}}(2)]V_{12}\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]|2,1)\}d\mathbf{r}_1d\mathbf{r}_2, \quad (2\text{-}5a)$$

$$A(A-1)(A-2)(V_{12}e^{-\lambda H_0}V_{13})_{00} =e^{-\lambda E_0}\int\cdots\int\sum_{\nu=1,2,3}(-1)^\nu P_\nu(abc)(1,2,3|\rho^3\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]V_{12}\exp[-\lambda H_{\text{osc}}(1)]V_{13} \times\exp[-\lambda H_{\text{osc}}(2)]|a,b,c)d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3, \quad (2\text{-}5b)$$

$$\tfrac{1}{4}A(A-1)(A-2)(A-3)(V_{12}e^{-\lambda H_0}V_{34})_{00} =\tfrac{1}{4}e^{-\lambda E_0}\int\cdots\int\sum_{\nu=1,2,3,4}(-1)^\nu P_\nu(abcd)(1,2,3,4|\rho^4\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]V_{12}V_{34} \times\exp[-\lambda H_{\text{osc}}(1)-\lambda H_{\text{osc}}(2)]|a,b,c,d)d\mathbf{r}_1\cdots d\mathbf{r}_4, \quad (2\text{-}5c)$$

where $H_0\psi_0=E_0\psi_0$, and $P_\nu(abc)$ simply permutes a, b, c over 1, 2, 3. Equation (1-6) is employed to handle $e^{-\lambda H_{\text{osc}}}$.

If V_{12} is merely a function of $\mathbf{r}_{12}=\mathbf{r}_1-\mathbf{r}_2$ we have $(1,2|\rho^2V_{12}|1,2)=V_{12}(1,2|\rho^2|1,2)$, but in general we shall consider an interaction operator with exchange character so that it will involve the projection operators

$$P_0(1,2)=(1/16)(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \quad \text{(singlet-even)}, \quad (2\text{-}6a)$$

$$P_1(1,2)=(1/16)(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \quad \text{(triplet-even)}, \quad (2\text{-}6b)$$

$$P_2(1,2)=(1/16)(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \quad \text{(singlet-odd)}, \quad (2\text{-}6c)$$

$$P_3(1,2)=(1/16)(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2) \quad \text{(triplet-odd)}, \quad (2\text{-}6d)$$

as well as the tensor operator

$$S_{12}=\boldsymbol{\sigma}_1\cdot\mathbf{n}_{12}\boldsymbol{\sigma}_2\cdot\mathbf{n}_{12}-\tfrac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2, \quad (2\text{-}6e)$$

and so we must perform a sum on spin and isobaric spin functions before taking V_{12} outside the density matrix. For a closed shell we may perform our sum over the spin, isobaric spin, and space quantum numbers independently. The results of this evaluation are displayed in Table I, II, and III. Table III has been abbreviated due to the equivalence of the sets of permutations

1324—1432—3214—4231, (2-7a)

3412—4321, (2-7b)

1342—1423—3241—4213, (2-7c)

2314—2431—3124—4132, (2-7d)

2413—3142—4123—2341, (2-7e)

3421—4312, (2-7f)

under the needed operations. Furthermore 2134 is readily obtained from 1243; and 2314 from 1342.

TABLE I. Evaluation of $(1,2|\rho^2\mathfrak{D}|a,b)$ in $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ space for needed projection operators.

$\mathfrak{D}\diagdown ab$	12	21
1	16	4
$P_0(12)$	3	−3
P_1	3	−3
P_2	1	1
P_3	9	9
$P_0(12)P_0(12)$	3	−3
$P_1\quad P_1$	3	−3
$P_2\quad P_2$	1	1
$P_3\quad P_3$	9	9
$P_i\quad P_{j\neq i}$	0	0

Tensor terms are of the form

$$(1,2|\rho^2S_{12}S_{1'2'}|a,b)=C_{ab}[\cos^2(n_{12},n_{1'2'})-\tfrac{1}{3}], \quad \text{(2-8a)}$$

$$(1,2,3|\rho^3S_{12}S_{1'3}|a,b,c)=-C_{abc}[\cos^2(n_{12},n_{1'3})-\tfrac{1}{3}], \text{(2-8b)}$$

$$(1,2,3,4|\rho^4S_{12}S_{34}|a,b,c,d)=C_{abcd}[\cos^2(n_{12},n_{34})-\tfrac{1}{3}], \quad \text{(2-8c)}$$

and tensor components in the potential will be multiplied by a projection operator to select tensor-even $[\frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)]$ or tensor-odd $[\frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)]$ states. Nonvanishing elements needed in the calculations are displayed in Table IV.

