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HELIUM ISOELECTRONIC SEQUENCE WAVE FUNCTIONS AND ENERGIES
FOR THE SECOND AND THIRD ROWS OF THE PERIODIC TABLE

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HELIUM ISOELECTRONIC SEQUENCE WAVE FUNCTIONS AND ENERGIES
FOR THE SECOND AND THIRD ROWS OF THE PERIODIC TABLE*

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April 24, 1964

ABSTRACT

A Green's function technique allows Schrödinger's equation to be written as an integral equation with a Green's function kernel. For the electrostatic atomic problem the Green's function is represented as a bilinear expansion of products of hydrogen-like wave functions. For the helium atom and for members of the helium isoelectronic sequence the integral equation is solved by expanding the wave function into a series of products of hydrogen-like wave functions. The helium isoelectronic sequence wave function expansion in hydrogen-like wave functions is shown to converge uniformly to the exact solution of the electrostatic Schrödinger's equation. The equations are simplified by truncation of sum-integrals that appear and the remaining implicit algebraic equations are solved by the use of a digital computer. The resulting wave functions and energies are presented for the first 18 members of the helium isoelectronic sequence, including the hydrogen negative ion. The calculated energies are accurate to within a few percent of the experimental values for helium and improve through the helium isoelectronic sequence ions to a few tenths of a percent for argon. Several bound states of the hydrogen negative ion are predicted. The calculated energies are closer to the experimental values than could be expected from the accuracy trend for the remainder of the helium isoelectronic sequence ions. In addition to the ground state wave functions and energies the wave functions and energies are presented for several excited states and states of multiple excitation. Results are compared with experimental values and the calculations of others.

I. INTRODUCTION

The quantum mechanical problem of the helium atom has received considerable attention.^{1,2} Several methods have been used to attack the problem.³⁻⁶ All techniques, except that of perturbation theory, are variational treatments and the energies calculated are quite good.⁷⁻⁹ This paper presents an alternate technique in which the resulting wave function is a series of products of hydrogen-like wave functions. The technique, in general, involves rewriting Schrodinger's equation in the form of an integral equation with a Green's function kernel. The Green's function is represented by a bilinear expansion of products of hydrogen-like wave functions. In an application to helium a double sum-integral appears. The resulting equations are reduced to a system of algebraic equations by expanding the helium wave function into a series of products of hydrogen-like wave functions and truncating the sum-integrals at one of several convenient points. The algebraic equations are then solved by digital computer with an eigenvalue-eigenvector code.

In the process of solving the integral equation it is shown that the helium isoelectronic sequence wave functions, and in general, all wave functions calculated by the method of this paper, are uniformly convergent. This gives support to the proposition that the wave functions obtained are useful in the calculation of other properties of an atom than energy eigenvalues.

The integral equation formulation of the general atomic problem is given in Section II. This formulation is presented for the electrostatic helium atom and members of the helium isoelectronic sequence in Section III. In this section the integral equation is solved by expressing the helium isoelectronic sequence wave functions as a product of hydrogen-like wave functions. In this way the wave functions appear in a useful analytic form. The resulting equations are simplified by truncating a double sum-integral that appears, at one of several convenient points. The remaining algebraic equations are solved by digital

computer. The system of algebraic equations is simplified in Section IV. The results are presented in Section V. Discussion of the accuracy of the results is discussed in Section VI.

II. THE INTEGRAL EQUATION

Schrodinger's equation¹⁰ may be written in the form

$$\left\{ H_0(\underline{\mu}, \underline{\rho}) + H_1(\underline{\mu}, \underline{\rho}) \right\} \psi_p(\underline{\rho}) = E_p' \psi_p(\underline{\rho}) \quad (1)$$

with appropriate boundary conditions. $\psi_p(\underline{\rho})$ is a column matrix wave function. The vector $\underline{\mu}$ represents all momentum coordinates including spin, and $\underline{\rho}$ represents all spatial coordinates. The number p represents the quantum state of the system, and E_p' the total energy. The "zero order" Hamiltonian $H_0(\underline{\mu}, \underline{\rho})$ is so chosen that, the equation

$$H_0(\underline{\mu}, \underline{\rho}) \phi_p(\underline{\rho}) = E_p \phi_p(\underline{\rho}) \quad (2)$$

plus the boundary conditions of (1) has a known solution $\phi_p(\underline{\rho})$, with energy eigenvalues E_p . $H_1(\underline{\mu}, \underline{\rho})$ is the "interaction Hamiltonian".

Equation (1) can be rewritten in the form,

$$\left\{ H_0(\underline{\mu}, \underline{\rho}) - E_p' \right\} \psi_p(\underline{\rho}) = - H_1(\underline{\mu}, \underline{\rho}) \psi_p(\underline{\rho}) . \quad (3)$$

Using a Green's function technique,¹¹ equation (3) can be rewritten as an integral equation,

$$\psi_p(\underline{\rho}) = \frac{1}{4\pi} \int G_p(\underline{\rho}, \underline{\rho}') H_1(\underline{\mu}', \underline{\rho}') \psi_p(\underline{\rho}') d\underline{\rho}', \quad (4)$$

in which $G_p(\underline{\mu}, \underline{\rho}')$ is a Green's function satisfying the equation,¹²

$$\left\{ H_0(\underline{\mu}, \underline{\rho}) - E_p' \right\} G_p(\underline{\rho}, \underline{\rho}') = - 4\pi \delta(\underline{\rho} - \underline{\rho}') , \quad (5)$$

plus the boundary conditions on (1). $G_p(\underline{\rho}, \underline{\rho}')$ may be represented by a bilinear expansion in $\phi_p(\underline{\rho})$ and $\phi_p^*(\underline{\rho}')$;¹³

$$G_p(\underline{r}, \underline{r}') = -4\pi \text{ l.i.m. } \sum_t \left\{ \phi_t(\underline{r}) \phi_t^*(\underline{r}') / (E_t - E_p) \right\}. \quad (6)$$

$\sum_t$ denotes summation over discrete values of t and integration over continuous values of t . The symbol l.i.m. is a notation for limit in the mean.¹⁴

III. APPLICATION TO HELIUM ISOELECTRONIC SEQUENCE ATOMS

For the electrostatic approximation to the helium isoelectronic sequence atoms the "zero order" Hamiltonian may be written as,

$$H_0(\underline{u}, \underline{p}) = -\frac{\hbar^2}{2m} \nabla_{\underline{r}_1}^2 - \frac{\hbar^2}{2m} \nabla_{\underline{r}_2}^2 - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2}. \quad (7)$$

The "interaction" Hamiltonian may be expressed as,

$$H_1(\underline{u}, \underline{p}) = e^2 \left\{ r_1^2 + r_2^2 - 2r_1 r_2 \cos \theta_{12} \right\}^{-1/2}. \quad (8)$$

The "zero order" energy is given by the equation,

$$E_p = E_{p_1 p_2} = -\frac{2Z^2 m e^4}{\hbar^2 n_{p_1}^2} - \frac{2Z^2 m e^4}{\hbar^2 n_{p_2}^2} \quad (9)$$

and, the "zero order" wave function may be written as,

$$\psi_p(\underline{r}) = \phi_{p_1}(\underline{r}_1) \phi_{p_2}(\underline{r}_2), \quad (10)$$

where $\phi_{p_1}(\underline{r}_1)$ and, $\phi_{p_2}(\underline{r}_2)$ are hydrogen-like wave functions. The letters p_1 and p_2 designate the quantum-state of the hydrogen-like systems.

