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RELATIVISTIC AND NON-RELATIVISTIC CONFIGURATION INTERACTION CALCULATIONS FOR ATOMS HAVING A CLOSED CORE AND TWO VALENCE SPIN-ORBITALS *

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PROGRAM SUMMARY

Title of program: SOCKITTOME 1

Catalogue number: AAKA

Computer for which the program is designed and others upon which it is operable:

Computer: CDC 6400. *Installation*: University of Colorado

Operating system or monitor under which the program is executed: 6400/6500/6600 Scope Version 3.1.3

Programming languages used: FORTRAN IV

High speed store required: $141\,000_8$ words. *No. of bits in a word*: 60

Is the program overlaid? No

No. of magnetic tapes required: None

What other peripherals are used? Card Reader; Line Printer

No. of cards in combined program and test deck: 3243

Card punching code: IBM 026

Keywords descriptive of problem and method of solution: Central Field Approximation, Configuration Interaction, Low-Z Pauli Approximation, Modified Hartree-Fock-Slater Equation, Linear Variation Technique, Self-Consistent Field.

Nature of physical problem

The problem is to obtain [1,2] wavefunctions for bound atomic levels which permit accurate calculation of energies and transition probabilities. The low-Z Pauli approximation [3], which is correct to orders $Z^3\alpha^2$ and $Z^4\alpha^2$ in the energy (the non-relativistic energy is of order Z^2) is used to approximate the atomic Hamiltonian. The anti-Hermitian part of those operators characteristic of the Dirac theory is dropped.

Method of solution

The wavefunction is expanded in single configuration functions which are eigenstates of S^2, L^2, J^2, J_z, and parity. All configurations in the expansion must have a closed core and two valence spin-orbitals. The single configuration functions are a linear combination of Slater determinants whose elements are of the central field type. The radial part of the elements is obtained from Lindgren's [4] modification of the Hartree-Fock-Slater [5] equation which is solved using the methods of Herman and Skillman [6]. (Three subprograms were originally written by Herman and Skillman in Fortran II. All statements incompatible with Fortran IV as defined in the Control Data 6400/6500/6600 Computer Systems Manual were altered so as to be compatible with Fortran IV.) The coefficients are obtained by application of the variational principle (linear variation technique). The program allows exclusion of any relativistic operators and consequently strictly non-relativistic calculations may also be done.

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Restrictions on the complexity of the problem

The program requires $141\,000_8$ high speed core locations at 60 bits per word. The 32 bits per word of the IBM 360 may not suffice.

Typical running time

The running time (all operators) for a test case (Ba I with the $6s^2$, 6s7s. $6p^2(^1S_0, ^3P_0)$, 6p7p. $5d^2$. 5d6d configurations for even parity and $J = 0$) was six minutes on the CDC 6400. A more realistic expansion (one containing 25-30 terms) would take about one hour of CDC 6400 computing time.

References

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[2] D. R. Beck, J. Chem. Phys., accepted for publication (Sept., 1969); Ph. D. thesis, Lehigh University (1968), unpublished.

[3] H. A. Bethe and E. E. Salpeter, Quantum mechanics of one- and two-electron atoms (Academic Press, New York, 1957) p. 181.

[4] E. R. Cohen and J. W. M. DuMond, Rev. Mod. Phys. 37 (1965) 537.

[5] E. U. Condon and G. H. Shortley, The theory of atomic spectra (Cambridge Univ. Press, New York, 1935).

[6] A. R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, 1960).

LONG WRITE-UP

1. THEORETICAL SUMMARY

A method for obtaining wavefunctions and energies of bound atomic levels, including correlation and relativistic effects, has been proposed by Zare [1] and by Beck [2]. This paper describes a program for applying these methods. For the atomic Hamiltonian, we use the low-Z Pauli approximation [3]. It is correct to orders $Z^3\alpha^2$ and $Z^4\alpha^2$ in the energy (the non-relativistic energy is of order Z^2). Here, we expand the relativistic Hamiltonian in powers of $Z\alpha$ and α, where α is the fine structure constant, taken [4] to be 1/137.0388.

For an atomic system with nuclear charge Z and N electrons, the Hamiltonian may be written as a sum of one-body and two-body operators. Let the energy be measured in Rydbergs and the distance in Bohr radii. We have then

$$H = \sum_{k=1}^{N} f_k + \sum_{k<l} g_{kl} \tag{1}$$

where

$$f_k = f_k(\mathrm{nr}) + f_k(\mathrm{mass}) + f_k(\mathrm{so}) + f_k(\mathrm{cd}) \tag{2a}$$

and

$$g_{kl} = g_{kl}(\mathrm{nr}) + g_{kl}(\mathrm{oo'}) + g_{kl}(\mathrm{so+so'}) + g_{kl}(\mathrm{css'}) + g_{kl}(\mathrm{ss'}) + g_{kl}(\mathrm{cd}) \,. \tag{2b}$$

In (2a) and (2b), $f_k(\mathrm{nr})$ and $g_{kl}(\mathrm{nr})$ are the non-relativistic one- and two-body operators, $f_k(\mathrm{mass})$ is the correction due to the variation of electron mass with velocity, $g_{kl}(\mathrm{oo'})$ is the orbit-orbit correction, $f_k(\mathrm{so})$ and $g_{kl}(\mathrm{so+so'})$ are the one- and two-body spin-orbit and spin-other-orbit interactions, $g_{kl}(\mathrm{css'})$ is the "contact" portion of the spin-spin interaction, $g_{kl}(\mathrm{ss'})$ is the remaining portion of the spin-spin interaction, and $f_k(\mathrm{cd})$ and $g_{kl}(\mathrm{cd})$ are the one- and two-body interactions characteristic of the Dirac theory for which no adequate physical interpretation has been given. These latter operators, sometimes known as the Darwin operators, are non-Hermitian. Earlier numerical calculations for Tl II[2] have shown that the contribution of the anti-Hermitian part to the atomic energy eigenvalues may be neglected.

The one- and two-body operators are given by

$$f_k(\mathrm{nr}) = -\nabla_k^2 - 2Z/r_k \qquad f_k(\mathrm{mass}) = -\tfrac{1}{4}\alpha^2\nabla_k^4$$

$$f_k(\mathrm{so}) = \alpha^2\,(Zr_k^{-3}\mathbf{r}_k \times -\mathrm{i}\nabla_k)\cdot \mathbf{s}_k \qquad f_k(\mathrm{cd}) = \pi Z\alpha^2\delta(\mathbf{r}_k) \tag{2c}$$

and by

$$g_{kl}(\mathrm{nr}) = 2/r_{kl} \qquad g_{kl}(\mathrm{oo'}) = -\alpha^2[r_{kl}^{-1}(-\mathrm{i}\nabla_k)\cdot(-\mathrm{i}\nabla_l) + r_{kl}^{-3}\mathbf{r}_{kl}\cdot(\mathbf{r}_{kl}\cdot-\mathrm{i}\nabla_k)(-\mathrm{i}\nabla_l)]$$

$$g_{kl}(\mathrm{so+so'}) = \alpha^2[-(r_{kl}^{-3}\mathbf{r}_{kl}\times-\mathrm{i}\nabla_k)\cdot\mathbf{s}_k + (2r_{kl}^{-3}\mathbf{r}_{kl}\times-\mathrm{i}\nabla_l)\cdot\mathbf{s}_k$$
$$+ (r_{kl}^{-3}\mathbf{r}_{kl}\times-\mathrm{i}\nabla_l)\cdot\mathbf{s}_l - (2r_{kl}^{-3}\mathbf{r}_{kl}\times-\mathrm{i}\nabla_k)\cdot\mathbf{s}_l]$$

$$g_{kl}(\mathrm{css'}) = -(\tfrac{16}{3})\pi\alpha^2\,(\mathbf{s}_k\cdot\mathbf{s}_l)\,\delta(\mathbf{r}_{kl})$$

$$g_{kl}(\mathrm{ss'}) = 2\alpha^2 r_{kl}^{-3}[\mathbf{s}_k\cdot\mathbf{s}_l - 3r_{kl}^{-2}(\mathbf{s}_k\cdot\mathbf{r}_{kl})(\mathbf{s}_l\cdot\mathbf{r}_{kl})]' \qquad g_{kl}(\mathrm{cd}) = -2\pi\alpha^2\,\delta(\mathbf{r}_{kl}) \,. \tag{2d}$$

Here, $\mathbf{r}_k$ is a vector pointing from the nucleus to the kth electron, $\mathbf{r}_{kl} = \mathbf{r}_k - \mathbf{r}_l$, and $\mathbf{s}_k$ is the spin vector of the kth electron. The prime bracket in $g_{kl}(\mathrm{ss'})$, when used in an integral over position space, is to be replaced by zero for $r_{kl} < \epsilon$. The integral is then evaluated, and the limit taken [3] as $\epsilon \to 0$. It is not necessary to perform this limiting process numerically if the form of the one-electron spin-orbitals is that described in this paper. In the orbit-orbit operator,

$$\boldsymbol{a}\cdot(\boldsymbol{a}\cdot\boldsymbol{b})\boldsymbol{c} \quad \text{means} \quad \sum_{i=1}^{3}\sum_{j=1}^{3} a_i a_j b_j c_i$$

where the subscripts refer to Cartesian components of the vector. Only the Hermitian part of $f_k(\mathrm{cd})$ and $g_{kl}(\mathrm{cd})$ is given in (2c) and (2d). The operators f_k and g_{kl} are such that the total angular momentum J^2, its projection J_z, and parity commute with H.

