

at $g^{(3)}$ can be made; it cannot, unfortunately, be used to measure the three-particle correlation function as an inverse Fourier transform cannot be taken.

A reasonable approximation to $g^{(3)}$ might be Kirkwood's superposition approximation.³ However, the limits on the integrals in (6) are such that they cannot be carried out in closed form even after this approximation is made so that a numerical calculation is necessary. Although calculations have not been performed, simple estimates of the integrals involved coupled with the fact that the incoherent scattering length is frequently larger than the coherent scattering length, lead us to believe that the second term generally dominates in expression (6). The assumption that multiple scattering is incoherent is the basis for other multiple-scattering corrections calculated using iterated applications of the single-scattering formula.⁵

⁵ See, for example, G. H. Vineyard, *Phys. Rev.* **96**, 93 (1954); and S. Chandrasekhar, *Radiative Transfer* (Clarendon Press, Oxford, 1950).

It is possible to extend the above analysis to the non-static case by introducing time-dependent correlation functions. A simple calculation following the method of Van Hove² shows that this case can be treated by making the substitutions

$$\begin{aligned} g^{(2)}(\mathbf{r}) &\rightarrow G(\mathbf{r}, t), \\ g^{(3)}(\mathbf{r}, \mathbf{r}') &\rightarrow G(\mathbf{r}, \mathbf{r}', t, 0), \end{aligned}$$

where $G(\mathbf{r}, t)$ is Van Hove's time-displaced two-particle correlation function and $G(\mathbf{r}, \mathbf{r}', t, t')$ is the probability that given a particle at the origin at $t=0$, there be particles at \mathbf{r} and \mathbf{r}' (per unit volume at \mathbf{r}, \mathbf{r}') at times t and t' .

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Analytic Wave Functions. IV. Inclusion of Correlation*

R. G. BREENE, JR.†

Space Science Laboratory, Missiles & Space Vehicles Department, General Electric Company, Philadelphia, Pennsylvania

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We have developed a general method for including correlation of the $2p$ electrons in our atomic wave function programs. In introducing correlation, an appeal has been made to the interelectronic coordinate method of doing so. Tables are given which enable one to write down the $2p$ correlated energy expression rapidly in terms of the radial integrals for any atoms having $2p$ electrons of the same magnetic quantum number. One then solves for the correlation parameter a , and the result follows. In the case of an atom or atomic state we were treating for the first time, this entire procedure would take place after our programs had been applied to the obtention of the effective nuclear charges. Only the $2p$ electrons have been considered by virtue of their importance to atomic interactions with exterior particles. We applied this to oxygen in its 3P ground state. We had previously obtained 2018.28 eV for the total energy. We now obtain 2039.81 eV. The experimental value is 2043.3.

I. INTRODUCTION

IN a series of papers¹ we have developed methods for machine computation of analytic atomic wave functions. Herein it is our purpose to develop a method of modifying these calculations so as to include the effects of electron correlation for the $2p$ electrons in as facile a manner as possible. We confine ourselves to the $2p$ electrons since we are most interested in the application of their results to exterior interaction.

The portions of the spatially-dependent interactions to which we shall pay particular attention are the

following: Two orbital electrons of opposite spin but the same $n\ell m$ have precisely the same spatial wave functions. We may anticipate that, due to the Coulombic interaction between them, the orbital electrons demonstrate an affinity for opposite sides of the atom. The changes in energy which result from wave function changes aimed at describing such affinity are called correlation energy. We designate the modification of the wave functions as the inclusion of correlation.

Three principal methods of including correlation in the computation of atomic wave functions have been applied to date.² (1) In the first, it is supposed that the two electrons in the same $n\ell m$ shell do not feel the same

† Consultant. 48 Maple Avenue, Centerville 59, Ohio.

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¹ R. G. Breene, Jr., *Phys. Rev.* **111**, 1111 (1958); **113**, 809 (1959); **119**, 1615 (1960).

² J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Vol. II.

nuclear charge. This has the practical effect of pushing out one orbit and pulling in the other, if we consider the orbits delineated by orbital wave function maxima. (2) The second method is based on the idea that complete orthonormal sets can describe almost anything and is called configuration interaction. The set members appealed to are the determinants of our earlier determination. This method is often equivalent to method (3). (3) In the last method, interelectronic coordinates are introduced to account for the correlation energy.