The space part of the density matrices is easily evaluated for closed oscillation shells.

$$(1|\rho_0|2)=\pi^{-\frac{3}{2}}\exp[-\tfrac{1}{2}(q_1^2+q_2^2)], \quad 1s\text{-shell} \quad \text{(2-9a)}$$

$$(1|\rho_1|2)=2\pi^{-\frac{3}{2}}\mathbf{q}_1\cdot\mathbf{q}_2\exp[-\tfrac{1}{2}(q_1^2+q_2^2)], \quad 1p\text{-shell} \quad \text{(2-9b)}$$

and so on.

The matrix elements of M needed in Eq. (1-3) are also easily obtained. Let $\exp(-q^2)\rightarrow\exp(-\gamma q^2)$ in the oscillator orbitals; then

$$\int\cdots\int|\psi_0|^2d\mathbf{r}_1\cdots d\mathbf{r}_A\rightarrow\gamma^{-(3/2)A}, \quad 1s\text{-shell}$$
$$\rightarrow\gamma^{-6}\gamma^{-(5/2)(A-4)}, \quad 1p\text{-shell} \quad \text{(2-10)}$$

$$(\sum q_k^2)_{00}=-\left(\frac{d}{d\gamma}\int\cdots\int|\psi_0|^2\right)_{\gamma=1}$$
$$=(3/2)A, \quad 1s\text{-shell}$$
$$=(5/2)A-4, \quad 1p\text{-shell} \quad \text{(2-11)}$$

$$(AQ^2)_{00}=\tfrac{3}{2}, \quad [(AQ^2)^2]_{00}=15/4, \quad \text{(2-12)}$$

and we finally have

$$M_{00}=\tfrac{3}{4}(A-1)\hbar\omega, \quad 1s\text{-shell}$$
$$=\tfrac{1}{4}(5A-11)\hbar\omega, \quad 1p\text{-shell.} \quad \text{(2-13)}$$

Likewise

$$[(\sum_k q_k^2)^2]_{00}=\left(\frac{d^2}{d\gamma^2}\int\cdots\int|\psi_0|^2\right)_{\gamma=1}$$
$$=\tfrac{3}{2}A(\tfrac{3}{2}A+1), \quad 1s\text{-shell}$$
$$=(\tfrac{5}{2}A-4)(\tfrac{5}{2}A-3), \quad 1p\text{-shell} \quad \text{(2-14)}$$

and

$$(M^2)_{00}=3(\hbar\omega/4)^2(3A-1)(A-1), \quad 1s\text{-shell}$$
$$=(\hbar\omega/4)^2(5A-11)(5A-9), \quad 1p\text{-shell} \quad \text{(2-15)}$$

$(MV)_{00}$ is simply obtained from V_{00}:

$$(MV)_{00}=-(\hbar\omega/2)\left(\frac{d}{d\gamma}V_{00}\right)_{\gamma=1}-(3/4)\hbar\omega(V_{00})_{\gamma=1}. \quad \text{(2-16)}$$

3. APPLICATION TO O^{16}

We shall consider an interaction operator that is composed of three distinct parts:

$$V_{12}=V_R(1,2)+V_C(1,2)+V_S(1,2)S_{12}. \quad \text{(3-1)}$$

V_R represents a repulsive core:

$$V_R(1,2)=J_R\exp(-r_{12}^2/R^2), \quad \text{(3-1a)}$$

with a short half-width; V_C is the central exchange potential $(r_0>R)$:

$$V_C(1,2)=(J_0P_0+J_1P_1+J_2P_2+J_3P_3)\times\exp(-r_{12}^2/r_0^2), \quad \text{(3-1b)}$$

TABLE II. Evaluation of $(1,2,3|\rho^3\mathfrak{D}|a,b,c)$ in $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ space for needed projection operators.