The vectors $\underline{r}_1 \sim (r_1, \theta_1, \phi_1)$ and $\underline{r}_2 \sim (r_2, \theta_2, \phi_2)$ are the distances from the center of mass to the first and second electrons, respectively. The letter m denotes the reduced mass of the electron, and e is the electrostatic unit of charge of the electron.

In the case of electrostatic helium isoelectronic sequence atom the Green's function is represented by;

$$G_p(\underline{\mu}, \underline{\rho}') = -4\pi \text{ l.i.m. } \sum_{t_1} \sum_{t_2} \left\{ \phi_{t_1}(\underline{r}_1) \phi_{t_2}(\underline{r}_2) \right. \\ \left. \phi_{t_1}^*(\underline{r}_1') \phi_{t_2}^*(\underline{r}_2') / (E_{t_1 t_2} - E_p') \right\}. \quad (11)$$

The Green's function as written in (11) does satisfy the boundary conditions of (1).

If one writes the Green's function as,

$$\left\{ G_p(\underline{\rho}, \underline{\rho}') \right\}_{N_1 N_2} = -4\pi \sum_{t_1}^{N_1} \sum_{t_2}^{N_2} \left\{ \phi_{t_1}(\underline{r}_1) \phi_{t_2}(\underline{r}_2) \right. \\ \left. \phi_{t_1}^*(\underline{r}_1') \phi_{t_2}^*(\underline{r}_2') / (E_{t_1 t_2} - E_p') \right\}, \quad (12)$$

then the wave function takes the form,

$$\left\{ \psi_p(\underline{\rho}) \right\}_{N_1 N_2} = \frac{1}{4\pi} \int \left\{ G_p(\underline{\rho}, \underline{\rho}') \right\}_{N_1 N_2} H_1(\underline{\mu}', \underline{\rho}') \psi_p(\underline{\rho}') d\rho', \quad (13)$$

and $\left\{ \psi_p(\underline{\rho}) \right\}_{N_1 N_2}$ converges uniformly to $\psi_p(\underline{\rho})$.¹⁵ The appropriate analytic form of $\left\{ \psi_p(\underline{\rho}) \right\}_{N_1 N_2}$ which satisfies the boundary conditions is,

$$\left\{ \psi_p(\underline{\rho}) \right\}_{N_1 N_2} = A_{p_1 p_2} \sum_{t_1}^{N_1} \sum_{t_2}^{N_2} M_{p_1 p_2 t_1 t_2} \phi_{t_1}(\underline{r}_1) \phi_{t_2}(\underline{r}_2). \quad (14)$$

Therefore, using the uniform convergence of $\left\{ \psi_p(\underline{\rho}) \right\}_{N_1 N_2}$ we have the equation

$$\psi_p(\underline{\rho}) = A_{p_1 p_2} \sum_{t_1} \sum_{t_2} M_{p_1 p_2 t_1 t_2} \phi_{t_1}(\underline{r}_1) \phi_{t_2}(\underline{r}_2). \quad (15)$$

Defining, $c_{t_1 t_2 p_1 p_2}$ by the equation

$$c_{t_1 t_2 p_1 p_2} = e^2 \iint \phi_{t_1}^*(r_1') \phi_{t_2}^*(r_2') (r_1'^2 + r_2'^2 - 2r_1' r_2' \cos \theta_{12}')^{-1/2} \phi_{p_1}(r_1') \phi_{p_2}(r_2') dr_1' dr_2', \quad (16)$$

and using (12) and (15) in (4), (the order of summation and integration may be reversed due to the uniform convergence of (15))¹⁶ one obtains,

$$M_{p_1 p_2 k_1 k_2} = \frac{1}{(E_{p_1 p_2}' - E_{k_1 k_2})} \sum_{s_1} \sum_{s_2} M_{p_1 p_2 s_1 s_2} \times c_{k_1 k_2 s_1 s_2}. \quad (17)$$

Rewriting equation (17) one obtains,

$$\sum_{s_1} \sum_{s_2} \left\{ c_{k_1 k_2 s_1 s_2} + (E_{k_1 k_2}' - E_{p_1 p_2}') \delta_{s_1 k_1} \delta_{s_2 k_2} \right\} \times M_{p_1 p_2 s_1 s_2}. \quad (18)$$

The delta functions are Kroniker deltas. After truncation of the double sum-integral the remaining equations are a system of algebraic equations that can be solved by well-known eigenvalue-eigenvector codes on a digital computer. A convenient truncation of these sum-integrals is apparent from the following table;

TABLE I. Quantum State Index Numbering Scheme

s	n	l	m
1	1	0	0
2	2	0	0
3	2	1	-1
4	2	1	0
5	2	1	1
6	3	0	0
7	3	1	-1
8	3	1	0
9	3	1	+1
10	3	2	-2
11	3	2	-1
12	3	2	0
13	3	2	1
14	3	2	2

The convenient points of truncation are those values of s that include all l 's and m 's of a particular n . These values of s are 1, 5, 14, 30, Different truncations will be denoted simply by the principal quantum number n .

IV. SIMPLIFICATION OF THE MATRIX EQUATION

Many of the interaction energy integrals are zero.¹⁷ The zeros arise through the Clebsch-Gordon coefficients which appear in the analytic solution of the integrals.¹⁷

The interaction energy matrix ($C_{p_1 p_2 l_1 l_2}$) can be reduced to a set of smaller matrices by the following process: The integral matrix is first condensed by omitting all of the columns that are headed by a zero in the first row. These columns will be multiplied by a zero element of the wave function expansion coefficient eigenvector. The rows corresponding to these columns are also omitted. The multiplication of these rows by the wave function expansion coefficient eigenvector results in zero, so these rows are omitted. This procedure produces the first matrix. The procedure is repeated starting with the first row untouched by the above procedure.

The above procedure produces several matrices all of whose elements are non-zero and of very much smaller size than the original. In this way very large interaction energy integral matrices can be handled.

V. RESULTS

The integrals of equation (16) were evaluated analytically and then numerically by digital computer. With these results and setting $n = 2$ the equations resulting from equation (18) was solved by digital computer using an eigenvalue-eigenvector code. The helium isoelectronic sequence energies calculated are given in the even numbered tables along with the experimental results and the results of other methods of calculation. The wave function constants (defined by $N_{p_1 p_2 k_1 k_2} = A_{p_1 p_2} M_{p_1 p_2 k_1 k_2}$) are given in the odd numbered tables.