Our intention is to extend our wave-function treatment to include correlation by the simplest method possible. Method (1) requires machine parameter variation of a more complex nature than our earlier work. Method (2) demands a tremendously extensive calculation, viz., work of the Mulliken group.³ We describe our application of method (3) in the next section.

II. WAVE FUNCTIONS FOR THE CORRELATED ORBITALS

We actually need only two orbitals, that for the $2p0$ and that for the $2p-1^+$. We outline our development of the $2p-1^+$ orbital—the shorter—and write down the $2p0$.

First, we recall that the portion of our wave function referring to the $2p1$ electrons (call them "1" and "2") is

$$r_1 r_2 \psi_1(2p1) \psi_2(2p1) = \frac{A^2}{2\pi} r_1^2 r_2^2 e^{-\frac{1}{2}Z_3(r_1+r_2)} \Theta_{11}(1) \Theta_{11}(2) e^{i(\varphi_1+\varphi_2)}.$$

We choose as our correlated orbital

$$r_1 r_2 \psi_{1,2}(2p1) = \frac{A_1}{2\pi} r_1^2 r_2^2 (1 + ar_{12}^2) e^{-\frac{1}{2}Z_3(r_1+r_2)} \times \Theta_{11}(1) \Theta_{11}(2) e^{i(\varphi_1+\varphi_2)}, \quad (1)$$

wherein a is the correlation coefficient whose value determines the amount of correlation introduced. We expand the interelectronic coordinate according to the law of cosines and then further expand $\cos\vartheta_{12}$ with the

TABLE I. The a_k table. These coefficients occur in the Coulomb energy expression.

	l	m	l'	m'	$k=0$	$k=2$
sp	1	0	0	0	1	0
	1	± 1	0	0	1	0
pp	1	0	1	0	1	4/25
	1	0	1	± 1	1	-2/25
	1	± 1	1	0	1	-2/25
	1	± 1	1	± 1	1	1/25

³ Technical Report 1959-60, Laboratory of Molecular Structure and Spectra, Department of Physics, The University of Chicago (unpublished).

TABLE II. The c_k table. These coefficients occur in the Coulomb energy expression. The subscript c refers to the correlated orbital.

	l_c	m_c	l'	m'	$k=0$	$k=2$
sp_c	1	0	0	0	272/25-28/5 $\sqrt{2}$	0
	1	± 1	0	0	68/25	0
pp_c	1	0	1	0	272/25-28/5 $\sqrt{2}$	-32/875+28 $\sqrt{2}$ /125
	1	0	1	± 1	272/25-28/5 $\sqrt{2}$	16/875-28/125 $\sqrt{2}$
	1	± 1	1	0	68/25	-248/875
	1	± 1	1	± 1	68/25	124/875

result

$$r_1 r_2 \psi_{1,2}(2p1) = \frac{A_1}{2\pi} r_1^2 r_2^2 [f_1(r_1 r_2) - 2af_2(r_1 r_2) (\cos\vartheta_1 \cos\vartheta_2 + \sin\vartheta_1 \sin\vartheta_2)] \Theta_{11}(1) \Theta_{11}(2) e^{i(\varphi_1+\varphi_2)}, \quad (2a)$$

$$f_1(r_1 r_2) = (1 + ar_1^2 + ar_2^2) e^{-\frac{1}{2}Z_3(r_1+r_2)}, \quad (2b)$$

$$f_2(r_1 r_2) = r_1 r_2 e^{-\frac{1}{2}Z_3(r_1+r_2)}. \quad (2c)$$

Now remark that

$$\cos\vartheta \Theta_{11} = \frac{\sqrt{3}}{2} \cos\vartheta \sin\vartheta = \frac{1}{\sqrt{5}} \Theta_{21}, \quad (3a)$$

$$\sin\vartheta \Theta_{11} = \frac{\sqrt{3}}{2} \sin^2\vartheta = \frac{2}{\sqrt{5}} \Theta_{22}. \quad (3b)$$

We may now write down our expression for the $2p1$ orbital. We also do so for the $2p0$.