$\mathfrak{D}\diagdown abc$	123	312	231	213	132	321
$P_0(12)P_0(13)$	9/4	−3	9/4	−9/4	3	−9/4
$P_1\quad P_1$	9/4	−3	9/4	−9/4	3	−9/4
$P_2\quad P_2$	1/4	1	1/4	1/4	1	1/4
$P_3\quad P_3$	81/4	9	81/4	81/4	9	81/4
$P_0\quad P_1$	9/4	0	9/4	−9/4	0	−9/4
$P_0\quad P_2$	3/4	0	−3/4	−3/4	0	3/4
$P_0\quad P_3$	27/4	0	−27/4	−27/4	0	27/4
$P_1\quad P_2$	3/4	0	−3/4	−3/4	0	3/4
$P_1\quad P_3$	27/4	0	−27/4	−27/4	0	27/4
$P_2\quad P_3$	9/4	0	9/4	9/4	0	9/4
1	64	4	4	16	16	16
$P_2\quad P_0$	3/4	0	−3/4	3/4	0	−3/4
$P_2\quad P_1$	3/4	0	−3/4	3/4	0	−3/4
$P_3\quad P_0$	27/4	0	−27/4	27/4	0	−27/4
$P_3\quad P_1$	27/4	0	−27/4	27/4	0	−27/4
$P_3\quad P_2$	9/4	0	9/4	9/4	0	9/4
$P_0(12)$	12	−3	−3	−12	3	3
$P_1(12)$	12	−3	−3	−12	3	3
$P_2(12)$	4	1	1	4	1	1
$P_3(12)$	36	9	9	36	9	9
$P_0(13)$	12	−3	−3	3	3	−12
$P_1(13)$	12	−3	−3	3	3	−12
$P_2(13)$	4	1	1	1	1	4
$P_3(13)$	36	9	9	9	9	36

TABLE III. Evaluation of $(1234|\rho^4\mathfrak{O}|abcd)$ in $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ space for needed projection operators. Absent permutations may be obtained from those given by simple symmetry considerations.

$\mathfrak{O}$ \ $abcd$	1234	1243	1324	2143	4321	1423	2413	4312
1	256	64	64	16	16	16	4	4
$P_0(12)P_0(34)$	9	−9	9/4	9	3	−9/4	9/4	−3
$P_0(12)P_1(34)$	9	−9	9/4	9	0	−9/4	9/4	0
$P_0(12)P_2(34)$	3	−3	3/4	−3	0	−3/4	−3/4	0
$P_0(12)P_3(34)$	27	−27	27/4	−27	0	−27/4	−27/4	0
$P_1(12)P_1(34)$	9	−9	9/4	9	3	−9/4	9/4	−3
$P_1(12)P_2(34)$	3	−3	3/4	−3	0	−3/4	−3/4	0
$P_1(12)P_3(34)$	27	−27	27/4	−27	0	−27/4	−27/4	0
$P_2(12)P_2(34)$	1	1	1/4	1	1	1/4	1/4	1
$P_2(12)P_3(34)$	9	9	9/4	9	0	9/4	9/4	0
$P_3(12)P_3(34)$	81	81	81/4	81	9	81/4	81/4	9
$P_0(12)$	48	−48	12	−12	3	−12	−3	−3
$P_1(12)$	48	−48	12	−12	3	−12	−3	−3
$P_2(12)$	16	16	4	4	1	4	1	1
$P_3(12)$	144	144	36	36	9	36	9	9

while V_S multiplies the tensor components:

$$V_S(1,2)=[\tfrac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_S+\tfrac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)J_A]\times(r_{12}/r_0)^2\exp[-(r_{12}/r_0)^2]. \quad \text{(3-1c)}$$

The specific radial forms chosen make the integrals reduce to a simple closed form, and furthermore qualitatively resembles the Gartenhaus potential.[10] Making the substitutions

$$\alpha^2q_{12}^2=r_{12}^2/r_0^2 \quad \text{and} \quad \beta^2q_{12}^2=r_{12}^2/R^2, \qquad \text{(3-2)}$$

we may express V_{00} and $(MV)_{00}$ for O^{16} in terms of the integrals

$$\mathcal{V}_1(\gamma,a)=\int\cdots\int(1|\rho|1)(2|\rho|2)\times\exp(-a^2q_{12}^2)d\mathbf{r}_1d\mathbf{r}_2$$
$$=\gamma^{-31}[\gamma^2+2a^2\gamma]^{-7/2}[16\gamma^2+40\gamma a^2+31a^4], \quad \text{(3-3a)}$$

$$\mathcal{V}_2(\gamma,a)=\int\cdots\int|(1|\rho|2)|^2\exp(-a^2q_{12}^2)d\mathbf{r}_1d\mathbf{r}_2$$
$$=\gamma^{-31}[\gamma^2+2a^2\gamma]^{-7/2}[4\gamma^2+16\gamma a^2+31a^4]. \quad \text{(3-3b)}$$