TABLE II. HYDROGEN NEGATIVE ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²)1s	-14.316587 EV	-14.295 EV ^A	-14.344 EV ^B
(1S,2S)2 ³ S	-11.902132 EV		
(1S,2S)2 ¹ S	-7.126372 EV		
(1S,2S)2 ³ P	-10.918178 EV		
(1S,2P)2 ¹ P	-9.947232 EV		
(2S ²)1s	-3.353351 EV	-4.210 EV ^A	
(2S,2P)3 ³ P	-3.149155 EV		
(2S,2P)1 ¹ P	-1.598073 EV		
(2P ²)3 ³ P	-2.343349 EV		
(2P ²)1 ¹ P	-1.769680 EV		

TABLE III. NON-ZERO HYDROGEN NEGATIVE ION

WAVE FUNCTION CONSTANTS

(1S ²)1s		(1S,2S)2 ¹ S		(2S ²)1s	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	-0.679349	N(1,2,1,1)	0.723263	N(2,2,1,1)	0.087635
N(1,1,1,2)	0.515054	N(1,2,1,2)	0.474605	N(2,2,1,2)	0.095321
N(1,1,2,1)	0.515054	N(1,2,2,1)	0.474605	N(2,2,2,1)	0.095321
N(1,1,2,2)	0.003748	N(1,2,2,2)	-0.158793	N(2,2,2,2)	0.867246
N(1,1,3,5)	-0.051347	N(1,2,3,5)	-0.019789	N(2,2,3,5)	0.272048
N(1,1,4,4)	0.051347	N(1,2,4,4)	0.019789	N(2,2,4,4)	-0.272049
N(1,1,5,3)	-0.051347	N(1,2,5,3)	-0.019789	N(2,2,5,3)	0.272048

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.705099	N(1,3,1,3)	0.707037	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.053256	N(1,3,2,3)	0.009884	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.705098	N(1,3,3,1)	0.707038		
N(1,3,3,2)	-0.053256	N(1,3,3,2)	0.009884		

(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.053256	N(2,3,1,3)	-0.009884	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.705098	N(2,3,2,3)	0.707038	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.053256	N(2,3,3,1)	-0.009884		
N(2,3,3,2)	-0.705098	N(2,3,3,2)	0.707038		

(2P ²)1 ¹ P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE IV. HELIUM ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-77.152813 EV	-78.983 EV ^C	-78.983 EV ^D
(1S,2S)2 ³ S	-57.830217 EV	-59.190 EV ^F	-59.170 EV
(1S,2S)2 ¹ S	-53.326942 EV	-58.373 EV ^F	-58.374 EV
(1S,2P)2 ³ P	-55.512251 EV		-58.025 EV
(1S,2P)2 ¹ P	-53.918681 EV		-57.772 EV
(2S ²) 1 ¹ S	-21.471516 EV	-21.710 EV ^A	
(2S,2P) 3 ³ P	-19.958831 EV		
(2S,2P) 1 ¹ P	-16.808345 EV		
(2P ²) 3 ³ P	-18.297104 EV		-21.338 EV
(2P ²) 1 ¹ P	-17.149767 EV		

TABLE V. NON-ZERO HELIUM
WAVE FUNCTION CONSTANTS

(1S ²) 1 ¹ S		(1S,2S)2 ¹ S		(2S ²) 1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.952136	N(1,2,1,1)	0.304029	N(2,2,1,1)	0.010681
N(1,1,1,2)	-0.214661	N(1,2,1,2)	0.672874	N(2,2,1,2)	0.029586
N(1,1,2,1)	-0.214661	N(1,2,2,1)	0.672874	N(2,2,2,1)	0.029586
N(1,1,2,2)	-0.014563	N(1,2,2,2)	-0.031520	N(2,2,2,2)	0.880907
N(1,1,3,5)	0.018817	N(1,2,3,5)	-0.018739	N(2,2,3,5)	0.272114
N(1,1,4,4)	-0.018817	N(1,2,4,4)	0.018739	N(2,2,4,4)	-0.272115
N(1,1,5,3)	0.018817	N(1,2,5,3)	-0.018739	N(2,2,5,3)	0.272114
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.706732	N(1,3,1,3)	0.707092	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.023027	N(1,3,2,3)	0.004447	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.706731	N(1,3,3,1)	0.707093		
N(1,3,3,2)	-0.023027	N(1,3,3,2)	0.004447		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.023027	N(2,3,1,3)	-0.004447	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.706732	N(2,3,2,3)	0.707093	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.023027	N(2,3,3,1)	-0.004447		
N(2,3,3,2)	-0.706732	N(2,3,3,2)	0.707093		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE VI. LITHIUM +1 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-195.789845 EV	-197.890 EV ^G	-198.038 EV
(1S,2S)2 ³ S	-137.784349 EV		-139.032 EV
(1S,2S)2 ¹ S	-132.548975 EV		-137.293 EV
(1S,2P)2 ³ P	-134.736702 EV		-135.773 EV
(1S,2P)2 ¹ P	-131.916252 EV		-135.838 EV
(2S ²) 1 ¹ S	-51.150248 EV		
(2S,2P)3 ³ P	-50.374552 EV		
(2S,2P)1 ¹ P	-45.628907 EV		
(2P ²) 3 ³ P	-47.851251 EV		
(2P ²) 1 ¹ P	-46.143260 EV		

TABLE VII. NON-ZERO LITHIUM +1 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.985963	N(1,2,1,1)	0.165885	N(2,2,1,1)	0.004920
N(1,1,1,2)	-0.117131	N(1,2,1,2)	0.695992	N(2,2,1,2)	0.018212
N(1,1,2,1)	-0.117131	N(1,2,2,1)	0.695993	N(2,2,2,1)	0.018212
N(1,1,2,2)	-0.010397	N(1,2,2,2)	-0.016460	N(2,2,2,2)	0.880856
N(1,1,3,5)	0.010473	N(1,2,3,5)	-0.014297	N(2,2,3,5)	0.272889
N(1,1,4,4)	-0.010473	N(1,2,4,4)	0.014297	N(2,2,4,4)	-0.272889
N(1,1,5,3)	0.010473	N(1,2,5,3)	-0.014297	N(2,2,5,3)	0.272888

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.706955	N(1,3,1,3)	0.707100	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.014675	N(1,3,2,3)	0.002869	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.706954	N(1,3,3,1)	0.707101		
N(1,3,3,2)	-0.014675	N(1,3,3,2)	0.002869		

(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.014675	N(2,3,1,3)	-0.002869	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.706954	N(2,3,2,3)	0.707101	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.014675	N(2,3,3,1)	-0.002869		
N(2,3,3,2)	-0.706954	N(2,3,3,2)	0.707101		

(2P ²)1 ¹ P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE VIII. BERYLLIUM +2 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-369.152107 EV	-371.238 EV ^G	-371.507 EV
(1S,2S)2 ³ S	-251.764500 EV		-252.949 EV
(1S,2S)2 ¹ S	-245.518114 EV		
(1S,2P)2 ³ P	-247.688053 EV		-249.620 EV
(1S,2P)2 ¹ P	-243.939657 EV		-247.871 EV
(2S ²) 1 ¹ S	-95.454512 EV		
(2S,2P)3 ³ P	-94.399780 EV		
(2S,2P)1 ¹ P	-88.059350 EV		
(2P ²) 3 ³ P	-91.035635 EV		
(2P ²) 1 ¹ P	-88.741160 EV		