The atomic wavefunctions, ψ, and energies, E, are found by solving the time-dependent Schrödinger equation for the Hamiltonian given in (1) and (2)

$$H\psi = E\psi \ . \tag{3}$$

The wavefunction is expanded in single configuration functions which are eigenstates of S^2, L^2, J^2, J_z and parity. All configurations in the expansion have a closed core and two valence spin-orbitals; configurations with core holes and continuum configurations are neglected. Denoting the approximation to ψ by Ψ, we have

$$\Psi(\epsilon, J, P) = \sum_{n^1l^1n^2l^2} \sum_{S,L} \alpha_{\epsilon JP}(n^1l^1n^2l^2SL)\ \chi(n^1l^1n^2l^2SLJ) \tag{4}$$

where

$$\chi(n^1l^1n^2l^2SLJ) = (-1)^{S+L+M_J}\,(2J+1)^{\frac{1}{2}} \sum_{M_S=-S}^{+S} \begin{pmatrix} S & L & J \\ M_S & M_J-M_S & -M_J \end{pmatrix} \zeta(n^1l^1n^2l^2SL, M_J-M_S, M_S) \tag{5}$$

and

$$\zeta(n^1l^1n^2l^2SL, M_J-M_S, M_S) = (-1)^{l^1+l^2+M_J}\,[2(2S+1)(2L+1)/N(n^1l^1n^2l^2)]^{\frac{1}{2}}$$
$$\times \sum_{m_S^1=-\frac{1}{2}}^{+\frac{1}{2}} \sum_{m^1=-l^1}^{+l^1} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S \\ m_S^1 & M_S-m_S^1 & -M_S \end{pmatrix} \begin{pmatrix} l^1 & l^2 & L \\ m^1 & -m^1+M_J-M_S & M_S-M_J \end{pmatrix} \Phi(n^1l^1m^1m_S^1; n^2l^2, -m^1+M_J-M_S, M_S-m_S^1) \tag{6}$$

The Φ's are Slater determinants ordered according to the convention adopted in Condon and Shortley [5]. Their elements have the form

$$r_k^{-1}\ P(n^il^i, r_k)\ Y_{l^im^i}(\theta_k, \phi_k)\ \eta_{m_s^i}(s_k) \tag{7}$$

and they constitute an orthonormal set, i.e.

$$\int_0^\infty dr_k\, P(n^il^i, r_k)\, P(n^jl^j, r_k) = \delta_{n^i,n^j} \qquad \text{when } l^i = l^j \ .$$

In (6),

$$N(n^1l^1n^2l^2) = 2 \text{ when } n^1l^1 \neq n^2l^2 \ ; \qquad N(n^1l^1n^2l^2) = 4 \text{ when } n^1l^1 = n^2l^2 \ . \tag{8}$$

The quantities $\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}$ are Wigner $3j$ symbols whose properties are given by Edmonds [6]. χ is an eigenstate of J_z with eigenvalue M_J (the argument M_J is supressed in (4) and (5) because the energy does not depend on this quantity). The properties of the $3j$ symbols in (5) and (6) require that: (i) $S = 0, 1$; (ii) $|l^1-l^2| \leq L \leq |l^1+l^2|$; and (iii) $|L-S| \leq J \leq |L+S|$.

The unknowns in $\Psi(\epsilon, J, P)$ are the radials, $P(nl, r)$, and the expansion coefficients, $\alpha_{\epsilon JP}$. The $P(nl, r)$ are obtained from Lindgren's [7] modification of the Hartree-Fock-Slater [8] equation

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r)\right] P(nl, r) = \epsilon_{nl}\, P(nl, r) \tag{9}$$

where for $r < r_0$

$$V(r) = -\frac{2Z}{r} + \frac{2}{r}\int_0^r \sum_{nl} b_{nl}[P(nl,t)]^2\,dt + 2\int_r^\infty \sum_{nl} b_{nl}[P(nl,t)]^2 t^{-1}\,dt - C\left\{\frac{81}{4\pi^2} r^{n-3}\left[\sum_{nl} b_{nl}P^2(nl,r)\right]^m\right\}^{\frac{1}{3}}; \tag{10}$$

and for $r \geq r_0$

$$V(r) = -2(Z-N+1)/r\ . \tag{11}$$

The value of r for which (10) and (11) are equal is r_0, and b_{nl} is the number of times the nl subshell appears in the configuration from which $V(r)$ is constructed. Continuum configurations can be constructed from solutions of (9) corresponding to positive ϵ_{nl}. The Coulombic tail of the potential, first introduced by Latter [9], produces compact bound radials which facilitate the rapid convergence of the expansion [1].

The radials, $P(nl,r)$, are known and the wavefunction, $\Psi(\epsilon,J,P)$, is normalized to unity. By applying the variational principle we obtain the secular equation

$$|H_{ij} - E\delta_{i,j}| = 0 \tag{12}$$

where i or j refers to a particular value of $n^1l^1n^2l^2SLJ$. Solving this equation is equivalent to diagonalizing the energy matrix, H_{ij}.

In table 1 we present expressions for an arbitrary matrix element between the symbolic configurations $n^1l^1n^2l^2$ and $\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2$ in terms of four quantities, three of which are listed below. The fourth quantity E(core), appears only in H_{ii} and is independent of i, since all radials are generated from the same $V(r)$. Removing E(core) from the secular equation by redefining the energy eigenvalues averts a possible source of large numerical error. For example, E(core) for Hg I is 20 000 times larger than the rest of H_{ii}. We will now define the quantities in Table 1.

The quantity I is given by

$$I(n^1l^1\bar{n}^1\bar{l}^1) = I_{\rm nr}(n^1l^1\bar{n}^1\bar{l}^1) + I_{\rm mass}(n^1l^1\bar{n}^1\bar{l}^1) + I_{\rm so}(n^1l^1\bar{n}^1\bar{l}^1) + I_{\rm cd}(n^1l^1\bar{n}^1\bar{l}^1) \tag{13}$$

where

$$I_{\rm nr}(n^1l^1\bar{n}^1\bar{l}^1) = -\delta_{l^1,l^1}\delta_{L,L}\delta_{S,S}\int_0^\infty dr\, P(n^1l^1,r)\left[\frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l^1(l^1+1)}{r^2}\right]P(\bar{n}^1\bar{l}^1,r)\ ; \tag{14}$$

$$I_{\rm mass}(n^1l^1\bar{n}^1\bar{l}^1) = -\frac{\alpha^2}{4}\delta_{l^1,\bar{l}^1}\delta_{S,S}\delta_{\bar{L},L}\int_0^\infty dr\, P(n^1l^1,r)\,P(\bar{n}^1\bar{l}^1,r)\,[\epsilon_{n^1l^1} - V(r)]\,[\epsilon_{\bar{n}^1\bar{l}^1} - V(r)]\ ; \tag{15}$$

$$I_{\rm so}(n^1l^1\bar{n}^1\bar{l}^1) = -(-1)^{l^1+l^x+L+\bar{L}+J} Z\alpha^2\,\delta_{l^1,\bar{l}^1}\left[\tfrac{3}{2}(2S+1)(2L+1)(2\bar{S}+1)(2\bar{L}+1)l^1(l^1+1)(2l^1+1)\right]^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix}\begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix}\begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix}\int_0^\infty dr\, R(n^1l^1,r)\frac{1}{r}R(\bar{n}^1\bar{l}^1,r)\ ; \tag{16}$$

$$I_{\rm cd}(n^1l^1\bar{n}^1\bar{l}^1) = \tfrac{1}{4}Z\alpha^2\,\delta_{\bar{S},S}\delta_{\bar{L},L}\delta_{l^1,\bar{l}^1}\delta_{l^1,0}\,R(n^1l^1,0)\,R(\bar{n}^1\bar{l}^1,0)\ . \tag{17}$$

In the above it is assumed that $P(n^1l^1,r)$ and $P(\bar{n}^1\bar{l}^1,r)$ have been obtained from (9) and that they have been generated from the same $V(r)$. To evaluate $R(nl,0)$, we use the small r expression, $R(nl,r) = A_{nl}r^l\{1 - Zr/(l+1)\}$, where A_{nl} is a constant. The quantity $\{\begin{smallmatrix} a & b & c \\ d & e & f \end{smallmatrix}\}$ is a Wigner $6j$ symbol [6] and $R(nl,r) = r^{-1}P(nl,r)$.

The A term is given by

$$A(n^1l^1\bar{n}^1\bar{l}^1) = A_{\rm nr}(n^1l^1\bar{n}^1\bar{l}^1) + A_{\rm oo'}(n^1l^1\bar{n}^1\bar{l}^1) + A_{\rm so+so'}(n^1l^1\bar{n}^1\bar{l}^1) + A_{\rm cd+css'}(n^1l^1\bar{n}^1\bar{l}^1) + A_{\rm ss'}(n^1l^1\bar{n}^1\bar{l}^1)\ . \tag{18}$$

In (18)

$$A_{\rm nr}(n^1l^1\bar{n}^1\bar{l}^1) = \delta_{l^1,\bar{l}^1}\delta_{\bar{S},S}\delta_{\bar{L},L}\sum_{n^kl^k}(\text{core})(2l^k+1)$$

$$\times\left[2R^0(n^kl^kn^1l^1;n^kl^k\bar{n}^1\bar{l}^1) - \sum_{l=0}^{\infty}\begin{pmatrix} l^1 & l & l^k \\ 0 & 0 & 0\end{pmatrix}^2 R^l(n^1l^1n^kl^k;n^kl^k\bar{n}^1\bar{l}^1)\right] \tag{19}$$

where

$$R^l(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = 2\int_0^\infty\int_0^\infty \frac{r_<^l}{r_>^{l+1}}P(n^1l^1,r_1)\,P(n^2l^2,r_2)\,P(\bar{n}^1\bar{l}^1,r_1)\,P(\bar{n}^2\bar{l}^2,r_2)\,dr_1\,dr_2\,; \tag{20}$$

$$A_{oo'}(n^1l^1\bar{n}^1\bar{l}^1) = -\delta_{S,\bar{S}}\delta_{L,\bar{L}}\delta_{l^1,\bar{l}^1}\sum_{n^kl^k}(\text{core})(2l^k+1)(1-\delta_{l^1+l^k,0})\left\{\sum_{z>0}\begin{pmatrix} l^1 & z & l^k \\ 0 & 0 & 0\end{pmatrix}^2\right.$$

$$\times\Big[z(z+1)[-T^{z+1}(1k;k\bar{1}) + T^{z-1}(1k;k\bar{1})] + (1-\delta_{l^k,0})[z(z+1) + l^k(l^k+1) - l^1(l^1+1)]$$

$$\times[U^{z+1}(1k;k\bar{1}) - U^{z-1}(1k;k\bar{1})] + (1-\delta_{l^1,0})[z(z+1) + l^1(l^1+1) - l^k(l^k+1)][U^{z+1}(k1;\bar{1}k) - U^{z-1}(k1;\bar{1}k)]$$

$$+ (1-\delta_{l^1,0})(1-\delta_{l^k,0})\frac{1}{z(z+1)}[l^1(l^1+1) - l^k(l^k+1) - z(z+1)][l^k(l^k+1) - l^1(l^1+1) - z(z+1)]$$

$$\times\Big[\frac{z(z+3)}{2z+3}[N^z(k1;\bar{1}k) + N^z(1k;k\bar{1})] - \frac{(z+1)(z-2)}{2z-1}[N^{z-2}(k1;\bar{1}k) + N^{z-2}(1k;k\bar{1})]\Big]\Big]$$

$$- 2(1-\delta_{l^1,0})(1-\delta_{l^k,0})\sum_{z>0}\frac{1}{z(z+1)}\begin{pmatrix} l^1 & z-1 & l^k \\ 0 & 0 & 0\end{pmatrix}^2$$

$$\times(l^1+l^k+z+1)(l^1-l^k+z)(l^k-l^1+z)(l^1+l^k-z+1)[N^{z-1}(1k;k\bar{1}) + N^{z-1}(k1;\bar{1}k)]\Big\} \tag{21}$$