$$r_1 r_2 \psi_{1,2}(2p\pm 1) = \frac{A_1}{2\pi} r_1^2 r_2^2 [f_1(r_1 r_2) \Theta_{11}(1) \Theta_{11}(2) - \frac{2}{5}a [\Theta_{21}(1) \Theta_{21}(2) + 4\Theta_{22}(1) \Theta_{22}(2)] f_2(r_1 r_2)] e^{\pm i(\varphi_1+\varphi_2)}, \quad (4a)$$

$$r_1 r_2 \psi_{1,2}(2p0) = \frac{A_0}{2\pi} r_1^2 r_2^2 [f_1(r_1 r_2) \Theta_{10}(1) \Theta_{10}(2) - a [3\Theta_{00}(1) \Theta_{00}(2) - (\frac{3}{5})^{1/2} \Theta_{00}(1) \Theta_{22}(2) - (\frac{3}{5})^{1/2} \Theta_{22}(1) \Theta_{00}(2) + \frac{4}{5} \Theta_{21}(1) \Theta_{21}(2) + \frac{1}{5} \Theta_{22}(1) \Theta_{22}(2)] f_2(r_1 r_2)], \quad (4b)$$

$$A_1 = \frac{Z_3^5}{24} \left[1 + \frac{120a}{Z_3^2} + \frac{7608}{Z_3^4} a^2 \right]^{-1/2}, \quad (4c)$$

$$A_0 = \frac{Z_3^5}{24} \left[1 + \frac{120a}{Z_3^2} + \frac{14952}{Z_3^4} a^2 \right]^{-1/2}. \quad (4d)$$

Determination of the normalization factors is obvious. If we look at Eq. (4a) we see that now some d wave has been mixed in with the p wave; this is if one considers only the angular part of the wave function. If one also considers the radial portion of the function

TABLE III. Additional Coulomb coefficients.

	l_c	m_c	l'_c	m'_c	$k=0$	$k=1$	$k=2$	$k=3$
f_k	1	± 1	1	0	$\frac{18\,496}{625} - \frac{272\sqrt{2}}{5}$	0	$\frac{1984}{30\,625}$	0
	1	± 1	1	± 1	$\frac{4624}{625}$	0	$\frac{15\,376}{30\,625}$	0
p_k	1	0	1	0	$\frac{322}{25} - \frac{64}{5\sqrt{2}}$	$-\left[\frac{1}{14\sqrt{2}} - \frac{297}{2048}\right]\pi^2$	$\frac{20}{1225}$	$\frac{5399\pi^2}{524\,288} - \frac{81\pi^2}{8192\sqrt{2}}$
	1	± 1	1	± 1	$\frac{68}{25}$	$\frac{9\pi^2}{512}$	$\frac{52}{245}$	$\frac{749\pi^2}{131\,072}$
q_k	1	0	1	0	$\frac{9\pi^2}{128}$	$\frac{51}{50} - \frac{\sqrt{2}}{5}$	$\frac{9\pi^2}{2048}$	$\frac{9}{2450}$
	1	± 1	1	± 1	$\frac{81\pi^2}{512}$	$\frac{2}{25}$	$\frac{81\pi^2}{8192}$	$\frac{18}{1225}$

one sees that $4d$, $5p$, and $5d$ have been mixed in with the $2p$. The equivalence to the configuration interaction approach is thus demonstrated.

III. THE COULOMB ENERGY CONTRIBUTIONS

We must now find the general expressions for the Coulomb energies associated only with the correlated orbitals. The energies associated with Coulomb interactions among uncorrelated orbitals remain given by the first paper in this series.¹ Straightforward algebraic manipulation of Eqs. (4) and the Coulomb operator leads us to the following expression for the Coulomb energy contribution of the correlated electrons:

$$\begin{aligned} \sum \sum_k a_k(l_c m_c, l'_c m'_c) F^k(n_c l_c, n'_c l'_c) &+ a^2 \sum \sum_k c_k(l_c m_c, l'_c m'_c) \\ &\times L^k(n_c l_c, n_l) + [\sum \sum_k a_k(l_c m_c, l'_c m'_c) M^k(n_c l_c, n_c l_c) \\ &+ a^2 \sum \sum_k g_k(l_c m_c, l'_c m'_c) W^k(n_c l_c, n_c l_c) \\ &+ a^4 \sum \sum_k f_k(l_c m_c, l'_c m'_c) N^k(n_c l_c, n_c l_c)] [\delta(m_c, m'_c \pm 1) \\ &+ \delta(m_c, m'_c \pm 2)] + [\sum \sum_k a_k(l_c m_c, l'_c m'_c) P^k(n_c l_c, n_c l_c) \\ &+ a^2 \sum \sum_k p_k(l_c m_c, l'_c m'_c) Q^k(n_c l_c, n_c l_c) \\ &- 2a \sum \sum_k q_k(l_c m_c, l'_c m'_c) V^k(n_c l_c, n_c l_c)] \delta(m_c, m'_c), \quad (5) \end{aligned}$$