TABLE IX. NON-ZERO BERYLLIUM +2 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.093591	N(1,2,1,1)	0.112212	N(2,2,1,1)	0.003075
N(1,1,1,2)	-0.079247	N(1,2,1,2)	0.702464	N(2,2,1,2)	0.013199
N(1,1,2,1)	-0.079247	N(1,2,2,1)	0.702464	N(2,2,2,1)	0.013199
N(1,1,2,2)	-0.007792	N(1,2,2,2)	-0.011023	N(2,2,2,2)	0.880652
N(1,1,3,5)	0.007195	N(1,2,3,5)	-0.011198	N(2,2,3,5)	0.273309
N(1,1,4,4)	-0.007195	N(1,2,4,4)	0.011198	N(2,2,4,4)	-0.273310
N(1,1,5,3)	0.007195	N(1,2,5,3)	-0.011198	N(2,2,5,3)	0.273309
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707025	N(1,3,1,3)	0.707103	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.010767	N(1,3,2,3)	0.002117	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707024	N(1,3,3,1)	0.707104		
N(1,3,3,2)	-0.010767	N(1,3,3,2)	0.002117		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.010767	N(2,3,1,3)	-0.002117	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707025	N(2,3,2,3)	0.707104	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.010767	N(2,3,3,1)	-0.002117		
N(2,3,3,2)	-0.707025	N(2,3,3,2)	0.707104		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE X. BORON +3 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-597.044167 EV	-599.273 EV ^H	-599.425 EV
(1S,2S)2 ³ S	-399.770638 EV		-401.643 EV
(1S,2S)2 ¹ S	-392.426327 EV		
(1S,2P)2 ³ P	-394.665749 EV		-397.274 EV
(1S,2P)2 ¹ P	-389.989513 EV		-394.663 EV
(2S ²) 1 ¹ S	-153.358158 EV		
(2S,2P)3 ³ P	-152.035076 EV		
(2S,2P)1 ¹ P	-144.101194 EV		
(2P ²) 3 ³ P	-147.820765 EV		
(2P ²) 1 ¹ P	-144.952467 EV		

TABLE XI. NON-ZERO BORON +3 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.996368	N(1,2,1,1)	0.034480	N(2,2,1,1)	0.002204
N(1,1,1,2)	-0.059572	N(1,2,1,2)	0.704466	N(2,2,1,2)	0.010359
N(1,1,2,1)	-0.050672	N(1,2,2,1)	0.704465	N(2,2,2,1)	0.010359
N(1,1,2,2)	-0.006190	N(1,2,2,2)	-0.008262	N(2,2,2,2)	0.880491
N(1,1,3,5)	0.005471	N(1,2,3,5)	-0.009147	N(2,2,3,5)	0.273567
N(1,1,4,4)	-0.005471	N(1,2,4,4)	0.009147	N(2,2,4,4)	-0.273567
N(1,1,5,3)	0.005471	N(1,2,5,3)	-0.009147	N(2,2,5,3)	0.273566

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707057	N(1,3,1,3)	0.707103	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.008503	N(1,3,2,3)	0.001678	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707054	N(1,3,3,1)	0.707106		
N(1,3,3,2)	-0.008503	N(1,3,3,2)	0.001678		

(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.008503	N(2,3,1,3)	-0.001678	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707056	N(2,3,2,3)	0.707105	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.008503	N(2,3,3,1)	-0.001678		
N(2,3,3,2)	-0.707056	N(2,3,3,2)	0.707105		

(2P ²)1 ¹ P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE XII. CARBON +4 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1S	-879.415802 EV	-881.841 EV ^P	-881.826 EV
(1S,2S)2 ³ S	-581.802742 EV		-582.949 EV
(1S,2S)2 ¹ S	-573.323486 EV		
(1S,2P)2 ³ P	-575.669678 EV		-577.510 EV
(1S,2P)2 ¹ P	-570.065216 EV		-574.028 EV
(2S ²) 1S	-224.872292 EV		
(2S,2P)3P	-223.280661 EV		
(2S,2P)1P	-213.752939 EV		
(2P ²) 3P	-218.216186 EV		
(2P ²) 1P	-214.774163 EV		

TABLE XIII. NON-ZERO CARBON +4 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 1S		(1S,2S)2 1S		(2S ²) 1S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.997670	N(1,2,1,1)	0.067058	N(2,2,1,1)	0.001706
N(1,1,1,2)	-0.047797	N(1,2,1,2)	0.705408	N(2,2,1,2)	0.008527
N(1,1,2,1)	-0.047797	N(1,2,2,1)	0.705407	N(2,2,2,1)	0.008527
N(1,1,2,2)	-0.005123	N(1,2,2,2)	-0.006599	N(2,2,2,2)	0.880370
N(1,1,3,3)	0.004412	N(1,2,3,3)	-0.007716	N(2,2,3,3)	0.273740
N(1,1,4,4)	-0.004412	N(1,2,4,4)	0.007716	N(2,2,4,4)	-0.273741
N(1,1,5,3)	0.004412	N(1,2,5,3)	-0.007716	N(2,2,5,3)	0.273740
(1S,2P)2 3P		(1S,2P)2 1P		(1S,2S)2 3S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	0.	N(1,3,1,3)	0.707105	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.	N(1,3,2,3)	0.001389	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.	N(1,3,3,1)	0.707105		
N(1,3,3,2)	0.	N(1,3,3,2)	0.001389		
(2S,2P) 3P		(2S,2P) 1P		(2P ²) 3P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.007025	N(2,3,1,3)	-0.001389	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707072	N(2,3,2,3)	0.707105	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.007025	N(2,3,3,1)	-0.001389		
N(2,3,3,2)	-0.707072	N(2,3,3,2)	0.707105		
(2P ²) 1P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XIV. NITROGEN +5 ION ENERGIES.

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-1216.248169 EV	-1218.768 EV ^F	-1218.755 EV
(1S,2S)2 ³ S	-797.860924 EV		-799.074 EV
(1S,2S)2 ¹ S	-788.227425 EV		
(1S,2P)2 ³ P	-790.699600 EV		-792.580 EV
(1S,2P)2 ¹ P	-784.166801 EV		-788.178 EV
(2S ²) 1 ¹ S	-379.975552 EV		
(2S,2P)3 ³ P	-378.136478 EV		
(2S,2P)1 ¹ P	-297.015060 EV		
(2P ²) 3 ³ P	-352.221973 EV		
(2P ²) 1 ¹ P	-298.206238 EV		