where

$$T^{z+1}(ab;cd) = \frac{\alpha^2}{2z+3}\int_0^\infty r_1^2\,dr_1\int_0^\infty r_2^2\,dr_2\,R(n^al^a,r_1)R(n^bl^b,r_2)\frac{r_<^{z+1}}{r_>^{z+2}}\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}R(n^cl^c,r_1)\,R(n^dl^d,r_2) \tag{22}$$

and

$$U^{z+1}(ab;cd) = \frac{\alpha^2}{2(2z+3)}\int_0^\infty r_1^2\,dr_1\int_0^\infty r_2^2\,dr_2\,R(n^al^a,r_1)\,R(n^bl^b,r_2)\frac{1}{r_1}\frac{r_<^{z+1}}{r_>^{z+2}}$$

$$\times[z\,\epsilon(r_1-r_2) - (z+3)\,\epsilon(r_2-r_1)]\frac{\partial}{\partial r_2}R(n^cl^c,r_1)\,R(n^dl^d,r_2) \tag{23}$$

and

$$N^{z-1}(ab;cd) = \frac{\alpha^2}{4}\int_0^\infty dr_1\int_0^\infty dr_2\,r_1^2r_2^2\,R(n^al^a,r_1)\,R(n^bl^b,r_2)\frac{r_2^{z-1}}{r_1^{z+2}}\epsilon(r_1-r_2)\,R(n^cl^c,r_1)\,R(n^dl^d,r_2)\,; \tag{24}$$

$$A_{so+so'}(n^1l^1\bar{n}^1\bar{l}^1) = (-1)^{L+\bar{L}+J+l^x+l^1}\delta_{l^1,\bar{l}^1}[(2S+1)(2L+1)(2\bar{S}+1)(2\bar{L}+1)]^{\frac{1}{2}}$$

$$\times \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix} 4[6l^1(l^1+1)(2l^1+1)]^{\frac{1}{2}} \begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix} \sum_{n^k l^k} (\text{core})(2l^k+1)\, N^0(1k;\bar{1}k)$$

$$+ (-1)^{l^x+l^1+L+\bar{L}+J}[(2S+1)(2\bar{S}+1)(2L+1)(2\bar{L}+1)]^{\frac{1}{2}} \tfrac{3}{2}\sqrt{6}\,\alpha^2\delta_{l^1,\bar{l}^1}(2l^1+1) \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix} \begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix}$$

$$\times \sum_{n^k l^k} (\text{core})(2l^k+1) \sum_{z>0} [z(z+1)(2z+1)]^{\frac{1}{2}} \begin{pmatrix} l^1 & z & l^k \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} l^1 & l^1 & 1 \\ z & z & l^k \end{Bmatrix} [V^{z-1}(1k;k\bar{1}) - V^{z-1}(k1;\bar{1}k)]$$

$$+ (-1)^{L+\bar{L}+l^x+l^1+J}[(2S+1)(2\bar{S}+1)(2L+1)(2\bar{L}+1)]^{\frac{1}{2}} \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix} \delta_{l^1,\bar{l}^1} \begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix}$$

$$\times 3\sqrt{6}(2l^1+1) \sum_{n^k l^k} (\text{core})(2l^k+1) \sum_{z>0} \left[\frac{2z+1}{z(z+1)}\right]^{\frac{1}{2}} \begin{pmatrix} l^1 & z & l^k \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} l^1 & l^1 & 1 \\ z & z & l^k \end{Bmatrix} \Big\{[l^1(l^1+1) - l^k(l^k+1) - z(z+1)]$$

$$\times [zN^z(1k;k\bar{1}) - (z+1)N^{z-2}(k1;\bar{1}k)] - [l^k(l^k+1) - l^1(l^1+1) - z(z+1)]\,[zN^z(k1;\bar{1}k) - (z+1)N^{z-2}(1k;k\bar{1})]\Big\}$$

$$- (-1)^{l^1+l^x+L+\bar{L}+J}[(2S+1)(2L+1)(2\bar{S}+1)(2\bar{L}+1)]^{\frac{1}{2}}\delta_{l^1,\bar{l}^1} \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix} \begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix}$$

$$\times 6\sqrt{6}(2l^1+1)[l^1(l^1+1)(2l^1+1)]^{\frac{1}{2}} \sum_{n^k l^k} (\text{core})(2l^k+1) \sum_{z>0} \frac{(2z+1)(2z-1)}{z+1}$$

$$\times \begin{pmatrix} l^1 & z-1 & l^k \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} l^1 & l^1 & 1 \\ z-1 & z & l^k \end{Bmatrix}^2 [N^{z-1}(1k;k\bar{1}) + N^{z-1}(k1;\bar{1}k)] \tag{25}$$

where

$$V^{z-1}(ab;cd) = \int_0^\infty dr_1 \int_0^\infty dr_2\, r_1^2 r_2^2\, R(n^a l^a, r_1)\, R(n^b l^b, r_2) \frac{r_<^{z-1}}{r_>^{z+2}} r_2 \frac{dR(n^c l^c, r_1)}{dr_1} R(n^d l^d, r_2)\,; \tag{26}$$

$$A_{cd+css'}(n^1l^1\bar{n}^1\bar{l}^1) = \frac{\alpha^2}{2}\delta_{l^1,\bar{l}^1}\delta_{\bar{L},L}\,\delta_{\bar{S},S} \sum_{n^k l^k} (\text{core})(2l^k+1) \int_0^\infty r^{-2}\,dr\, P(n^1l^1,r)\, P(\bar{n}^1\bar{l}^1,r)\, P^2(n^k l^k,r)\,; \tag{27}$$

$$A_{ss'}(n^1l^1\bar{n}^1\bar{l}^1) = 0\,. \tag{28}$$

In the above, $\bar{1}$ refers to $\bar{n}^1\bar{l}^1$, $r_<$ is the smaller of r_1 and r_2, and $\epsilon(r_1-r_2) = 1$ if $r_1 \geq r_2$ and is zero otherwise. In (16) and (25), l^x is the azimuthal quantum number common to the two valence subshells not appearing as arguments in I or A (see Table 1).

To simplify presentation of the quantity E, let

$$E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = E^{\mathrm{I}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) + E^{\mathrm{II}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) \ . \tag{29}$$

By multiplying $E^{\mathrm{I}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)$ by $(-1)^{\bar{S}+\bar{L}+\bar{l}^1+\bar{l}^2}$ and interchanging $\bar{n}^2\bar{l}^2$ and $\bar{n}^1\bar{l}^1$ ($\bar{l}^1$ and $\bar{l}^2$ are also interchanged) in the resulting product, $E^{\mathrm{II}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)$ is obtained. It should be noted that $N(n^1l^1n^2l^2) = N(n^2l^2n^1l^1)$, etc. (See eq. (8).) Thus

$$E^{\mathrm{I}} = E^{\mathrm{I}}_{\mathrm{nr}} + E^{\mathrm{I}}_{\mathrm{oo'}} + E^{\mathrm{I}}_{\mathrm{so+so'}} + E^{\mathrm{I}}_{\mathrm{cd+css'}} + E^{\mathrm{I}}_{\mathrm{ss'}} \tag{30}$$

where the common argument is $n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2$. In (30)

$$E^{\mathrm{I}}_{\mathrm{nr}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = \delta_{\bar{S},S}\,\delta_{\bar{L},L}\,(-1)^{l^1+\bar{l}^1+L}\left[\frac{4(2l^1+1)(2l^2+1)(2\bar{l}^1+1)(2\bar{l}^2+1)}{N(n^1l^1n^2l^2)\,N(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)}\right]^{\frac{1}{2}}$$

$$\times \sum_{l=0}^{\infty} \begin{pmatrix} l^1 & l & \bar{l}^1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l^2 & l & \bar{l}^2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l^1 & l^2 & L \\ \bar{l}^2 & \bar{l}^1 & l \end{Bmatrix} R^l(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) \ ; \tag{31}$$

$$E^{\mathrm{I}}_{\mathrm{oo'}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = -(-1)^L\,\delta_{\bar{S},S}\,\delta_{\bar{L},L}\left[\frac{4(2l^1+1)(2l^2+1)(2\bar{l}^1+1)(2\bar{l}^2+1)}{N(n^1l^1n^2l^2)\,N(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)}\right]^{\frac{1}{2}}$$

$$\times \Big\{(1-\delta_{1,\bar{1}})(1-\delta_{2,\bar{2}})\,(-1)^{l^1+\bar{l}^1}\sum_{k>0} \begin{pmatrix} l^1 & k & \bar{l}^1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l^2 & k & \bar{l}^2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l^1 & \bar{l}^1 & k \\ \bar{l}^2 & l^2 & L \end{Bmatrix}$$

$$\times \Big[\, k(k+1)\,[T^{k+1}(12;\bar{1}\bar{2}) - T^{k-1}(12;\bar{1}\bar{2})] + [l^1(l^1+1) - \bar{l}^1(\bar{l}^1+1) - k(k+1)]\,[U^{k+1}(12;\bar{1}\bar{2}) - U^{k-1}(12;\bar{1}\bar{2})]$$

$$+ [l^2(l^2+1) - \bar{l}^2(\bar{l}^2+1) - k(k+1)]\,[U^{k+1}(21;\bar{2}\bar{1}) - U^{k-1}(21;\bar{2}\bar{1})] + [l^1(l^1+1) - \bar{l}^1(\bar{l}^1+1) - k(k+1)]$$

$$\times [l^2(l^2+1) - \bar{l}^2(\bar{l}^2+1) - k(k+1)]\left\{\frac{-(k+3)}{(k+1)(2k+3)}\,[N^k(12;\bar{1}\bar{2}) + N^k(21;\bar{2}\bar{1})] + \frac{(k-2)}{k(2k-1)}\,[N^{k-2}(12;\bar{1}\bar{2}) + N^{k-2}(21;\bar{2}\bar{1})]\right\}\Big]$$

$$+ 2(-1)^{l^1+\bar{l}^1}\sum_{k>0}\frac{1}{k(k+1)} \begin{pmatrix} l^1 & k-1 & \bar{l}^1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l^2 & k-1 & \bar{l}^2 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l^1 & \bar{l}^1 & k \\ \bar{l}^2 & l^2 & L \end{Bmatrix} [(l^1+\bar{l}^1+k+1)(l^1-l^1+k)$$

$$\times (l^1-\bar{l}^1+k)(l^1+\bar{l}^1-k+1)(l^2+\bar{l}^2+k+1)(\bar{l}^2-l^2+k)(l^2-\bar{l}^2+k)(l^2+\bar{l}^2-k+1)]^{\frac{1}{2}}\,[N^{k-1}(12;\bar{1}\bar{2}) + N^{k-1}(21;\bar{2}\bar{1})]\Big\} \ ; \tag{32}$$