TABLE IV. The b_k coefficients. These enter Eq. (7) for the exchange contributions. The upper and lower signs must be taken together.

	l	m	l'_c	m'_c	$k=0$	$k=1$	$k=2$
sp_c	0	0	1	0	0	$1/3$	0
	0	0	1	± 1	0	$1/3$	0
pp_c	1	0	1	0	1	0	$4/25$
	1	0	1	± 1	0	0	$3/25$
	1	± 1	1	0	0	0	$3/25$
	1	± 1	1	∓ 1	0	0	$6/25$

where the first sum in each case is over the correlated pairs. It is unfortunate that eight terms must be involved in this equation, but the difference in the radial integrals makes this rather difficult to avoid.

In Tables I, II, and III we list the coefficients in the series of Eq. (5). Some of these coefficients may appear a bit more formidable than those appearing in the Slater tables.⁴ This is due to the odd decomposition of the spherical harmonics which we may remark in Eq. (4), that is to say, one is now mixing $\exp(-i\varphi_1)$ with $\Theta_{22}(1)$.

The following are the general forms for the radial integrals in Eq. (5).

$$F^k(n_c l_c, n'_c l'_c) = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_3^4 f_1^2(r_1 r_3) \times R_{n'_c l'_c}(r_2) dr_1 dr_2 dr_3, \quad (6a)$$

$$L^k(n_c l_c, n'_c l'_c) = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_3^4 f_2^2(r_1 r_3) \times R_{n'_c l'_c}(r_2) dr_1 dr_2 dr_3, \quad (6b)$$

$$M^k(n_c l_c, n_c l_c) = A_i^2 A_j^2 \int \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \times f_1^2(r_1 r_3) f_1^2(r_2 r_4) dr_1 dr_2 dr_3 dr_4, \quad (6c)$$

$$W^k(n_c l_c, n_c l_c) = A_i^2 A_j^2 \int \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \times f_1^2(r_1 r_3) f_2^2(r_2 r_4) dr_1 dr_2 dr_3 dr_4, \quad (6d)$$

⁴ J. C. Slater, Phys. Rev. **34**, 1293 (1929).

$$N^k(n_{cl_c}, n_{cl_c}) = A_i^2 A_j^2 \int \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \\ \times f_2^2(r_1 r_3) f_2^2(r_2 r_4) dr_1 dr_2 dr_3 dr_4, \quad (6e)$$

$$P^k(n_{cl_c}, n_{cl_c}) = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}} r_1^4 r_2^4 f_1^2(r_1 r_2) dr_1 dr_2, \quad (6f)$$

$$Q^k(n_{cl_c}, n_{cl_c}) = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}} r_1^4 r_2^4 f_2^2(r_1 r_2) dr_1 dr_2, \quad (6g)$$

$$V^k(n_{cl_c}, n_{cl_c}) = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}} r_1^4 r_2^4 \\ \times f_1(r_1 r_2) f_2(r_1 r_2) dr_1 dr_2. \quad (6h)$$

The general forms for these integrals are available to the reader on request.

IV. THE EXCHANGE ENERGY CONTRIBUTIONS

We next determine the general expression for the exchange energy contributions associated with the correlated orbitals. Again the contributions from pairs of uncorrelated orbitals remain unchanged. Quite straightforward manipulations of Eqs. (4) and the exchange operator yield the following expression for the exchange energy contribution of the correlated electrons:

$$\mathbf{S} \sum_k b_k(l_c m_c, l' m') G^k(n_{cl_c}, n' l') + a^2 \mathbf{S} \sum_k \alpha_c(l_c m_c, l' m') \\ \times A^k(n_{cl_c}, n' l') + [\mathbf{S} \sum_k \gamma_k(l_c m_c, l_c m_c') B^k(n_{cl_c}, n_{cl_c}) \\ + a^2 \mathbf{S} \sum_k \kappa_k(l_c m_c, l_c m_c') T^k(n_{cl_c}, n_{cl_c}) \\ + a^4 \mathbf{S} \sum_k \delta_k(l_c m_c, l_c m_c') D^k(n_{cl_c}, n_{cl_c})], \quad (7)$$

wherein the summation symbol \mathbf{S} refers to a sum over pairs of the same spin.