TABLE IV. Density matrices for the tensor operator described by Eq. (2-8). All absent elements vanish.

Operator	Density matrix element
$\frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)C_{12}$	4
$\frac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)C_{21}$	−4
$\frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)C_{12}$	12
$\frac{1}{4}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)C_{21}$	12
$\frac{1}{16}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_3)C_{312}$	4
$\frac{1}{16}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_3)C_{132}$	−4
$\frac{1}{16}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_3)C_{312}$	−12
$\frac{1}{16}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_3)C_{132}$	−12
$\frac{1}{16}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(1-\boldsymbol{\tau}_3\cdot\boldsymbol{\tau}_4)C_{4321}$	4
$\frac{1}{16}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(1-\boldsymbol{\tau}_3\cdot\boldsymbol{\tau}_4)C_{4312}$	−4
$\frac{1}{16}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(3+\boldsymbol{\tau}_3\cdot\boldsymbol{\tau}_4)C_{4321}$	12
$\frac{1}{16}(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)(3+\boldsymbol{\tau}_3\cdot\boldsymbol{\tau}_4)C_{4312}$	12

Then

$$V_{00}=\tfrac{1}{2}J_R\{16\mathcal{V}_1(1,\beta)-4\mathcal{V}_2(1,\beta)\}+\tfrac{1}{2}(3J_0+3J_1)\{\mathcal{V}_1(1,\alpha)+\mathcal{V}_2(1,\alpha)\}+\tfrac{1}{2}(J_2+9J_3)\{\mathcal{V}_1(1,\alpha)-\mathcal{V}_2(1,\alpha)\}, \quad \text{(3-3c)}$$

and $(MV)_{00}$ is easily obtained from Eq. (2-16).

The matrix elements $(VeV)_{00}$ involve the integrals

$$I_{ij}(a,b)=\int\cdots\int(1,2|\rho^2\exp[-a^2q_{12}^2]\exp[-\lambda H_{\text{osc}}(1)-\lambda H_{\text{osc}}(2)]\exp[-b^2q_{12}^2]\times\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]|i,j)d\mathbf{q}_1d\mathbf{q}_2, \quad \text{(3-4a)}$$

$$I_{ijk}(a,b)=\int\cdots\int(1,2,3|\rho^3\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]\exp[-a^2q_{12}^2]\exp[-\lambda H_{\text{osc}}(1)]\times\exp[-b^2q_{13}^2]\exp[-\lambda H_{\text{osc}}(2)]|i,j,k)d\mathbf{q}_1d\mathbf{q}_2d\mathbf{q}_3, \quad \text{(3-4b)}$$

$$I_{ijkl}(a,b)=\int\cdots\int(1,2,3,4|\rho^4\exp[\lambda H_{\text{osc}}(1)+\lambda H_{\text{osc}}(2)]\exp[-a^2q_{12}^2-b^2q_{34}^2]\times\exp[-\lambda H_{\text{osc}}(1)-\lambda H_{\text{osc}}(2)]|i,j,k,l)d\mathbf{q}_1\cdots d\mathbf{q}_4, \quad \text{(3-4c)}$$

$$T_{ij}(\alpha)=\tfrac{1}{2}(k/2\pi g)^3\int\cdots\int(1,2|\rho^2\exp[-\alpha^2(q_{12}^2+v_{12}^2)][(\mathbf{q}_{12}\cdot\mathbf{v}_{12})^2-\tfrac{1}{3}q_{12}^2v_{12}^2]\exp[\lambda H_{\text{osc}}(1')+\lambda H_{\text{osc}}(2')]|i',j')\exp[-(\tfrac{1}{2}g)(q_1^2+v_1^2-2k\mathbf{q}_1\cdot\mathbf{v}_1+q_2^2+v_2^2-2k\mathbf{q}_2\cdot\mathbf{v}_2)]d\mathbf{q}_1d\mathbf{q}_2d\mathbf{v}_1d\mathbf{v}_2, \quad \text{(3-4d)}$$