$$E^{\mathrm{I}}_{\mathrm{so+so'}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = \left[\frac{4(2l^1+1)(2l^2+1)(2\bar{l}^1+1)(2\bar{l}^2+1)}{N(n^1l^1n^2l^2)N(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)}\right]^{\frac{1}{2}}(-1)^{J+L+1+l^1+\bar{l}^2}\sqrt{6}\,[1+2(-1)^{\bar{S}+S}]$$

$$\times[(2S+1)(2L+1)(2\bar{S}+1)(2\bar{L}+1)]^{\frac{1}{2}}\begin{Bmatrix} S & \bar{S} & 1\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} S & L & J\\ \bar{L} & \bar{S} & 1\end{Bmatrix}\left\{\sum_{k>0}\left[\frac{2k+1}{k(k+1)}\right]^{\frac{1}{2}}\begin{pmatrix} l^1 & k & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l^2 & k & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} 1 & L & \bar{L}\\ k & l^1 & \bar{l}^1\\ k & l^2 & \bar{l}^2\end{Bmatrix}\right.$$

$$\times[\tfrac{1}{2}\alpha^2k(k+1)[V^{k-1}(12;\bar{1}\bar{2}) - (-1)^{\bar{S}+S}V^{k-1}(21;\bar{2}\bar{1})] + [l^1(l^1+1) - \bar{l}^1(\bar{l}^1+1) - k(k+1)][kN^k(12;\bar{1}\bar{2}) - (k+1)N^{k-2}(21;\bar{2}\bar{1})]$$

$$- (-1)^{\bar{S}+S}[l^2(l^2+1) - \bar{l}^2(\bar{l}^2+1) - k(k+1)][kN^k(21;\bar{2}\bar{1}) - (k+1)N^{k-2}(12;\bar{1}\bar{2})]] + 2\sum_{k>0}(2k+1)\,[2k-1]^{\frac{1}{2}}$$

$$\times\left[[\bar{l}^1(\bar{l}^1+1)(2\bar{l}^1+1)]^{\frac{1}{2}}\begin{pmatrix} l^1 & k-1 & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l^1 & \bar{l}^1 & k\\ 1 & k-1 & \bar{l}^1\end{Bmatrix}\left\{-(2k-1)^{\frac{1}{2}}\begin{pmatrix} l^2 & k-1 & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} \bar{l}^2 & l^2 & k-1\\ \bar{l}^1 & l^1 & k\\ \bar{L} & L & 1\end{Bmatrix}N^{k-1}(12;\bar{1}\bar{2})\right.\right.$$

$$+\left[\frac{k(2k+3)}{k+1}\right]^{\frac{1}{2}}\begin{pmatrix} l^2 & k+1 & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} \bar{l}^2 & l^2 & k+1\\ \bar{l}^1 & l^1 & k\\ \bar{L} & L & 1\end{Bmatrix}N^{k-1}(21;\bar{2}\bar{1})\Big\} + (-1)^{\bar{S}+S+\bar{L}+L}\,[\bar{l}^2(\bar{l}^2+1)(2\bar{l}^2+1)]^{\frac{1}{2}}$$

$$\times\begin{pmatrix} l^2 & k-1 & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l^2 & \bar{l}^2 & k\\ 1 & k-1 & \bar{l}^2\end{Bmatrix}\left\{-(2k-1)^{\frac{1}{2}}\begin{pmatrix} l^1 & k-1 & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} \bar{l}^1 & l^1 & k-1\\ \bar{l}^2 & l^2 & k\\ \bar{L} & L & 1\end{Bmatrix}N^{k-1}(21;\bar{2}\bar{1})\right.$$

$$\left.\left.+\left[\frac{k(2k+3)}{k+1}\right]^{\frac{1}{2}}\begin{pmatrix} l^1 & k+1 & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} \bar{l}^1 & l^1 & k+1\\ \bar{l}^2 & l^2 & k\\ \bar{L} & L & 1\end{Bmatrix}N^{k-1}(12;\bar{1}\bar{2})\right\}\right]\Bigg\}\ ; \tag{33}$$

$$E_{\mathrm{cd+css'}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = \alpha^2\left[\frac{4(2l^1+1)(2l^2+1)(2\bar{l}^1+1)(2\bar{l}^2+1)}{N(n^1l^1n^2l^2)N(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)}\right]^{\frac{1}{2}}\delta_{\bar{L},L}\,\delta_{\bar{S},S}\,\delta_{S,0}$$

$$\times\begin{pmatrix} l^1 & l^2 & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} \bar{l}^1 & \bar{l}^2 & L\\ 0 & 0 & 0\end{pmatrix}\int_0^\infty r^{-2}\,\mathrm{d}r\,P(n^1l^1,r)\,P(\bar{n}^1\bar{l}^1,r)\,P(n^2l^2,r)\,P(\bar{n}^2\bar{l}^2,r) \tag{34}$$

where the full contribution to E is given;

$$E^{\mathrm{I}}_{\mathrm{ss'}}(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2) = 4\left[\frac{5(2L+1)(2\bar{L}+1)(2l^1+1)(2l^2+1)(2\bar{l}^1+1)(2\bar{l}^2+1)}{N(n^1l^1n^2l^2)N(\bar{n}^1\bar{l}^1\bar{n}^2l^2)}\right]^{\frac{1}{2}}(-1)^{l^1+l^2+L+J}$$

$$\times\delta_{\bar{S},S}\delta_{S,1}\begin{Bmatrix} S & \bar{S} & 2\\ \bar{L} & L & J\end{Bmatrix}\sum_p(-1)^p\left[\frac{(2p+5)!}{(2p)!}\right]^{\frac{1}{2}}\left[\begin{pmatrix} l^1 & p & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l^2 & p+2 & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l^1 & \bar{l}^1 & p\\ l^2 & \bar{l}^2 & p+2\\ L & \bar{L} & 2\end{Bmatrix}N^p(21;\bar{2}\bar{1})\right.$$

$$\left.+(-1)^{L+\bar{L}}\begin{pmatrix} l^2 & p & \bar{l}^2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l^1 & p+2 & \bar{l}^1\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} l^2 & \bar{l}^2 & p\\ l^1 & \bar{l}^1 & p+2\\ L & \bar{L} & 2\end{Bmatrix}N^p(12;\bar{1}\bar{2})\right]. \tag{35}$$

In the above, $\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$ is a $9j$ symbol [6] and the quantity $\delta_{1,\bar{1}} = 1$ if $n^1l^1 = \bar{n}^1\bar{l}^1$ and $\delta_{1,\bar{1}} = 0$ if $n^1l^1 \neq \bar{n}^1\bar{l}^1$. This completes the definitions of the quantities appearing in Table 1.

Table 1

Expressions for the matrix element $(\chi(n^1l^1n^2l^2SLJ),\ H\chi(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2\bar{S}\bar{L}J)) = T$ in terms of I, A, and $E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)$.

1. When $n^1l^1 = \bar{n}^1\bar{l}^1$ and $n^2l^2 = \bar{n}^2\bar{l}^2$

$$T = E(\text{core}) + (-1)^{\bar{S}+S+\bar{L}+L}\,[I(n^2l^2n^2l^2) + A(n^2l^2n^2l^2)] + I(n^1l^1n^1l^1) + A(n^1l^1n^1l^1) + E(n^1l^1n^2l^2;n^1l^1n^2l^2)\,.$$

2. When $(n^1l^1n^2l^2) \neq (\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)$ [a]

$$T = E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)\,.$$

3. When $n^1l^1 \neq \bar{n}^1l^1$ and $n^2l^2 = \bar{n}^2l^2$

$$T = [N(n^1l^1n^2l^2)\,N(\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)/4]^{\frac{1}{2}}[I(n^1l^1\bar{n}^1\bar{l}^1) + A(n^1l^1\bar{n}^1\bar{l}^1)] + E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1n^2l^2)\,.$$

4. When $n^1l^1 = \bar{n}^1\bar{l}^1$ and $n^2l^2 \neq \bar{n}^2\bar{l}^2$

$$T = (-1)^{\bar{S}+S+\bar{L}+L}\,[N(n^1l^1n^2l^2)\,N(n^1l^1\bar{n}^2\bar{l}^2)/4]^{\frac{1}{2}}[I(n^2l^2\bar{n}^2\bar{l}^2) + A(n^2l^2\bar{n}^2\bar{l}^2)] + E(n^1l^1n^2l^2;n^1l^1\bar{n}^2\bar{l}^2)\,.$$

5. When $n^1l^1 \neq \bar{n}^2\bar{l}^2$ and $n^2l^2 = \bar{n}^1\bar{l}^1$

$$T = (-1)^{l^2+\bar{l}^2+\bar{S}+\bar{L}}\,[N(n^1l^1n^2l^2)\,N(n^2l^2\bar{n}^2\bar{l}^2)/4]^{\frac{1}{2}}[I(n^1l^1\bar{n}^2\bar{l}^2) + A(n^1l^1\bar{n}^2\bar{l}^2)] + E(n^1l^1n^2l^2;n^2l^2\bar{n}^2\bar{l}^2)\,.$$

6. When $n^1l^1 = \bar{n}^2\bar{l}^2$ and $n^2l^2 \neq \bar{n}^1\bar{l}^1$

$$T = (-1)^{l^1+\bar{l}^1+S+L}\,[N(n^1l^1n^2l^2)\,N(\bar{n}^1\bar{l}^1n^1l^1)/4]^{\frac{1}{2}}[I(n^2l^2\bar{n}^1\bar{l}^1) + A(n^2l^2\bar{n}^1\bar{l}^1)] + E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1n^1l^1)\,.$$

[a] e.g. $n^1l^1 \neq \bar{n}^1\bar{l}^1$ and $n^1l^1 \neq \bar{n}^2\bar{l}^2$

2. NUMERICAL METHODS AND ACCURACY

The numerical procedures can be divided into three basic parts: (i) self-consistent solution of (9); (ii) evaluation of the matrix elements given in Table 1, and (iii) diagonalization of the matrix and determination of the eigenvectors. A book on the self-consistent solution of (9), including a computer program, has been written by Herman and Skillman [10] (subprograms HRSK, SCHEQ, and CRØSYM, in a slightly modified form, formed their deck). Therefore, we will only briefly summarize the numerical methods used, assuming a familiarity with that book.