TABLE XV. NON-ZERO NITROGEN +5 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.998381	N(1,2,1,1)	0.056395	N(2,2,1,1)	0.001387
N(1,1,1,2)	-0.039844	N(1,2,1,2)	0.705923	N(2,2,1,2)	0.007247
N(1,1,2,1)	-0.039844	N(1,2,2,1)	0.705924	N(2,2,2,1)	0.007247
N(1,1,2,2)	-0.004366	N(1,2,2,2)	-0.005490	N(2,2,2,2)	0.380277
N(1,1,3,5)	0.003696	N(1,2,3,5)	-0.006667	N(2,2,3,5)	0.273864
N(1,1,4,4)	-0.003696	N(1,2,4,4)	0.006667	N(2,2,4,4)	-0.273865
N(1,1,5,3)	0.003696	N(1,2,5,3)	-0.006667	N(2,2,5,3)	0.273864
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707084	N(1,3,1,3)	0.707103	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.005985	N(1,3,2,3)	0.001186	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.707079	N(1,3,3,1)	0.707108		
N(1,3,3,2)	-0.005985	N(1,3,3,2)	0.001186		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.005985	N(2,3,1,3)	-0.001186	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707081	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.005985	N(2,3,3,1)	-0.001186		
N(2,3,3,2)	-0.707081	N(2,3,3,2)	0.707106		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XVI. OXYGEN +6 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-1637.533615 EV	-1609.507 EV ^H	-1610.234 EV
(1S,2S)2 ³ S	-1047.945190 EV		-1049.318 EV
(1S,2S)2 ¹ S	-1037.146301 EV		
(1S,2P)2 ³ P	-1039.755661 EV		-1041.770 EV
(1S,2P)2 ¹ P	-1032.294525 EV		-1036.436 EV
(2S ²) 1 ¹ S	-408.731121 EV		
(2S,2P)3 ³ P	-396.602711 EV		
(2S,2P)1 ¹ P	-393.887623 EV		
(2P ²) 3 ³ P	-399.838058 EV		
(2P ²) 1 ¹ P	-395.248745 EV		

TABLE XVII. NON-ZERO OXYGEN +6 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.998810	N(1,2,1,1)	0.048335	N(2,2,1,1)	0.001166
N(1,1,1,2)	-0.034152	N(1,2,1,2)	0.706236	N(2,2,1,2)	0.006302
N(1,1,2,1)	-0.034152	N(1,2,2,1)	0.706236	N(2,2,2,1)	0.006302
N(1,1,2,2)	-0.003803	N(1,2,2,2)	-0.004698	N(2,2,2,2)	0.880205
N(1,1,3,5)	0.003180	N(1,2,3,5)	-0.005867	N(2,2,3,5)	0.273957
N(1,1,4,4)	-0.003180	N(1,2,4,4)	0.005867	N(2,2,4,4)	-0.273958
N(1,1,5,3)	0.003180	N(1,2,5,3)	-0.005867	N(2,2,5,3)	0.273957
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707090	N(1,3,1,3)	0.707104	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.005213	N(1,3,2,3)	0.001034	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.707085	N(1,3,3,1)	0.707108		
N(1,3,3,2)	-0.005213	N(1,3,3,2)	0.001034		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.005213	N(2,3,1,3)	-0.001034	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707088	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.005213	N(2,3,3,1)	-0.001034		
N(2,3,3,2)	-0.707088	N(2,3,3,2)	0.707106		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XVIII. FLUORINE +7 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-2053.268005 EV	-2070.005 EV ^F	-2069.884 EV
(1S,2S)2 ³ S	-1332.055359 EV		-1347.265 EV
(1S,2S)2 ¹ S	-1320.084061 EV		
(1S,2P)2 ³ P	-1322.837646 EV		-1338.664 EV
(1S,2P)2 ¹ P	-1314.448151 EV		-1332.393 EV
(2S ²) 1 ¹ S	-521.076012 EV		
(2S,2P)3 ³ P	-518.679306 EV		
(2S,2P)1 ¹ P	-504.370586 EV		
(2P ²) 3 ³ P	-511.064667 EV		
(2P ²) 1 ¹ P	-505.901680 EV		

TABLE XIX. NON-ZERO FLUORINE +7 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999089	N(1,2,1,1)	0.042284	N(2,2,1,1)	0.001004
N(1,1,1,2)	-0.029379	N(1,2,1,2)	0.706439	N(2,2,1,2)	0.005574
N(1,1,2,1)	-0.029379	N(1,2,2,1)	0.706439	N(2,2,2,1)	0.005574
N(1,1,2,2)	-0.003367	N(1,2,2,2)	-0.004105	N(2,2,2,2)	0.880147
N(1,1,3,5)	0.002790	N(1,2,3,5)	-0.005237	N(2,2,3,5)	0.274030
N(1,1,4,4)	-0.002790	N(1,2,4,4)	0.005237	N(2,2,4,4)	-0.274031
N(1,1,5,3)	0.002790	N(1,2,5,3)	-0.005237	N(2,2,5,3)	0.274030
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707095	N(1,3,1,3)	0.707103	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.004618	N(1,3,2,3)	0.000917	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707088	N(1,3,3,1)	0.707110		
N(1,3,3,2)	-0.004618	N(1,3,3,2)	0.000917		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.004618	N(2,3,1,3)	-0.000917	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707092	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.004618	N(2,3,3,1)	-0.000917		
N(2,3,3,2)	-0.707092	N(2,3,3,2)	0.707106		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XX. NEON +8 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-2553.447998 EV	-1193.826 EV ^H	
(1S,2S)2 ³ S	-1650.191422 EV		
(1S,2S)2 ¹ S	-1637.043152 EV		
(1S,2P)2 ³ P	-1639.945847 EV		
(1S,2P)2 ¹ P	-1630.627930 EV		
(2S ²) 1 ¹ S	-647.031105 EV		
(2S,2P) 3 ³ P	-644.366249 EV		
(2S,2P) 1 ¹ P	-628.463936 EV		
(2P ²) 3 ³ P	-635.901535 EV		
(2P ²) 1 ¹ P	-630.164818 EV		

TABLE XXI. NON-ZERO NEON +8 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999261	N(1,2,1,1)	0.037577	N(2,2,1,1)	0.005881
N(1,1,1,2)	-0.026555	N(1,2,1,2)	0.705576	N(2,2,1,2)	0.004998
N(1,1,2,1)	-0.026555	N(1,2,2,1)	0.705579	N(2,2,2,1)	0.004998
N(1,1,2,2)	-0.003021	N(1,2,2,2)	-0.003645	N(2,2,2,2)	0.880100
N(1,1,3,5)	0.002485	N(1,2,3,5)	-0.004729	N(2,2,3,5)	0.274090
N(1,1,4,4)	-0.002485	N(1,2,4,4)	0.004720	N(2,2,4,4)	-0.274089
N(1,1,5,3)	0.002485	N(1,2,5,3)	-0.004729	N(2,2,5,3)	0.274086
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707096	N(1,3,1,3)	0.707105	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.004144	N(1,3,2,3)	0.000823	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.707093	N(1,3,3,1)	0.707103		
N(1,3,3,2)	-0.004144	N(1,3,3,2)	0.000823		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.004144	N(2,3,1,3)	-0.000823	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707095	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.004144	N(2,3,3,1)	-0.000823		
N(2,3,3,2)	-0.707095	N(2,3,3,2)	0.707106		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XXII. SODIUM +9 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1S	-3168.074127 EV		
(1S,2S)2 ³ S	-2602.353775 EV		
(1S,2S)2 ¹ S	-1988.025238 EV		
(1S,2P)2 ³ P	-1991.080017 EV		
(1S,2P)2 ¹ P	-1980.833664 EV		
(2S ²) 1S	-786.596786 EV		
(2S,2P)3P	-783.663605 EV		
(2S,2P)1P	-766.167686 EV		
(2P ²) 3P	-774.349197 EV		
(2P ²) 1P	-766.038755 EV		