[10] S. Gartenhaus, Phys. Rev. **100**, 900 (1955).

$$T_{ijk}(\alpha)=(k/2\pi g)^{\frac{3}{2}}\int\cdots\int(1,2,3|\rho^3\exp[\lambda H_{\rm osc}(1)+\lambda H_{\rm osc}(2)]\exp[-\alpha^2q_{12}^2-\alpha^2(\mathbf{v}_1-\mathbf{q}_3)^2]$$
$$\times\{[q_{12}\cdot(\mathbf{v}_1-\mathbf{q}_3)]^2-\tfrac{1}{3}q_{12}^2(\mathbf{v}_1-\mathbf{q}_3)^2\}\exp[-\lambda H_{\rm osc}(2)]|i,j,k)\exp[-(\tfrac{1}{2}g)(q_1^2+v_1^2-2k\mathbf{q}_1\cdot\mathbf{v}_1)]$$
$$\times d\mathbf{q}_1d\mathbf{q}_2d\mathbf{q}_3d\mathbf{v}_1, \quad (3\text{-}4e)$$

$$T_{ijkl}(\alpha)=\tfrac{1}{2}\int\cdots\int(1,2,3,4|\rho^4\exp[\lambda H_{\rm osc}(1)+\lambda H_{\rm osc}(2)]\exp[-\alpha^2(q_{12}^2+q_{34}^2)][(\mathbf{q}_{12}\cdot\mathbf{q}_{34})^2-\tfrac{1}{3}q_{12}^2q_{34}^2]$$
$$\times\exp[-\lambda H_{\rm osc}(1)-\lambda H_{\rm osc}(2)]|i,j,k,l)d\mathbf{q}_1\cdots d\mathbf{q}_4. \quad (3\text{-}4f)$$

The contributions to $(VeV)_{00}$ may now be written down quite generally for any closed oscillator shell, employing the $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ space evaluations given in Tables I–IV:

$$(V_Ce^{-\lambda H_0}V_C)_{00}+e^{-\lambda E_0}|(V_C)_{00}|^2$$
$$=e^{-\lambda E_0}\{(1/2)[3(J_0^2+J_1^2)+J_2^2+9J_3^2][I_{12}(\alpha,\alpha)-2I_{132}(\alpha,\alpha)+I_{4321}(\alpha,\alpha)]+(1/2)[3(J_0^2+J_1^2)-J_2^2-9J_3^2]$$
$$\times[I_{21}(\alpha,\alpha)-2I_{312}(\alpha,\alpha)+I_{4312}(\alpha,\alpha)]+(1/4)[3(J_0+J_1)+J_2+9J_3]^2[I_{123}(\alpha,\alpha)-I_{1324}(\alpha,\alpha)]$$
$$+(1/4)[3(J_0+J_1)-J_2-9J_3]^2[I_{231}(\alpha,\alpha)-I_{2413}(\alpha,\alpha)]+(1/2)[3(J_0+J_1)+J_2+9J_3]$$
$$\times[3(J_0+J_1)-J_2-9J_3][I_{213}(\alpha,\alpha)-I_{1423}(\alpha,\alpha)]\}, \quad (3\text{-}5a)$$

$$(V_Re^{-\lambda H_0}V_R)_{00}+e^{-\lambda E_0}|(V_R)_{00}|^2$$
$$=e^{-\lambda E_0}J_R^2\{64[I_{123}(\beta,\beta)-I_{1324}(\beta,\beta)]-32[I_{213}(\beta,\beta)-I_{1423}(\beta,\beta)]+8[I_{12}(\beta,\beta)-2I_{132}(\beta,\beta)-I_{4321}(\beta,\beta)]$$
$$+4[I_{231}(\beta,\beta)-I_{2413}(\beta,\beta)]-2[I_{21}(\beta,\beta)-2I_{312}(\beta,\beta)-I_{4312}(\beta,\beta)]\}, \quad (3\text{-}5b)$$