Two different meshes (X and R in Bohr units) are used as an independent variable. The X mesh, which is the same for all atoms, is given by

$$X(I) = 0.1(2^N-1) + 0.0025*2^N*(I - 40*N - 1) \quad (36)$$

where

$$N = (I-1)/40 \ . \quad (37)$$

In (37) the result is truncated to an integer. Within a block (fixed N) the mesh is linear, in going from one block to the next, the interval between two adjacent points is doubled. Each block has 40 points. A mesh of 601 points (15 blocks) is sufficient for the calculations described here. The relation between the R (independent variable r) and the X meshes is

$$R(I) = C*X(I) \quad (38)$$

where

$$C = (1/2)(3\pi/4)^{2/3}Z^{-(1/3)} \ . \quad (39)$$

If configuration interaction is to be included, a high degree of self-consistency is not critical. Consequently, the self-consistency requirement of Herman and Skillman (TØL = 0.001) was used.

In the SCHEQ subprogram the methods outlined by Hartree [11] as well as the Numerov [10] integration method are used to solve (9). Integrals are evaluated in SCHEQ and HRSK using the 6 point Newton-Cotes scheme [10] which is obtained from the forward interpolation formula of Newton [12] by integrating it over five intervals. The trial energy eigenvalue is adjusted in one of four ways [10] until the ratio of the change of the eigenvalue to the eigenvalue drops below some threshold (THRESH). Assigning a value of 0.000 01 to THRESH produces sufficiently accurate results. A test made with THRESH = 0.000 000 1 and an X mesh obtained by halving the interval between two adjacent points in a block and doubling the number of points per block, had little effect on the results. Such a change will alter $V(r)$ slightly as well.

Kelly [13] has modified SCHEQ to include spatially diffuse radials of many nodes (up to 25s). The most spatially diffuse radial used by the authors [2], having the greatest number of nodes, was the 15s of Hg I. For this radial, the difference in the results obtained from the two versions of SCHEQ was insignificant. It appears that the basic difference between the two versions is in the way the trial energy is adjusted. Conceivably, a poor trial input for the energy might result in a failure of the original version of SCHEQ to solve the radial equation whereas Kelly's modified SCHEQ would achieve a solution. We decided to retain the original version, since it has been more thoroughly investigated. However, the modifications required to incorporate Kelly's changes into the program would be straightforward. We have found, for Ba I, that the inward integrations for certain d and f radials do not start at large enough values of r (Kelly [13] seems to have experienced a similar problem). This has been corrected by beginning the inward integrations at $(5 + 3l/2)$ times the matching radius for all radials except the 1s.

2.1. *Evaluation of the matrix elements*

In general, the numerical formulas used are accurate up to order h^6 (the spacing), which is the accuracy of the 5 point Newton-Cotes formula. Other formulas are used for points near the beginning and end of the mesh and in regions of "r-space" where block changes occur. Evaluation of $dR(nl, r)/dr$ is achieved (in BRIP) using a 7 point Stirling formula except for special mesh points. Derivatives for the second and third mesh points are obtained by differentiating the 7 point Newton forward interpolation formula. For the first mesh point ($r=0$), we differentiate the analytic expression for $R(nl, r)$: $A_{nl}\, r^l[1 - Zr/(l+1)]$. Due to the large number of subtractions occurring, the numerical differentiation results are, in general, less accurate than the integration results. However, the integrals containing derivatives do not comprise the major contributions to the matrix elements. We have evaluated

$$\int_0^\infty dr\, R(6p, r)\, \frac{dR(7p, r)}{dr}$$

and

$$-\int_0^\infty dr\, R(7p, r)\, \frac{dR(6p, r)}{dr} \quad \text{(for Tl II)}$$

and found that the results differ by 1.4%. The

authors feel that the present differentiation accuracy is satisfactory, but suggest that if numerical inaccuracies are suspected, the differentiation process should be re-examined.

Single integrals of the form

$$\int_0^\infty dr\, f(r)$$

are evaluated (by SINT) using the 5 point Newton-Cotes formula. Integration ceases when the integrand is zero (ICUT) or when the end of the mesh is reached. Radials and their derivatives are assumed to be zero beyond the NKKKth mesh point.

The outer integration of the double integral

$$\int_0^\infty f(r)\, dr \int_0^r g(s)\, ds$$

is performed by SINT. Subprogram DINTI does the inner integrations required, using the 5 point Newton-Cotes formula for most values of r. To evaluate the inner integral for the three smallest values of r ($r=0$ excluded), we integrate the 5 point Newton forward interpolation formula over one, two, and three intervals, which means we are sampling points having larger values of s than those included in the region of integration. Blocks are spanned by taking the larger spacing as the common one and dropping out certain points in the block having the smaller spacing. We also provide DINTI with information as to which mesh points f (ICUT7) and g (ICUT5) are first zero. If ICUT7 > ICUT5 then

$$\int_0^r g(s)\, ds = \int_0^{R(\mathrm{ICUT5})} g(s)\, ds$$

$$\text{for} \quad R(\mathrm{ICUT5}) \leq r \leq R(\mathrm{ICUT7}) .$$

This saves considerable computing time. Since the greatest share of the computing time is spent evaluating the double integrals, SINT, DINTI, DINTD need to be as efficient as possible.

To evaluate the inner integrations of

$$\int_0^\infty f(r)\, dr \int_r^\infty g(s)\, ds ,$$

a separate subprogram, DINTD, was designed. Use of DINTI and SINT

$$\text{(i.e. } \int_r^\infty g(s)\, ds = \int_0^\infty g(s)\, ds - \int_0^r g(s)\, ds\text{)}$$

to evaluate the inner integrals, yielded a result for $F^6(6f, 6f)$ (a special case of (20)) which was negative and thus clearly invalid. A test was made of DINTD using the mesh of (36) and a mesh in which the intervals were halved and the number of points per block was doubled. The results were in good agreement.

DINTD uses the 5 point Newton-Cotes formula except for special points. The upper limit is set equal to R(ICUT), the first point at which g is non-zero. Near the end of the mesh, the inner integral is evaluated by integrating the 5 point backward Newton interpolation formula [12] over one, two, and three intervals. Blocks are spanned by taking the smaller spacing as the common one and obtaining the required additional points in the larger block using the 5 point Newton forward interpolation formula. The integrations are then performed using either the 5 or the 6 point Newton-Cotes formula (whichever requests an integral already evaluated).

In addition to the evaluation of the radial integrals described above, various angular terms are needed to compute the matrix elements of Table 1. The $3j$ symbols are calculated (in BRIP) using Edmonds' [6] Table 2. For the arguments of the Wigner nj (n = 3, 6, 9) symbols encountered, the digit capacity of the CDC 6400 and 6600 allows direct, accurate calculation of the symbols. Subprograms W6J and W6JB calculate the $6j$ symbol, while W9J calculate the $9j$ symbol. All three are limited to integer arguments. Explicit values are used for all symbols containing half-integer arguments (i.e. those associated with the spin quantum numbers). If any argument of the $6j$ symbol is zero, then we use eq. (6.3.2) of Edmonds [6]; if any argument is one, we use Table 5 of Edmonds. If neither condition is satisfied, then eq. (6.3.7) (the general formula) of Edmonds is used. Whenever possible, the $6j$ symbols are arranged so that their lowest argument falls in the second row, first column (lower left hand corner); this speeds up computation of the symbol.

If any argument of the $9j$ symbol is zero, we use eq. (6.4.14) of Edmonds. All other $9j$ symbols using Edmonds' eq. (6.4.3). The evaluation of a $9j$ symbol requires, on the average, 0.05 sec of computing time. A rapid computational technique originated by Caswell and Maximon [14] is used. There are six different arrangements of the $9j$ symbol arguments (the value of the $9j$ symbol differing at most by a phase factor) which give different combinations of $6j$ symbols appearing in Edmonds' eq. (6.4.3). The arrangement giving the least number of expansion terms is used (it is automatically computed by W9J).

The number of terms can differ considerably with the arrangement used [14]. If the user desires to compute $6j$ or $9j$ symbols with large arguments (>10), then the methods [14] by which the sums are cut off in eqs. (6.3.7) and (6.4.3) of Edmonds are of interest (overflow may occur without such cutoffs). The $6j$ symbol of (31) and the $9j$ symbols of (35) were evaluated for various arguments and the results were in good agreement with the results obtained analytically.

2.2. *Diagonalization*

Householder's method [15] is used to reduce the matrix to tridiagonal form. The eigenvalues are then isolated using Sturm sequencing [15] and the eigenvectors are found by Wilkinson's [15] method.

Two checks are provided in the program to test the output of MLEW. The first check compares the trace and the sum of the eigenvalues and the second check compares $H\Psi/E$ to Ψ for a chosen (IMPVEC) eigenvector. A second diagonalizer ‡ has been used to test MLEW and the results are in good agreement.

3. PROGRAM STRUCTURE

Except for the Herman and Skillman subprograms [10], the structure of the program is simple. The only complexity is one of detail arising from the nature of the theoretical results. In Table 2, information is provided on the subprogram flow from which flow chart may be constructed. The program is in two parts. The first part, whose central subprogram is HRSK, solves (9) self-consistently. The second segment, whose central program is BRIP, calculates and diagonalizes the energy matrix H_{ij}. Except for the sharing of subprograms SCHEQ and CRØSYM and common storage (see Tables 3 and 4), the two segments are independent. The internal flow of the first segment has been adequately described by Herman and Skillman [10]. The flow in the BRIP subprogram is outlined in the following paragraphs.

The factorials are calculated and stored in common block WIGNER. They are used in subprograms W6JB and W9J. Next, the $3j$ symbols are calculated and stored. Then the extra radials (those not found in the first segment) are obtained, using SCHEQ, and stored. Next, all the derivatives, $dR(nl,r)/dr$, are calculated and

‡ Subprogram UNSYMEIG, CO-OP Class/Index Code: F4 WISC UNSYMEIG.

Table 2
Subprogram flow

Subprogram	Called by
HRSK	BETHE
SCHEQ	HRSK, BRIP
CRØSYM	HRSK, BRIP
CEI	BRIP
W9J	BRIP
TKUKX	BRIP
W6J	BRIP
W6JB	W9J, W6J
SINT	CEI, TKUKX, SNK, VBSUB1, CSSPIN, BRIP
DINTD	CEI, TKUKX, VKSUB1
DINTI	CEI, TKUKX, SNK, VKSUB1
SNK	BRIP
VKSUB1	BRIP
CSSPIN	BRIP
BRIP	BETHE
ZERØ	HRSK, SCHEQ, VKSUB1, BRIP
SECØND	BRIP
MLEW	BRIP

stored (none were calculated in the first segment).