TABLE XXIII. NON-ZERO SODIUM +9 ION

WAVE FUNCTION CONSTANTS

(1S ²)1S		(1S,2S)2 ¹ S		(2S ²)1S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999418	N(1,2,1,1)	0.033811	N(2,2,1,1)	0.000785
N(1,1,1,2)	-0.023895	N(1,2,1,2)	0.705678	N(2,2,1,2)	0.004529
N(1,1,2,1)	-0.023895	N(1,2,2,1)	0.705680	N(2,2,2,1)	0.004530
N(1,1,2,2)	-0.002739	N(1,2,2,2)	-0.003277	N(2,2,2,2)	0.880060
N(1,1,3,5)	0.002240	N(1,2,3,5)	-0.004310	N(2,2,3,5)	0.274135
N(1,1,4,4)	-0.002240	N(1,2,4,4)	0.004310	N(2,2,4,4)	-0.274137
N(1,1,5,3)	0.002240	N(1,2,5,3)	-0.004310	N(2,2,5,3)	0.274135

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707099	N(1,3,1,3)	0.707104	N(1,2,1,2)	0.707107
N(1,3,2,3)	0.003759	N(1,3,2,3)	0.000747	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.707094	N(1,3,3,1)	0.707109		
N(1,3,3,2)	-0.003759	N(1,3,3,2)	0.000747		

(2S,2P)3P		(2S,2P)1P		(2P ²)3P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.003759	N(2,3,1,3)	-0.000747	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707097	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.003759	N(2,3,3,1)	-0.000747		
N(2,3,3,2)	-0.707097	N(2,3,3,2)	0.707106		

(2P ²)1P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE XXIV. MAGNESIUM +10 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-3717.143751 EV	-3742.527 EV ^H	-3745.735 EV
(1S,2S)2 ³ S	-2388.541716 EV		
(1S,2S)2 ¹ S	-2373.230396 EV		
(1S,2P)2 ³ P	-2376.240356 EV		
(1S,2P)2 ¹ P	-2365.065552 EV		-2393.775 EV
(2S ²) 1 ¹ S	-939.772758 EV		
(2S,2P) 3 ³ P	-936.571457 EV		
(2S,2P) 1 ¹ P	-917.481895 EV		
(2P ²) 3 ³ P	-926.407021 EV		
(2P ²) 1 ¹ P	-919.522835 EV		

TABLE XXV. NON-ZERO MAGNESIUM +10 ION

WAVE FUNCTION CONSTANTS

(1S ²) 1 ¹ S		(1S,2S) 2 ¹ S		(2S ²) 1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999519	N(1,2,1,1)	0.030730	N(2,2,1,1)	0.000707
N(1,1,1,2)	-0.021713	N(1,2,1,2)	0.706753	N(2,2,1,2)	0.004141
N(1,1,2,1)	-0.021718	N(1,2,2,1)	0.706753	N(2,2,2,1)	0.004141
N(1,1,2,2)	-0.002505	N(1,2,2,2)	-0.002976	N(2,2,2,2)	0.880027
N(1,1,3,5)	0.002040	N(1,2,3,5)	-0.003959	N(2,2,3,5)	0.274175
N(1,1,4,4)	-0.002040	N(1,2,4,4)	0.003959	N(2,2,4,4)	-0.274177
N(1,1,5,3)	0.002040	N(1,2,5,3)	-0.003959	N(2,2,5,3)	0.274175
(1S,2P) 2 ³ P		(1S,2P) 2 ¹ P		(1S,2S) 2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	0.	N(1,3,1,3)	0.707106	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.	N(1,3,2,3)	0.000684	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.	N(1,3,3,1)	0.707106		
N(1,3,3,2)	0.	N(1,3,3,2)	0.000684		
(2S,2P) 3 ³ P		(2S,2P) 1 ¹ P		(2P ²) 3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.003439	N(2,3,1,3)	-0.000684	N(3,4,3,4)	-0.707107
N(2,3,2,3)	0.707098	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.003439	N(2,3,3,1)	-0.000684		
N(2,3,3,2)	-0.707098	N(2,3,3,2)	0.707106		
(2P ²) 1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XXVI. ALUMINUM +11 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-4330.657288 EV		-4414.487 EV
(1S,2S)2 ³ S	-2808.756073 EV		
(1S,2S)2 ¹ S	-2792.060059 EV		
(1S,2P)2 ³ P	-2795.426361 EV		
(1S,2P)2 ¹ P	-2783.322937 EV		-2816.535 EV
(2S ²) 1 ¹ S	-1106.559156 EV		
(2S,2P)3 ² P	-1103.089523 EV		
(2S,2P)1 ¹ P	-1082.406448 EV		
(2P ²) 3 ² P	-1092.075241 EV		
(2P ²) 1 ¹ P	-1084.617416 EV		

TABLE XXVII. NON-ZERO ALUMINUM +11 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999596	N(1,2,1,1)	0.028163	N(2,2,1,1)	0.000643
N(1,1,1,2)	-0.019905	N(1,2,1,2)	0.705811	N(2,2,1,2)	0.003815
N(1,1,2,1)	-0.019905	N(1,2,2,1)	0.705808	N(2,2,2,1)	0.003815
N(1,1,2,2)	-0.002308	N(1,2,2,2)	-0.002726	N(2,2,2,2)	0.879999
N(1,1,3,5)	0.001872	N(1,2,3,5)	-0.003661	N(2,2,3,5)	0.274209
N(1,1,4,4)	-0.001872	N(1,2,4,4)	0.003661	N(2,2,4,4)	-0.274210
N(1,1,5,3)	0.001872	N(1,2,5,3)	-0.003661	N(2,2,5,3)	0.274209
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707102	N(1,3,1,3)	0.707104	N(1,2,1,2)	0.707105
N(1,3,2,3)	0.003169	N(1,3,2,3)	0.000631	N(1,2,2,1)	-0.707108
N(1,3,3,1)	0.707097	N(1,3,3,1)	0.707109		
N(1,3,3,2)	-0.003169	N(1,3,3,2)	0.000631		
(2S,2P)3 ² P		(2S,2P)1 ¹ P		(2P ²)3 ² P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.003169	N(2,3,1,3)	-0.000631	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707100	N(2,3,2,3)	0.707106	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.003169	N(2,3,3,1)	-0.000631		
N(2,3,3,2)	-0.707100	N(2,3,3,2)	0.707106		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XXVIII. SILICON +12 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-5098.612915	EV	
(1S,2S)2 ³ S	-3262.996552	EV	
(1S,2S)2 ¹ S	-3245.114156	EV	
(1S,2P)2 ³ P	-3248.638580	EV	
(1S,2P)2 ¹ P	-3235.636873	EV	
(2S ²) 1 ¹ S	-1236.955698	EV	
(2S,2P) 3 ³ P	-1283.218002	EV	
(2S,2P) 1 ¹ P	-1260.941350	EV	
(2P ²) 3 ³ P	-1271.353867	EV	
(2P ²) 1 ¹ P	-1263.322159	EV	