$$(V_Ce^{-\lambda H_0}V_R)_{00}+(V_C)_{00}(V_R)_{00}e^{-\lambda E_0}$$
$$=J_Re^{-\lambda E_0}\{(1/2)[3(J_0+J_1)+J_2+9J_3][I_{12}(\alpha,\beta)-2I_{132}(\alpha,\beta)+I_{4321}(\alpha,\beta)]+(1/2)[3(J_0+J_1)-J_2-9J_3]$$
$$\times[I_{21}(\alpha,\beta)-2I_{312}(\alpha,\beta)+I_{4312}(\alpha,\beta)]+4[3(J_0+J_1)+J_2+9J_3][I_{123}(\alpha,\beta)-I_{1324}(\alpha,\beta)]$$
$$-[3(J_0+J_1)-J_2-9J_3][I_{231}(\alpha,\beta)-I_{2413}(\alpha,\beta)]+4[3(J_0+J_1)-J_2-9J_3][I_{213}(\alpha,\beta)-I_{2314}(\alpha,\beta)]$$
$$-[3(J_0+J_1)+J_2+9J_3][I_{321}(\alpha,\beta)-I_{1423}(\alpha,\beta)]\}, \quad (3\text{-}5c)$$

$$\Big(\sum_{i<j}V_S(i,j)S_{ij}e^{-\lambda H_0}\sum_{i<j}V_S(i,j)S_{ij}\Big)_{00}$$
$$=4e^{-\lambda E_0}\alpha^4\{(J_S^2+3J_A^2)[T_{12}(\alpha)-T_{132}(\alpha)+T_{4321}(\alpha)]+(J_S^2-3J_A^2)[T_{21}(\alpha)-T_{312}(\alpha)+T_{4312}(\alpha)]\}. \quad (3\text{-}5d)$$

Explicit evaluation of the space integrals appears to be rather arduous, but labor is minimized by noting that one needs only the integral

$$\int\cdots\int\exp\Big[-\sum_{i,j=1}^{4}c_{ij}\mathbf{r}_i\cdot\mathbf{r}_j\Big]d\mathbf{r}_1\cdots d\mathbf{r}_4=\frac{\pi^6}{[\det|c_{ij}|]^{\frac{3}{2}}}, \quad (3\text{-}6)$$

and various combinations of its derivatives with respect to the c_{ij}. For O^{16} the integrals are (we let $t=e^{-2\mu}$):

$$I_{12}(a,b)=C_1^3\{4+3C_1^2[4+a^2b^2(1/t^2+8+t^2)]+15C_1^4[a^4+b^4-4a^4b^4-4a^2b^2t^2(a^2+b^2-a^2b^2t^2)]\},$$
$$I_{132}(a,b)=C_2^3\{4+3C_2^2[4+a^2b^2(1/t^2+4)]+15C_2^4[a^4+b^4+a^2b^2(a^2+b^2)]+105C_2^6a^4b^4(1+a^2)(1+b^2)t^2\},$$
$$I_{4321}(a,b)=C_3^3\{4+3C_3^2[4+a^2b^2(t^2+1/t^2)]+15C_3^4[a^4+b^4+a^2b^2(2a^2+2b^2+3a^2b^2)]\},$$
$$I_{21}(a,b)=C_1^3\{4+3C_1^2[a^2b^2(1/t^2+8+t^2)]+15C_1^4[a^4+b^4-4a^4b^4-4a^2b^2t^2(a^2+b^2-a^2b^2t^2)]\},$$
$$I_{312}(a,b)=C_2^3\{4+3C_2^2[a^2b^2(1/t^2+4)]+15C_2^4[a^4+b^4+a^2b^2(a^2+b^2)]+105C_2^6a^4b^4(1+a^2)(1+b^2)t^2\},$$
$$I_{4312}(a,b)=C_3^3\{4+3C_3^2[a^2b^2(t^2+1/t^2)]+15C_3^4[a^4+b^4+a^2b^2(2a^2+2b^2+3a^2b^2)]\},$$
$$I_{123}(a,b)=C_2^3\{64+3C_2^2[-22(a^2+b^2)-(61a^2b^2)+16a^2b^2t^2]+15C_2^4[a^2b^2(-11-5[a^2+b^2]-3a^2b^2-5t^2$$
$$-3t^2[a^2+b^2]-(4a^2b^2t^2)-2(a^2+b^2)]+105C_2^6a^4b^4(1+a^2)(1+b^2)t^2\}, \quad (3\text{-}7)$$
$$I_{1324}(a,b)=C_3^3\{64+3C_3^2[-22(a^2+b^2)-61a^2b^2]+15C_3^4[a^2b^2(-11-5a^2-5b^2-3a^2b^2)-2(a^2+b^2)]\},$$
$$I_{231}(a,b)=C_2^3\{4+3C_2^2[2a^2b^2(2-3t^2)]+15C_2^4[a^2b^2(3a^2+3b^2+9a^2b^2+t^2-8a^2b^2t^2)+a^4+b^4]$$
$$+105C_2^6a^4b^4(1+a^2)(1+b^2)t^2\},$$