In Tables IV and V we list the coefficients in the various terms of Eq. (7). The general form of the

TABLE V. The α_k coefficients. These are related to exchange contributions.

	l	m	l'_c	m'_c	$k=0$	$k=1$	$k=2$	$k=3$
sp_c	0	0	1	0	$\frac{152}{15} - \frac{32\sqrt{3}}{5\sqrt{5}}$	$\frac{3\pi^2}{160}$	0	$\frac{3\pi^2}{12\,800}$
	0	0	1	0	0	$\frac{27\pi^2}{320}$	$\frac{4}{125}$	$\frac{9\pi^2}{10\,240}$
pp_c	1	0	1	± 1	0	$\frac{4}{125}$	$\frac{27\pi^2}{2560}$	$\frac{288}{18\,375}$
	1	± 1	1	0	0	$\frac{432}{125} - \frac{32\sqrt{2}}{25}$	$\frac{27\pi^2}{2560}$	$\frac{48}{6125}$
	1	± 1	1	∓ 1	0	0	$\frac{135\pi^2}{2048}$	$\frac{72}{2675}$

radial integrals is

$$G^k(n_{cl_c}, n' l') = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^2 r_2^2 r_3^4 f_1(r_1 r_3) \\ \times f_1(r_2 r_3) R_{n' l'}(r_1) R_{n' l'}(r_2) dr_1 dr_2 dr_3, \quad (8a)$$

$$A^k(n_{cl_c}, n' l') = A^2 \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^2 r_2^2 r_3^4 f_2(r_1 r_3) \\ \times f_2(r_2 r_3) R_{n' l'}(r_1) R_{n' l'}(r_2) dr_1 dr_2 dr_3, \quad (8b)$$

$$B^k(n_{cl_c}, n_{cl_c}) = A^4 \int \int \int \int \frac{r_{<}^k}{r_{>}^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \\ \times f_1(r_1 r_3) f_1(r_1 r_4) f_1(r_2 r_3) \\ \times f_1(r_2 r_4) dr_1 dr_2 dr_3 dr_4, \quad (8c)$$

TABLE VI. The γ_k , δ_k , and κ_k coefficients. Signs must be taken together.

	l_c	m_c	l'_c	m'_c	$k=0$	$k=1$	$k=2$	$k=3$
γ_k	1	0	1	± 1	0	0	$\frac{3}{25}$	0
	1	± 1	1	∓ 1	0	0	$\frac{6}{25}$	0
δ_k	1	0	1	± 1	0	$\frac{23\,346\pi^2}{128\,000} - \frac{27\pi^2}{80\sqrt{2}}$	$\frac{29\,376 - 8064\sqrt{2}}{91\,875} - \frac{\pi^2}{2400}$	$\frac{5\,117\,661\pi^2}{393\,216\,000}$
	1	± 1	1	∓ 1	0	0	$\frac{55\,392}{30\,625}$	$\frac{135}{16\,384}$
κ_k	1	0	1	± 1	0	$\frac{434 - 32\sqrt{2}}{125}$	$\frac{27\pi^2}{1280}$	$\frac{144}{6125}$
	1	± 1	1	∓ 1	0	0	$\frac{405\pi^2}{3072}$	$\frac{16}{1225}$

$$D^k(n_c l_c, n_c l_c) = A^4 \int \int \int \int \frac{r <^k}{r >^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \\ \times f_2(r_1 r_3) f_2(r_1 r_4) f_2(r_2 r_3) \\ \times f_2(r_2 r_4) dr_1 dr_2 dr_3 dr_4, \quad (8d)$$

$$T^k(n_c l_c, n_c l_c) = A^4 \int \int \int \int \frac{r <^k}{r >^{k+1}(1,2)} r_1^4 r_2^4 r_3^4 r_4^4 \\ \times f_1(r_1 r_3) f_1(r_2 r_3) f_2(r_1 r_4) \\ \times f_2(r_2 r_4) dr_1 dr_2 dr_3 dr_4. \quad (8e)$$

The general forms for these integrals are available to the reader on request.