TABLE XXIX. NON-ZERO SILICON +12 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999656	N(1,2,1,1)	0.025992	N(2,2,1,1)	0.000590
N(1,1,1,2)	-0.018371	N(1,2,1,2)	0.706854	N(2,2,1,2)	0.003536
N(1,1,2,1)	-0.018371	N(1,2,2,1)	0.706852	N(2,2,2,1)	0.003536
N(1,1,2,2)	-0.002139	N(1,2,2,2)	-0.002515	N(2,2,2,2)	0.879974
N(1,1,3,5)	0.001729	N(1,2,3,5)	-0.003404	N(2,2,3,5)	0.274238
N(1,1,4,4)	-0.001729	N(1,2,4,4)	0.003404	N(2,2,4,4)	-0.274239
N(1,1,5,3)	0.001729	N(1,2,5,3)	-0.003404	N(2,2,5,3)	0.274238
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707104	N(1,3,1,3)	0.707103	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.002939	N(1,3,2,3)	0.000585	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707097	N(1,3,3,1)	0.707110		
N(1,3,3,2)	-0.002939	N(1,3,3,2)	0.000585		
(2S,2P) 3 ³ P		(2S,2P) 1 ¹ P		(2P ²) 3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.002939	N(2,3,1,3)	-0.000585	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707101	N(2,3,2,3)	0.707107	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.002939	N(2,3,3,1)	-0.000585		
N(2,3,3,2)	-0.707101	N(2,3,3,2)	0.707107		
(2P ²) 1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XXX. PHOSPHORUS +13 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-5871.012329	EV	
(1S,2S)2 ³ S	-3751.262878	EV	
(1S,2S)2 ¹ S	-3732.193390	EV	
(1S,2P)2 ³ P	-3735.876892	EV	
(1S,2P)2 ¹ P	-3721.916534	EV	
(2S ²) 1 ¹ S	-1480.962860	EV	
(2S,2P)3 ³ P	-1476.957016	EV	
(2S,2P)1 ¹ P	-1453.086807	EV	
(2P ²) 3 ³ P	-1464.242920	EV	
(2P ²) 1 ¹ P	-1455.63734	EV	

TABLE XXXI. NON-ZERO PHOSPHORUS +13 ION

WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999703	N(1,2,1,1)	0.024131	N(2,2,1,1)	0.000544
N(1,1,1,2)	-0.017056	N(1,2,1,2)	0.706887	N(2,2,1,2)	0.003295
N(1,1,2,1)	-0.017056	N(1,2,2,1)	0.706889	N(2,2,2,1)	0.003295
N(1,1,2,2)	-0.001994	N(1,2,2,2)	-0.002334	N(2,2,2,2)	0.879953
N(1,1,3,3)	0.001607	N(1,2,3,3)	-0.003181	N(2,2,3,3)	0.274263
N(1,1,4,4)	-0.001607	N(1,2,4,4)	0.003181	N(2,2,4,4)	-0.274264
N(1,1,5,3)	0.001607	N(1,2,5,3)	-0.003181	N(2,2,5,3)	0.274263
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707107	N(1,3,1,3)	0.707101	N(1,2,1,2)	0.707108
N(1,3,2,3)	0.002740	N(1,3,2,3)	0.000546	N(1,2,2,1)	-0.707106
N(1,3,3,1)	0.707096	N(1,3,3,1)	0.707112		
N(1,3,3,2)	-0.002740	N(1,3,3,2)	0.000546		
(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.002740	N(2,3,1,3)	-0.000546	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707101	N(2,3,2,3)	0.707107	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.002740	N(2,3,3,1)	-0.000546		
N(2,3,3,2)	-0.707101	N(2,3,3,2)	0.707107		
(2P ²)1 ¹ P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

TABLE XXXII. SULPHUR +14 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1 ¹ S	-6697.853213	EV	
(1S,2S)2 ³ S	-4273.555237	EV	
(1S,2S)2 ¹ S	-4253.297546	EV	
(1S,2P)2 ³ P	-4257.141296	EV	
(1S,2P)2 ¹ P	-4242.252502	EV	
(2S ²) 1 ¹ S	-1688.580322	EV	
(2S,2P)3 ³ P	-1684.306351	EV	
(2S,2P)1 ¹ P	-1658.842621	EV	
(2P ²) 3 ³ P	-1670.741776	EV	
(2P ²) 1 ¹ P	-1661.563187	EV	

TABLE XXXIII. NON-ZERO SULPHUR +14 ION
WAVE FUNCTION CONSTANTS

(1S ²)1 ¹ S		(1S,2S)2 ¹ S		(2S ²)1 ¹ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999741	N(1,2,1,1)	0.022518	N(2,2,1,1)	0.000505
N(1,1,1,2)	-0.015916	N(1,2,1,2)	0.706917	N(2,2,1,2)	0.003085
N(1,1,2,1)	-0.015916	N(1,2,2,1)	0.706916	N(2,2,2,1)	0.003085
N(1,1,2,2)	-0.001866	N(1,2,2,2)	-0.002177	N(2,2,2,2)	0.879934
N(1,1,3,5)	0.001501	N(1,2,3,5)	-0.002986	N(2,2,3,5)	0.274284
N(1,1,4,4)	-0.001501	N(1,2,4,4)	0.002986	N(2,2,4,4)	-0.274286
N(1,1,5,3)	0.001501	N(1,2,5,3)	-0.002986	N(2,2,5,3)	0.274285

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707103	N(1,3,1,3)	0.707106	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.002566	N(1,3,2,3)	0.000511	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707101	N(1,3,3,1)	0.707108		
N(1,3,3,2)	-0.002566	N(1,3,3,2)	0.000511		

(2S,2P)3 ³ P		(2S,2P)1 ¹ P		(2P ²)3 ³ P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.002566	N(2,3,1,3)	-0.000511	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707102	N(2,3,2,3)	0.707107	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.002566	N(2,3,3,1)	-0.000511		
N(2,3,3,2)	-0.707102	N(2,3,3,2)	0.707107		

(2P ²)1 ¹ P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE XXXIV. CHLORINE +15 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1S	-7579.136902	EV	
(1S,2S)2 ³ S	-4329.872742	EV	
(1S,2S)2 ¹ S	-4808.426758	EV	
(1S,2P)2 ³ P	-4812.431274	EV	
(1S,2P)2 ¹ P	-4796.613892	EV	
(2S ²) 1S	-1909.808182	EV	
(2S,2P)3P	-1905.266068	EV	
(2S,2P)1P	-1878.208601	EV	
(2P ²) 3P	-1890.851547	EV	
(2P ²) 1P	-1881.099304	EV	

TABLE XXXV. NON-ZERO CHLORINE +15 ION
WAVE FUNCTION CONSTANTS

(1S ²) 1S		(1S,2S)2 ¹ S		(2S ²) 1S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999773	N(1,2,1,1)	0.021108	N(2,2,1,1)	0.000472
N(1,1,1,2)	-0.014920	N(1,2,1,2)	0.706940	N(2,2,1,2)	0.002900
N(1,1,2,1)	-0.014920	N(1,2,2,1)	0.706939	N(2,2,2,1)	0.002900
N(1,1,2,2)	-0.001755	N(1,2,2,2)	-0.002040	N(2,2,2,2)	0.879917
N(1,1,3,5)	0.001408	N(1,2,3,5)	-0.002613	N(2,2,3,5)	0.274302
N(1,1,4,4)	-0.001408	N(1,2,4,4)	0.002613	N(2,2,4,4)	-0.274305
N(1,1,5,3)	0.001408	N(1,2,5,3)	-0.002613	N(2,2,5,3)	0.274305