$$I_{2413}(a,b)=C_3^3\{4+3C_3^2[4a^2b^2]+15C_3^4[a^2b^2(3a^2+3b^2+9a^2b^2)+a^4+b^4]\},$$

$$I_{213}(a,b)=I_{321}(b,a)=C_2^3\{16+3C_2^2[-8a^2-7a^2b^2]+15C_2^4[a^2b^2(-1+a^2+7b^2+5a^2b^2)+a^4+4b^4 -a^2b^2t^2(6b^2+5a^2b^2)]+105C_2^6a^4b^4(1+a^2)(1+b^2)t^2\},$$

$$I_{2314}(a,b)=I_{1423}(b,a)=C_3^3\{16+3C_3^2[-8a^2-7a^2b^2]+15C_3^4[a^2b^2(-1+a^2+7b^2+5a^2b^2)+a^4+4b^4]\},$$

$$T_{12}(\alpha)=(5/2)C_1^7[1/t^2+18+7t^2]+(35/2)C_1^9[-8\alpha^2-6\alpha^4+6t^2-16\alpha^2t^2-12\alpha^4t^2+18\alpha^4t^4] +(315/2)C_1^{11}(8\alpha^4t^2)[(1+\alpha^2)^2-2t^2(1+\alpha^2)\alpha^2+t^4\alpha^4],$$

$$T_{132}(\alpha)=(5/2)C_2^7[2/t^2+28+6t^2]+(35/2)C_2^9[-12\alpha^2-7\alpha^4+t^2(-5-8\alpha^2-13\alpha^4)] +(315/2)C_2^{11}\{t^2[(1+\alpha^2)^2+\alpha^4]\times[(1+\alpha^2)^2+4\alpha^4]+t^4[(1+\alpha^2)^4-2\alpha^8]\}+(3465/2)C_2^{13}t^4\alpha^8(1+\alpha^2)^2,$$

$$T_{4321}(\alpha)=(5/2)C_3^7[t^2+1/t^2+10]+(35/2)C_3^9[-4\alpha^2-2\alpha^4], \tag{3-8}$$

$$T_{21}(\alpha)=(5/2)C_1^7[1/t^2+2-5t^2]+(35/2)C_1^9[-8\alpha^2-6\alpha^4+4t^2\alpha^4+2t^4\alpha^4]+(315/2)C_1^{11}[8\alpha^4t^2] \times[(1+\alpha^2)^2-2t^2\alpha^2(1+\alpha^2)+\alpha^4t^4],$$

$$T_{312}(\alpha)=(5/2)C_2^7[2/t^2+2+4t^2]+(35/2)C_2^9[-12\alpha^2-7\alpha^4+8t^2\alpha^4]+(315/2)C_2^{11}(2t^2\alpha^4)[2+\alpha^2-\alpha^4] +(3465/2)C_2^{13}\alpha^8(1+\alpha^2)^2t^4,$$

$$T_{4312}(\alpha)=(5/2)C_3^7(1/t^2+t^2)+(35/2)C_3^9(-4\alpha^2-2\alpha^4),$$

where

$$C_1=[(1+2a^2)(1+2b^2)-4a^2b^2t^2]^{-\frac{1}{2}},\quad C_2=[(1+2a^2)(1+2b^2)-a^2b^2t^2]^{-\frac{1}{2}},\quad C_3=[(1+2a^2)(1+2b^2)]^{-\frac{1}{2}}. \tag{3-9}$$

(In T terms $a=b=\alpha$.)