In subprogram BRIP the area spanned by DØ LØØPS "77" and "7004" (DØ LØØP's are designated by the statement number appearing in the DØ statement) calculates all the energy matrix elements needed. We determine which two χ's (see eq. (5)) are involved in the matrix element. This is equivalent to determining the configurations and values of $S, L, \bar{S}, \bar{L}$ used. By comparing the two configurations, we find the entry of Table 1 which must be evaluated. Depending on the nature of the entry, the program decides how many of the quantities $I(n^1l^1\bar{n}^1\bar{l}^1)$, $A(n^1l^1\bar{n}^1\bar{l}^1)$, $E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)$ must be evaluated and what their arguments are. There are six areas positioned inside the DØ LØØPS (to save computing time) that are responsible for the calculation of the non-relativistic and relativistic contributions to I, A, and E. These areas call subprograms to evaluate the double integrals, $6j$ and $9j$ symbols. Depending upon the nature of the specific entry in Table 1 the program flow is directed to one of the six areas. After the calculation is completed, control passes back and another non-relativistic or relativistic contribution to I, A, or E is evaluated. This process continues until all contributions to the matrix element H_{ij} have been obtained. Then calculation of a new matrix element begins. After DØ LØØPS "77" and "7004" have been exhausted, the H_{ij} matrix is diagonalized and the eigenvectors and eigenvalues are found. Control then passes back to the main program, BETHE, which exits.

Table 3
Arrangement of unlabelled common.

Name	Relative address	Function
RSCØRE(601)		core part of charge density
XNUM(601)	0	numerator of Pratt formula
RSVALE(601)		valence part of charge density
DENM(601)	602	denominator of Pratt formula
RU2(601)	1203	input potential ($U(r)$ or $rV(r)$)
SNLØ(601)		work area for $P(nl, r)$
RDER(13000)	1804	derivatives of $R(nl, r) = r^{-1} P(nl, r)$
RU(601)	2405	$rV(r)$ where $V(r)$ is the HFS potential
RUEXCH(601)	3006	atomic exchange potential
XI(601)	3607	Coulomb part of output $rV(r)$
XJ(601)	4208	entire output $rV(r)$
RSATØM		total charge density
QQ(601)	4809	$V(r) + l(l+1)/r^2 - \epsilon_{nl}$
RUINL1(601)	5410	input $rV(r)$, I-1 iteration
RUFNL1(601)	6011	output $rV(r)$, I-1 iteration
RUINL2(601)	6612	input $rV(r)$, I iteration
RUFNL2(601)	7213	output $rV(r)$, I iteration
RU3(601)	7814	second input potential (for interpolation)
WWNL(30)	8415	occupation numbers of subshells
X(601)	8445	independent variable (from Thomas Fermi theory)
GNU(4, 5)	9046	work area for calculation of PSLØPE and interpolation

Table 4
Arrangement of labelled common.

Name	Relative address	Function
	Common Block BREIT	
R(601)	0	independent variable r; $R(I) = C*X(I)$
SNL(13000)	602	the $P(nl, r)$
NKKK(30)	13602	the number of non-zero calculated mesh points for each radial
MTAB7(30)	13632	the first point of the Ith radial is in the MTAB7(I)th location of SNL
V(601)	13662	the HFS potential, $V(r)$
NNLZ(30)	14263	$100*n+10*l$ where n and l are the principal and azimuthal quantum numbers of the subshell
EE(30)	14293	the eigenvalues of the HFS equation; negative for bound states
PSLØPE(30)	14323	$(P(nl, r)/r^{l+1})$ at $r = 0$
Z	14353	nuclear charge
C	14354	factor to convert from X to R mesh
THRESH	14355	eigenvalue accuracy criterion
NCSPVS	14356	total number of radials desired
MESH	14357	number of points in X and R meshes
	Common Block WIGNER	
FACT(31)	0	the factorials, 0-30

3.1. *Restrictions on program use*

The program requires $141\,000_8$ high speed core locations, at 60 bits per word. The 32 bits per word of the IBM 360 may not suffice ‡. This can be checked by redoing the test run given here on the IBM 360. The total computing time required depends on (i) the size of the expansion (ii) the number of subshells in the core and (iii) whether or not the two-body relativistic operators are included. In practice, the amount of computing time needed on a CDC 6400 ranges from a few minutes to 3/2 hours. For large runs with all operators present, about 90% of the time is spent in setting up the H_{ij} matrix (evaluation of the double integrals and $9j$ symbols is responsible for most of this). To estimate the time needed for a calculation with many expansion terms, the same calculation can be performed with a smaller number of expansion terms (see the test run results). This permits the calculation of the time required per matrix element. By multiplying this time and the number of independent matrix elements together (N.B.: H_{ji} is found by setting it equal to H_{ij}), one can obtain a fairly reliable time estimate.

No radial or derivative may have more than 601 mesh points. The DIMENSIØN statements in tables 3 and 4, as well as the dimensions of the arrays A and B of subprograms SINT, DINTI, and DINTD and the dimension of the array H (block spacings) contain this restriction.

There can be a total of only 30 radials and 19 non-core radials (core radials are those common to all configurations). The arrays ZARI, ZARA, BTHA, and BTHI and Tables 3 and 4 contain these limitations. The size of arrays SNL and RDER is determined by the number of radials and radial derivatives, and the number (NKKK) of mesh points for which each radial and its derivative is calculated to be non-zero. The present dimension of SNL and RDER, 13 000, appears suitable for systems of up to 80 electrons (e.g. Hg I). If this dimension is exceeded, the instruction on card 1806 will abort the job (very little time will be wasted).

The present program can handle configurations comprised of a closed core and two valence spin-orbitals. No general provisions have been made for configurations comprised of a closed core, 1 hole, and 1 electron, although these may be handled on a special-case basis. It appears that configurations with holes in p, d, and f subshells will often contribute significantly to the energy eigenvalues. Such configurations will not have the same E(core) as the configurations having a closed core and two valence spin-orbitals. If we denote their core energy as E'(core), then E'(core) - E(core) must be added to their diagonal matrix element. Calculation of this quantity involves the subtraction of two large numbers and consequently additional accuracy will be lost. For example, it was found that the $5d^9 6s^2 6p$ configuration must [2] be added to the odd parity Tl II expansions.

Only subshells having s, p, d, or f azimuthal quantum numbers are permitted in the program because of the limited number of factorials and $3j$ symbols generated. The extension to g or higher azimuthal quantum numbers is straightforward but space consuming. The storage of the radial integrals of (24) in VEC would have to be altered. The largest factorials needed in the calculation of $3j$, $6j$, and $9j$ symbols can be determined using the methods of Caswell and Maximon [14].

Calculations have been made only for expansion terms with total L's ≤ 3, i.e., S, P, D, and F term values. The program can handle total L's ≤ 6 (which is the largest L that an ff' configuration can produce). The dimensions of the NUR1 and NUR2 arrays limit the number of configurations to 20. The dimensions of the arrays HAM, HAM5, VEC, EIG, and JSL limit the size of the matrix to 35×35. This limitation is also expressed on cards 2313 and 2914.

ZARI stores $I_{nr}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (14)], ZARA stores $A_{nr}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (19)], BTHI(1, I) stores $\alpha^{-2} I_{\text{mass}}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (15)], BTHI(2, I) stores $\alpha^{-2} I_{\text{cd}}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (17)], BTHI(3, I) stores $Z[\frac{3}{2} l^1 (l^1+1)(2l^1+1)]^{\frac{1}{2}} \times$ the radial integral of $I_{\text{so}}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (16)], BTHA(1, I) stores $A_{\text{cd+css}'}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (27)], BTHA(2, I) stores $W^{-1} A_{\text{so+so}'}(n^1 l^1 \bar{n}^1 \bar{l}^1)$ [eq. (25)], where

$$W = (-1)^{L+\bar{L}+J+l^1+l^x} [(2S+1)(2L+1)(2\bar{S}+1)(2\bar{L}+1)]^{\frac{1}{2}} \times \begin{Bmatrix} S & \bar{S} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} L & \bar{L} & 1 \\ l^1 & l^1 & l^x \end{Bmatrix} \begin{Bmatrix} S & L & J \\ \bar{L} & \bar{S} & 1 \end{Bmatrix}$$

‡ Dr. John H. Wood, University of California at Los Alamos, New Mexico, has called to our attention that $F^0(1s, 2s)$ differed from $F^0(2s, 1s)$ when calculated using subroutine DINT described in ref. [1] on an IBM 7094. This problem does not exist with the present radial integration routines when used on a CDC-6600/6400. Moreover, the use of DINTI and DINTD should reduce, if not eliminate, the problem on a smaller-word-length computer.

and BTHA(3, I) stores $A_{00'}(n^1l^1\bar{n}^1\bar{l}^1)$ [eq. (21)]. It is thus possible to reconstruct the contribution that a particular operator makes to the $I(n^1l^1\bar{n}^1\bar{l}^1)$ and $A(n^1l^1\bar{n}^1\bar{l}^1)$ parts of any matrix element. However, the valence-valence parts of the matrix element $[E(n^1l^1n^2l^2;\bar{n}^1\bar{l}^1\bar{n}^2\bar{l}^2)]$ are neither printed out nor stored (there are just too many of them to make this practical). To determine the effect of a given operator on the eigenvalues and eigenvectors a complete new calculation must be done, deleting the operator under investigation. This is performed simply by setting the relevant NYCALC variable to zero. It is not possible to delete any non-relativistic operator. For Tl II, it was found [2] that the two-body relativistic operators were not very important. A substantial part of the computing time is due to the presence of these operators.

3.2. *Input and output*

Much of the input and output follows the program developed by Herman and Skillman [10]. Schematically, the input format is

		Card number
(1)	READ Heading Card	84
(2)	READ KEY, TØL, THRESH, MESH, IPRATT, MAXIT, KUT	91
(3)	READ IPUNCH, QC, QN, QM	93
(4)	IF KEY = 0, READ RU2(M), M = 1,437,4	124
	IF KEY = 1, READ RU3(M), M = 1,441	128
	IF KEY = 2, READ RU2(M), M = 1,441 and	118
	READ RU3(M), M = 1,441	119
(5)	READ Z, NCØRES, NVALES, IØN	132
(6)	READ NNLZ(I), WWNL(I), EE(I), I = 1, NCØRES+NVALES	146
(7)	READ JTØT, NØCØNF, NADSØ, NPRNT, IMPVEC, NCØRES, NVSE	1699
(8)	READ NYCALC(K2), K2 = 1, 7	1712
(9)	READ NUR1(K2), NUR2(K2), K2 = 1, NØCØNF	1725
(10)	READ NNLZ(K2), EE(K2), K2 = NCSPVS+1, NCSPVS+NADSØ	1767
(11)	READ MXSIZE, JSL(I4), I4 = 1, MXSIZE	1914

Entries (1)-(6) are read from HRSK, and the remaining entries are read from BRIP. There will rarely be more than 70 data cards. In the following paragraphs, selection of the data will be discussed. The information provided by Herman and Skillman [10] will not be repeated.