V. THE CENTRAL ENERGY CONTRIBUTION

The central portion of the spinless Hamiltonian may be quite easily computed for our case using Eqs. (4). The results are as follows:

$$I_{2pm} = -\frac{1}{2} A_m^2 \{I_0 + I_1 + I_2 + B_m a^2 I_3 + B_m(l) a^2 I_4\}, \quad (9a)$$

$$I_0 = -\left[26 \frac{3!}{Z_3^8} + 114a \frac{3!4!}{Z_3^{10}} + 479a^2 \frac{2!6!}{Z_3^{12}} \right], \quad (9b)$$

$$I_1 = 2Z \left[3 \frac{4!}{Z_3^9} + 5a \frac{4!5!}{Z_3^{11}} + \frac{a^2}{Z_3^{12}} \left(3!7! + 24 \frac{4!6!}{Z_3} \right) \right], \quad (9c)$$

$$I_2 = -2 \left[\frac{2!4!}{Z_3^8} + a(2+5a) \frac{4!4!}{Z_3^{10}} + 46a^2 \frac{4!5!}{Z_3^{12}} \right], \quad (9d)$$

$$I_3 = -171 \frac{3!5!}{Z_3^{12}} + 2 \frac{5!6!}{Z_3^{13}} Z, \quad (9e)$$

$$I_4 = -\frac{4!6!}{Z_3^{12}}, \quad (9f)$$

$$B_0 = 272/25, \quad B_0(l) = 192/25, \\ B_1 = 68/25, \quad B_1(l) = 120/25. \quad (9g)$$

Equations (9) complete the requirements for expressions for the various energy contributions.

VI. APPLICATION TO OXYGEN

We shall consider very briefly application of the correlation treatment to the 3P state of oxygen arising from four $2p$ electrons. For this state we may take a single determinant representation, and the reader is referred to the first paper in this series¹ for specifics.

In what follows we have cut off the expansion of the operator at $k=2$. In the energy expressions we include only those terms relating to the correlated orbitals and different from our earlier result:

$$4F^0(2p_c, 1s) + 4F^0(2p_c, 2s) + 4F^0(2p_c, 2p) - \frac{2}{25} F^2(2p_c, 2p) \\ + P^0(2p_c, 2p_c) + \frac{1}{25} P^2(2p_c, 2p_c) - 2a \left\{ \frac{81\pi^2}{512} V^0(2p_c, 2p_c) \right. \\ \left. + \frac{2}{25} V^1(2p_c, 2p_c) + \frac{81\pi^2}{8192} V^2(2p_c, 2p_c) \right\} \\ + a^2 \left\{ \frac{272}{25} L^0(2p_c, 1s) + \frac{272}{25} L^0(2p_c, 2s) + \frac{272}{25} L^0(2p_c, 2p) \right. \\ - \frac{248}{875} L^2(2p_c, 2p) + \frac{68}{25} Q^0(2p_c, 2p_c) + \frac{9\pi^2}{512} Q^1(2p_c, 2p_c) \\ \left. + \frac{52}{245} Q^2(2p_c, 2p_c) \right\} - \frac{2}{3} G^1(2p_c, 1s) - \frac{2}{3} G^1(2p_c, 2s) \\ - \frac{9}{25} G^2(2p_c, 2p) - a^2 \left\{ \left(\frac{54\pi^2}{320} \right) A^1(2p_c, 1s) \right. \\ \left. + \left(\frac{54\pi^2}{320} \right) A^1(2p_c, 2s) + \frac{4}{125} A^1(2p_c, 2p) \right. \\ \left. + \frac{783\pi^2}{10240} A^2(2p_c, 2p) + [A^2(2p_c, 1s) \right. \\ \left. + A^2(2p_c, 2s)] \frac{8}{125} \right\} + 2I_{2p1}. \quad (10)$$

Now we do not go through the obvious arithmetical details, but one may readily obtain a polynomial in a for the energy of the atom by adding similar expressions to Eq. (10) for the exchange and central energies. One differentiates this, solves for a , and the introduction of correlation is complete. For the 3P state a is obtained as 0.3078. The total atomic energy is now 2039.81 eV, where without correlation we had obtained 2018.28 eV. The experimental value is 2043.3 eV.

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