(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707110	N(1,3,1,3)	0.707099	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.002413	N(1,3,2,3)	0.000481	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707095	N(1,3,3,1)	0.707114		
N(1,3,3,2)	-0.002413	N(1,3,3,2)	0.000481		

(2S,2P)3P		(2S,2P)1P		(2P ²)3P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.002413	N(2,3,1,3)	-0.000481	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707103	N(2,3,2,3)	0.707107	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.002413	N(2,3,3,1)	-0.000481		
N(2,3,3,2)	-0.707103	N(2,3,3,2)	0.707107		

(2P ²) 1P	
COMPONENT	VALUE
N(3,4,3,4)	0.707107
N(3,4,4,3)	0.707107

TABLE XXXVI. ARGON +16 ION ENERGIES

STATE	G.F. METHOD	OTHER METHODS	EXPERIMENTAL
(1S ²) 1s	-7579.136992 EV		
(1S,2S)2 ³ S	-4329.872742 EV		
(1S,2S)2 ¹ S	-4650.426758 EV		
(1S,2P)2 ³ P	-4812.431274 EV		
(1S,2P)2 ¹ P	-4796.613892 EV		
(2S ²) 1s	-1909.808182 EV		
(2S,2P) 3P	-1905.266068 EV		
(2S,2P) 1P	-1878.208001 EV		
(2P ²) 3P	-1890.851547 EV		
(2P ²) 1P	-1881.599374 EV		

TABLE XXXVII. NON-ZERO ARGON +16 ION

WAVE FUNCTION CONSTANTS

(1S ²)1s		(1S,2S)2 ¹ S		(2S ²)1s	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,1,1,1)	0.999773	N(1,2,1,1)	0.021108	N(2,2,1,1)	0.000472
N(1,1,1,2)	-0.014920	N(1,2,1,2)	0.705940	N(2,2,1,2)	0.002900
N(1,1,2,1)	-0.014920	N(1,2,2,1)	0.705939	N(2,2,2,1)	0.002900
N(1,1,2,2)	-0.001755	N(1,2,2,2)	-0.002040	N(2,2,2,2)	0.879917
N(1,1,3,5)	0.001408	N(1,2,3,5)	-0.002813	N(2,2,3,5)	-0.274302
N(1,1,4,4)	-0.001408	N(1,2,4,4)	0.002813	N(2,2,4,4)	-0.274305
N(1,1,5,3)	0.001408	N(1,2,5,3)	-0.002813	N(2,2,5,3)	0.274305
(1S,2P)2 ³ P		(1S,2P)2 ¹ P		(1S,2S)2 ³ S	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(1,3,1,3)	-0.707110	N(1,3,1,3)	0.707099	N(1,2,1,2)	0.707106
N(1,3,2,3)	0.002413	N(1,3,2,3)	0.000481	N(1,2,2,1)	-0.707107
N(1,3,3,1)	0.707095	N(1,3,3,1)	0.707114		
N(1,3,3,2)	-0.002413	N(1,3,3,2)	0.000481		
(2S,2P)3P		(2S,2P)1P		(2P ²)3P	
COMPONENT	VALUE	COMPONENT	VALUE	COMPONENT	VALUE
N(2,3,1,3)	0.002413	N(2,3,1,3)	-0.000481	N(3,4,3,4)	0.707107
N(2,3,2,3)	0.707103	N(2,3,2,3)	0.707107	N(3,4,4,3)	-0.707107
N(2,3,3,1)	-0.002413	N(2,3,3,1)	-0.000481		
N(2,3,3,2)	-0.707103	N(2,3,3,2)	0.707107		
(2P ²)1P					
COMPONENT	VALUE				
N(3,4,3,4)	0.707107				
N(3,4,4,3)	0.707107				

VI. DISCUSSION

The helium isoelectronic sequence energies calculated by the method of this paper are larger than the corresponding experimental or most reported theoretical values. There are three reasons for this: (a) the convergence of the energy eigenvalue for calculations of this type is slow,¹⁸ (b) the truncation of the double sum-integrals that appear eliminates contributions from other terms in the series,¹⁹ and, (c) the variational techniques which have been used to calculate nearly all of the reported theoretical values of the energies minimize the energy. The variational wave functions are in general accurate only when used to calculate energies while the Green's function technique produces wave functions of generally equal accuracy for all properties of the system because of the property of uniform convergence.

The Green's function method of this paper gives a ground state energy for helium, -77.15 eV, 1.8% in error, which is more accurate than that of the first order perturbation theory, -74.8 eV, or the screening constant variation, -74.4 eV,²⁰ about the same accuracy as determined by Hartree, -77.6 eV,²¹ but less accurate than variational approaches.⁷⁻⁹ Even though these variational techniques are more accurate they require more computer time.

A reason for good accuracy with few terms can be seen from an investigation of configurational interaction,⁵ for the helium atom, to which the Green's function technique is related. Expanding a three-parameter Hylleraas type wave function into a series of Legendre polynomials to investigate the contributions to the total wave function of hydrogen-like wave functions with different angular momenta, the contributions were found to be;¹⁹

$\ell=0$	0.995076
$\ell=1$	0.004792
$\ell=2$	0.000108
$\ell=3$	0.000012
$\ell \geq 4$	< 0.000012

The corresponding contributions to the energy were;

$l=0$	-5.72823 Rydbergs
$l=1$	- .06992
$l=2$	- .00478
$l \geq 3$	- .00110

This shows the slow energy convergence of this type of series.

Thus it is seen that configurational interaction adds all contributions of a particular angular momentum state at once, while the method of this paper adds these terms in the order of contribution to the wave function thus resulting in fewer terms for the same accuracy.

The variational calculations for the single excited states of helium are again more accurate than the calculations and results of this paper, and again for the reasons already mentioned, but here the method of this paper has a distinct advantage over other methods. From TABLE V the wave function expansion coefficients are seen to be orthonormal. A problem in the variational calculations is to find a basis set, for the variation, which is orthonormal after variation. This orthonormality is a natural consequence of the method of this paper.

States of multiple excitations have been evaluated by the method of this paper. Although the truncation of the double sums limited the accuracy of the wave functions for these states, fair accuracy for the energy was obtained. Other calculations for these states have been made.^{22,23}

The percentage error in the energy eigenvalue calculations becomes smaller with increasing atomic number. This is as expected, since the ions become more and more hydrogen-like. The relative error for various ions is nearly constant at a few electron volts for the $n = 2$ truncation.

It is interesting to note that the ground state energy calculated for the hydrogen negative-ion is only one-fourth of an electron volt from the experimental value. The error in this case should be expected to be larger than the error for the ground state of the helium atom, not smaller. In addition several bound states

are predicted for the negative-ion, while only two have been reported experimentally.²⁴ The fortunate or accidental accuracy of the calculations and their predictions can only be cleared up by more elaborate calculations, as this alone will provide better energies and wave functions.

VII. ACKNOWLEDGMENTS

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FOOTNOTES

- * Part of the results presented in this paper were originally calculated by a different computational technique and are to be published. J. E. Swain and B. Curnutte, Jr., Helium Wave Functions and Energies Using a Green's Function Technique, to be published.
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FOOTNOTES (Continued)

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