If the numerical atomic potential on a 441 mesh is known (from a previous run) read it in (KEY = 1). If this potential is unknown then read in a suitable [10] normalized atomic potential, $U(r)$, on a 110 mesh (KEY = 0). It has been our experience than when MESH is greater than 441, the HRSK subprogram may fail to function if the 110 mesh potential is used.

The authors have never used the KEY = 2 option.

NOTE ADDED IN PROOF: This possible failure may be averted by making the following changes to the version of the deck which is in the possession of Computer Physics Communications. Card 326 is removed and replaced with the cards:
RATIO = 1.0 and IF(RUZM .NE. XJ(LIMIT))
RATIO = (RUZM-RU(LIMIT))/(RUZM-XJ(LIMIT)).
have never used the KEY = 2 option.

TØL = 0.001 and THRESH = 0.00001 appear to be satisfactory for all runs. MESH is an estimate of the maximum number of mesh points required for the calculation. In the absence of definite information this should be set to 601; very little machine time will be wasted due to overestimation because all numerical processes stop once the last calculated point, NKKK, of $P(nl, r)$ and $dR(nl, r)/dr$ has been reached. We concur with the suggestion of Herman and Skillman and recommend that the user set IPRATT equal to 2. MAXIT can vary from 20 to 100 depending on how accurate the input potential is and what atomic system is being calculated (F^- takes about 100 iterations). We recommend that KUT be set equal to zero so that the Coulomb tail [9] is matched to $V(r)$ (see eq. (11)).

QC, QN, and QM correspond to the Lindgren [7] parameters C, n, m [eq. (10)]. With all parameters equal to 1, we have the normal [10] Hartree-Fock-Slater potential. With (C, n, m) = (0.8, 1.15, 1.0) we have the so-called universal potential of Lindgren [7]. This Lindgren potential is a useful trial potential for whatever atomic system is being investigated. With (C, n, m) = (2./3., 1.0, 1.0) we have the "two-thirds" potential [16]. Starting from the universal parameters, variations in C and n (it was never necessary to vary m) may be performed to determine which set of parameters gives the most rapid convergence rate of the expansion. For Hg I, the combinations (0.75, 1.12, 1.), (0.85, 1.18, 1.), (0.775, 1.135, 1.), and (0.7, 1.09, 1.) were used [2], the latter set being the best. A simple way

to choose improved Lindgren parameters is as follows: prepare the deck for a normal run, keeping the number of expansion terms to a minimum (use only the 4 or 5 most important). If relativistic calculations are to be made include only the one-body relativistic operators. For each set of parameters, compute E_2-E_1, where E_1 and E_2 are algebraically the two lowest eigenvalues. The set of parameters giving the result closest to the experimental measurement is used. The authors have found that the error in E_2-E_1 calculated at this stage is unreliable; the error may increase (for a while) as the size of the expansion increases. This method has the drawback that it relies on experimental data. A more appealing method is described later. Unless the user wishes to optimize the rate of convergence, we recommend using the universal Lindgren parameters $C = 0.8$, $n = 1.15$, $m = 1$.

NCØRES+NVALES is the number of subshells in the configuration used to construct the potentail; the individual values are not important except that both must be positive and non-zero. ION = Z-N, where Z is the nuclear charge and N is the number of electrons. NNLZ (= $100*n+10*l$) gives the n and l of the subshell, WWNL gives the number of electrons in the subshell, and EE is the energy eigenvalue guess in Rydbergs (negative for bound radials). In order to obtain energy differences by subtracting two system energy eigenvalues corresponding to different values of J and/or parity (and hence different computer runs), the same $V(r)$ must be used to generate the radials for each computer run. Consequently the configuration chosen to construct $V(r)$ must be the same for all runs in which energy comparisons are to be made. This configuration is usually one which is thought to be most dominant in one of the eigenvectors of interest (see the test run). For Mg I, the $3s^2$ configuration was used [1] for ^1S terms, but we could have just as well used 3s3p or 3s3d.

For the strongly bound states (EE < -0.01), SCHEQ is remarkably insensitive to the estimate of the energy eigenvalues. There are three sources from which estimates may be obtained. First, the results of Herman and Skillman [10] may be used. These are most useful for ground states of neutral systems. Second, estimates may be made from experimental measurements [17]. The quantity -EE$_{nl}$ is roughly the energy, in Rydbergs, necessary to remove the nlth electron from the configuration X nl, leaving the configuration X (the precise form of X is unimportant for the estimation). The position of the configuration is computed by first taking the appropriate weighted average of the levels associated with a given term (obtaining the term position) and then appropriately averaging the terms to obtain the configuration position. The process produces a sufficiently accurate estimate for all computations provided that the existing experimental measurements are reliable. Finally, the energy eigenvalues may be estimated by extrapolating the results for the $(n-m)l \ldots (n-1)l$ radials in the same potential.

The choice and number of configurations and terms to be included in the expansions is a matter of trial and error, unless the amount of core and computing time available is essentially unlimited (all configurations must have the same parity; the program makes no parity test). Usually, the first estimate of the configurations and terms for the expansions is sufficient to produce moderately accurate results. We have observed some trends which will aid in making this selection. If the dominant configuration is X $nln'l'$ then configurations of the form (we exclude configurations obtained by only varying n or n') X $\bar{n}\bar{l}\bar{n}'\bar{l}'$ are important. This is particularly true when $\bar{n} = n$ and $\bar{n}' = n'$ (the two configurations then belong to the same complex) [18]. The lowest values that $\bar{n}$ and $\bar{n}'$ can take on consistent with the closed core and azimuthal quantum numbers should also be included. For the Mg I calculation [1] in which 3s3p was the dominant configuration, the additional configurations (of this type) used were: 3p3d (same complex), 3d4p, 3p4d, and 3d4f. For a Ba I calculation in which the $6s^2$ configuration is dominant (see the test run), we might use $6p^2$ (same complex), 6p7p, 6p8p, 6p9p, 6p10p, $5d^2$, 5d6d, 5d7d, 5d8d, $6d^2$ (same complex), $4f^2$, $7s^2$, 7s8s, etc. Even though $6d^2$ and $6s^2$ belong to the same complex, the strength of their interaction is weaker than that of the $6s^2$ and $5d^2$ interaction. The latter interaction is stronger because the two configurations are closer in energy and there is more overlapping of radials than in the former case. We also find that it is important to include single excitations of the dominant configuration having the forms X $(n+m)l\ n'l'$ and X $nl(n'+m')l'$, where $m, m' \leq 4$ (the cutoff is somewhat arbitrary). For Mg I, the single excitations 3s4p, 3s5p, 3s6p, 3p4s were used [1]. For Ba I ($6s^2$ dominant) the single excitations 6s7s, 6s8s, 6s9s, 6s10s might be used. If the dominant term is ^{2S+1}L then other permitted terms [see eq. (6)] should only be included if the ^{2S+1}L term associated with the same configuration interacts strongly with the ^{2S+1}L term of the dominant configuration. The importance of a term other

than the dominant one depends on the strength of the one-body spin-orbit interaction. In Mg I, where spin-orbit interactions are small [1], only one term (^{2S+1}L) needs to be included in the expansions. For Hg I where the one-body spin-orbit interactions are large and $6s^2$ and $6p^2$ interact strongly, it is necessary to include $6p^2\ ^3P_0$ in the expansion in which $6s^2\ ^1S_0$ is dominant. To estimate the importance of a configuration one can do an abbreviated calculation using only the one-body relativistic operators (if a relativistic calculation is desired) and a few configurations. If the expansion coefficient of the configuration under investigation is small ($< 10^{-3}$ in magnitude) in the eigenvector of interest, then the configuration may be deleted. However, such a configuration may be quite important in the calculation of absolute line strengths [1] and thus must be retained if line strength calculations are to be performed. If other atomic quantities are to be calculated the configuration's effect on these quantities should be checked before deleting it. The choice of configurations and terms is the most difficult problem confronting the user.

NADSO is the number of additional radials needed to construct all expansion configurations excluding those radials used to construct $V(r)$. NCORES (in BRIP) is the number of closed subshells common to all configurations. JSL designates the term value and configuration number according to the formula 100*NO+10*S+L where NO is the configuration number, S and L have their usual meanings.

Schematically, the output format for a successful run is [10]

		Card number
(1)	PRINT Hollerith statement	28
*(2)	PRINT Hollerith statement	85
*(3)	PRINT QC,QN,QM	94
*(4)	PRINT KEY,TØL,THRESH,MESH,KUT	102
*(5)	IF KEY=0, PRINT RU2(M),M=1,437,4 with label	125-126
	IF KEY=1, PRINT RU3(M),M,1,441 with label	129-130
*(6)	PRINT EE(I),I=1,NCØRES+NVALES with label	147-148
(7)	PRINT NITER,Z,DELTA,IDELTA,X(IDELTA),ICUT,X(ICUT) for each self-consistent iteration with label	229,317
†(8)	IF DENM(I)=0 and/or SNLØ(I)=0 PRINT IDIV	354
*(9)	PRINT Z,NCØRES,NVALES,IØN	434
†(10)	IF IPUNCH ≠ 0 PRINT RUINL2(M),M=1,441	456
	DØ LØØP: M=1,NCØRES+NVALES PRINT NLZ,XL,EE(M),WWNL(M),KKK,PSLØPE(M)	461
	PRINT SNL(I),I=MTAB7(M),MTAB7(M)+KKK-1	464
(11)	PRINT Hollerith statement	1697
*(12)	PRINT JTØT,NØCØNF,NADSØ,NCØRES	1702
*(13)	PRINT NYCALC	1713
*(14)	PRINT EE(K2),K2=NCSPVS+1,NCSPVS+NADSØ with label	1769
(15)	DØ LØØP: K2=1,NADSØ PRINT NNLZ(NCSPVS+K2),KKK,EE(NCSPVS+K2)	1780
	†IF NCSPVS+K2 > NPRNT, PRINT SNL(K1),K1=MTAB7(NCSPVS+K2),MTAB7(NCSPVS+K2)+KKK-1	1785
(16)	PRINT PSLØPE(K5),K5=NCSPVS+1,NCSPVS+NADSØ with label	1804
*(17)	DØ LØØP: J3=1,NØCØNF PRINT J3,NNLZ(NUR1(J3)),NNLZ(NUR2(J3))	1814
*(18)	PRINT JSL(I3),I3=1,MXSIZE	1915
(19)	PRINT YUPER2	2905
(20)	PRINT ((INC,JNC,HAM(INC,JNC),INC=JNC,MXSIZE),JNC=1,MXSIZE) with label	2907,2910
(21)	PRINT EIG(JNC,1),JNC=1,MXSIZE with label	2915,2917
(22)	DØ LØØP: JNC=1,MXSIZE PRINT VEC(INC,JNC),INC=1,MXSIZE with label	2922
(23)	PRINT Z71,Z81	2930
(24)	PRINT IMPVEC,EIG(INC,3),INC=1,MXSIZE	2944
(25)	PRINT EIG(1,4)	2952
(26)	IF NVSE ≠ 0	
	DØ LØØP: INC=2,NCSPVS+NADSØ-NCØRES+1	
	DØ LØØP: JNC=2,INC	
	IF LQUAN(NNLZ(INC+NCØRES-1)) = LQUAN(NNLZ(JNC+NCØRES-1))	
	PRINT NNLZ(INC+NCØRES-1),NNLZ(JNC+NCØRES-1),ZARI(ILK7),ZARA(ILK7), (BTHI(ISP,ILK7),ISP=1,3),(BTHA(ISP,ILK7),ISP=1,3) with label	2956,2966,2967
	where ILK7=ZBLØC(INC,JNC)	
(27)	PRINT Hollerith statement: NØRMAL EXIT	33

* input variables.
† does not appear as part of test run output.