4. THE POTENTIAL

The interaction operator of Eq. (3-1) is simplified by assuming a Serber mixture:

$$J_2=J_3=0,\quad J_0=J_1=J_C,\quad J_A=0. \tag{4-1}$$

We then determine the five parameters J_C, J_R, J_S, r_0, and R to give a reasonable representation of nuclei in the first s-shell. The values

$$J_C=-58.65\text{ Mev},\quad J_S=-107.29\text{ Mev},$$
$$J_R=+189.75\text{ Mev},$$
$$r_0=1.54\times10^{-13}\text{ cm}\equiv1.54\text{ fermis}, \tag{4-2}$$

and

$$R=r_0/\sqrt{8}$$

yield binding energies (by our second-order perturbation method[6])

$$\text{B.E.}(H^2)=2.16\text{ Mev}, \tag{4-3a}$$

$$\text{B.E.}(H^3)=8.48\text{ Mev}, \tag{4-3b}$$

$$\text{B.E.}(He^4)=28.42\text{ Mev}, \tag{4-3c}$$

and an electric quadrupole moment of 2.72×10^{-27} cm^2 in H^2. The resulting wave function for the three-body system yields a Coulomb energy difference in H^3-He^3 of 0.74 Mev, compared with an experimental value of 0.76 Mev. The D-state admixture in H^2 is computed to be 7%.

The charge distribution in the s-shell closely resembles a Gaussian shape since the zero-order wave function is Gaussian, however configuration mixing introduces deviations from a pure Gaussian distribution. The computed rms radii are: 1.92 fermis for H^2, 1.60 f for H^3, and 1.46 f for He^4; in reasonable agreement with experiments[11] performed on H^2 and He^4. One must keep in mind, with regard to these latter results, that it is actually the size of the system that one varies to minimize the energy. The curve is very flat in the neighborhood of the eigenvalue, and consequently a small correction to the energy from higher orders in the perturbation expansion could result in much larger corrections to the sizes computed here.

The use of the second-order perturbation theory places some restrictions on our potential. For a sufficiently strong repulsive core the J_C^2 terms in second order would be dominant, and attractive. One must take care that the attractive terms from the core appearing in second order are much smaller than the zero-order repulsive effect.[8] Ways to cope with a stronger core in a calculation such as this have been discussed by Clark and Feenberg,[12] and by Dabrowski.[13]

A two-body spin-orbit term in the potential would make zero contribution to the nuclei considered here (as long as one goes only to second-order terms), and consequently we have not considered such a term.

5. RESULTS FOR O^{16}

Employing the interaction operator of Sec. 4, and the matrix elements of Sec. 3, we have solved Eq. (1-4) for O^{16}. We obtain a binding energy of 129.2 Mev compared to an experimental value of 127.16 Mev. Agreement is not quite so good as it appears at first glance since we have neglected Coulomb forces which in O^{16} contribute nearly -14 Mev to the binding energy.

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Consequently in this calculation one should shoot for a number near 141 Mev, and we are about 8% short.

The zero-order contribution to the binding energy is 87.8 Mev (that is $E_0-\frac{3}{2}\hbar\omega=-87.8$ Mev, where $\hbar\omega=17.25$ Mev). The tensor force provides an additional contribution of 36.4 Mev in the second order, and the remaining 5.0 Mev comes from the remaining central terms in second order. It is interesting that the second-order effects of the central terms are so slight. This appears to be at least partly due to the fact that these terms are "smothered" by the larger contribution of the tensor force.

The rms radius is calculated to be 2.33 fermis; a bit too small for the experimental value of 2.64 fermis.[11,14] Here again the charge distribution is in zero order simply the oscillator function for the first p shell.

We find that $N^2-1=0.22$, so that mixing of configurations higher than the zero order is

$$(N^2-1)/N^2=0.18, \quad (5\text{-}1)$$

or about 18%. This means that the simple oscillator shell-model[15,16] wave function comprises about 82% of our eigenstate. The small configuration mixing is especially interesting in light of the fact that our potential yields a 7% D-state admixture in H^2, and hence appears to overrate configuration mixing.

The overshoot in radius can possibly be traced back to the fact that we are forced to use a repulsive core in this calculation which is weak by modern standards.[10,17,18]

The procedure described in this paper is currently being applied to Ca^{40} and O^{17}.

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