Entries (1) and (27) are printed from BETHE, entries (2)-(10) are printed from HRSK, entries (11)-(26) are printed from BRIP. See the test run for an example of the edited output.

4. MODIFICATIONS TO THE PROGRAM

The present deck permits one to do a non-relativistic calculation simply by setting the NYCALC array to zero. However, if only non-relativistic calculations are desired, then considerable storage can be saved by making the following modifications: drop subprograms W9J, TKUKX, W6J, W6JB, SNK, VKSUB1, and CSSPIN, drop the array RDER and rearrange common block storage. Further storage may be saved by omitting arrays BTHA, BTHI, and W3J. In BRIP the following modifications are required: (i) the section computing the factorials must be removed and common block WIGNER can be deleted; (ii) the section computing the $3j$ symbols must be removed; (iii) the section computing the derivatives must be removed; (iv) Table 1, which begins on card 1921, is modified so that no references are made to statements 401, 601, and 826; (v) cards 2165-2245, 2301-2541, 2590-2900 must be removed.

We anticipate that many users may wish to apply the program to systems of fewer than 80 electrons. To save storage locations, the maximum number of mesh points may be decreased from 601 (in integral mutiples of 40) and/or the number of radials (derivatives) may be decreased. There is a corresponding decrease in the storage required for the SNL and RDER arrays. If the number of mesh points saved is N_M and the savings in both SNL and RDER is 2 N_{RS} (identical savings in each) then the total number of locations saved is

$$N_{RS} + 2N_M + 14803$$
$$- \text{Maximum}\,[9065 - 15N_M,\ 14803 - 3N_M - N_{RS}]\ .$$

A few more locations may be saved by reducing the dimensions of ZARA, ZARI, BTHA, and BTHI. In addition to changing the various dimension statements (Tables 3 and 4) the following cards have to be revised: 97, 98, 134, 135, 243, 244, 553, 1469, 1591, 1695, 1790, 1806, 1808.

Certain problems may require an increase in the number of radials (derivatives) An estimate of the number of points in a core radial (derivative) may be obtained from Herman and Skillman [10]. One should use 601 as an estimate for the number of points in valence radials (derivatives). The necessary changes can be deduced from the above information. If insufficient locations in SNL(RDER) have been provided, then card 1806 will abort the run.

If one or more of the arrays RDER, R, SNL, and V is to be written on tape or punched on cards, then introduce the appropriate output statement after card 2902. These arrays are complete at this time and remain intact throughout the remainder of the program. If the matrix HAM is desired, then it should be obtained before diagonalization (i.e. after card 2913). Arrays ZARA, ZARI, BTHA, BTHI and W3J are available after DØ LØØP "77" is completed. The most useful results that might be stored on cards or tape are the eigenvectors and eigenvalues, for they can be used to compute other atomic quantities such as electric dipole line strengths. We have found that for systems with large relativistic effects, (e.g. Hg I) it is necessary to use a relativistic $\dot{X}$, $\{\, i\dot{X} = [H, X]$ where H is the Hamiltonian and X is the length operator$\}$, if the velocity form of the absolute line strength is to be computed.

E versus N curves may be computed in BRIP. An E versus N curve is obtained by observing how the energy eigenvalue associated with a particular level varies with the number of expansion terms. By examining the rate of convergence of such curves in the regions of intermediate and large values of N, a choice of Lindgren [7] parameters can be made. The effect of an expansion term on the energy eigenvalue can also be determined. Note that this method is more precise than the analysis based upon coefficient magnitudes in the eigenvector. It has not proved useful to fit the tail of such a curve with an analytic function and then extrapolate to $N = \infty$ to obtain an estimate of the error involved in deleting discrete configurations. Conclusions based on E versus N curves are invalid when an important configuration has been omitted from the expansion.

At present SECØND is a dummy subprogram. If a subprogram which provides timing information is available to the user, then SECØND can be replaced. Similarly ZERØ can be replaced with a system subprogram which sets all entries in an array to zero.

We expect that each user will encounter different kinds of problems and we have therefore carefully documented the program to permit easy modification.

ACKNOWLEDGMENTS

We wish to express our indebtness to F. Herman and S. Skillman upon whose excellent work this program is built.

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TEST RUN OUTPUT

```
CONFIGURATION INTERACTION WITH PAULI-BREIT HAMILTONIAN  USING PROGRAM BETHE.

J=0,EVEN PARITY  8A 1  ALL OPERATORS PRESENT   UNIVERSAL POTENTIAL

LINDGREN PARAMETERS.  C =     8.00000000E-01   N =     1.15000000E+00   M =     1.00000000E+00

KEY = 1       TOL =  .001000      THRESH =  .00001000      MESH = 601      KUT = 0

INPUT POTENTIAL RU2 AND/OR RU3  FOLLOWS

-1.1200000E+02 -1.1166000E+02 -1.1132000E+02 -1.1098000E+02 -1.1065000E+02 -1.1031000E+02 -1.0997000E+02 -1.0964000E+02
-1.0930000E+02 -1.0897000E+02 -1.0864000E+02 -1.0831000E+02 -1.0798000E+02 -1.0765000E+02 -1.0733000E+02 -1.0701000E+02
-1.0669000E+02 -1.0637000E+02 -1.0606000E+02 -1.0574000E+02 -1.0543000E+02 -1.0512000E+02 -1.0482000E+02 -1.0451000E+02
-1.0421000E+02 -1.0391000E+02 -1.0361000E+02 -1.0331000E+02 -1.0302000E+02 -1.0273000E+02 -1.0244000E+02 -1.0215000E+02
-1.0187000E+02 -1.0158000E+02 -1.0130000E+02 -1.0102000E+02 -1.0074000E+02 -1.0046000E+02 -1.0019000E+02 -9.9917000E+01
-9.9645290E+01 -9.9107450E+01 -9.8576080E+01 -9.8051010E+01 -9.7532080E+01 -9.7019140E+01 -9.6512060E+01 -9.6010720E+01
-9.5515020E+01 -9.5024840E+01 -9.4540090E+01 -9.4060650E+01 -9.3586440E+01 -9.3117340E+01 -9.2653250E+01 -9.2194060E+01
-9.1739660E+01 -9.1289940E+01 -9.0844790E+01 -9.0404100E+01 -8.9967750E+01 -8.9535660E+01 -8.9107710E+01 -8.8683810E+01
-8.8263860E+01 -8.7847780E+01 -8.7435470E+01 -8.7026880E+01 -8.6621910E+01 -8.6220500E+01 -8.5822600E+01 -8.5428120E+01
-8.5037030E+01 -8.4649270E+01 -8.4264780E+01 -8.3883520E+01 -8.3505450E+01 -8.3130510E+01 -8.2758680E+01 -8.2389910E+01
-8.2024150E+01 -8.1301590E+01 -8.0590670E+01 -7.9891110E+01 -7.9202650E+01 -7.8525010E+01 -7.7857930E+01 -7.7201140E+01
-7.6554380E+01 -7.5917410E+01 -7.5289970E+01 -7.4671810E+01 -7.4062690E+01 -7.3462400E+01 -7.2870710E+01 -7.2287410E+01
-7.1712280E+01 -7.1145160E+01 -7.0585840E+01 -7.0034160E+01 -6.9489960E+01 -6.8953090E+01 -6.8423390E+01 -6.7900740E+01
-6.7385000E+01 -6.6876060E+01 -6.6373790E+01 -6.5878070E+01 -6.5388810E+01 -6.4905880E+01 -6.4429190E+01 -6.3958620E+01
-6.3494080E+01 -6.3035470E+01 -6.2582670E+01 -6.2135590E+01 -6.1694120E+01 -6.1258180E+01 -6.0827640E+01 -6.0402410E+01
-5.9982400E+01 -5.9157700E+01 -5.8352700E+01 -5.7566690E+01 -5.6799000E+01 -5.6049040E+01 -5.5316200E+01 -5.4599920E+01
-5.3899730E+01 -5.3215170E+01 -5.2545790E+01 -5.1891150E+01 -5.1250890E+01 -5.0624630E+01 -5.0011970E+01 -4.9412550E+01
-4.8826010E+01 -4.8252020E+01 -4.7690190E+01 -4.7140170E+01 -4.6601610E+01 -4.6074180E+01 -4.5557490E+01 -4.5051210E+01
-4.4554990E+01 -4.4068510E+01 -4.3591410E+01 -4.3123370E+01 -4.2664080E+01 -4.2213230E+01 -4.1770520E+01 -4.1335640E+01
-4.0908340E+01 -4.0488360E+01 -4.0075440E+01 -3.9669330E+01 -3.9269830E+01 -3.8876740E+01 -3.8489840E+01 -3.8109190E+01
-3.7734190E+01 -3.7001440E+01 -3.6290690E+01 -3.5600830E+01 -3.4931020E+01 -3.4280880E+01 -3.3649630E+01 -3.3036350E+01
-3.2440820E+01 -3.1862470E+01 -3.1300660E+01 -3.0754700E+01 -3.0223870E+01 -2.9707460E+01 -2.9204720E+01 -2.8714940E+01
-2.8237430E+01 -2.7771550E+01 -2.7316720E+01 -2.6872440E+01 -2.6438220E+01 -2.6013660E+01 -2.5598430E+01 -2.5192190E+01
-2.4794670E+01 -2.4405630E+01 -2.4024860E+01 -2.3652170E+01 -2.3287380E+01 -2.2930340E+01 -2.2580890E+01 -2.2238900E+01
-2.1904220E+01 -2.1576730E+01 -2.1256270E+01 -2.0942740E+01 -2.0635980E+01 -2.0335860E+01 -2.0042250E+01 -1.9755000E+01
-1.9473990E+01 -1.8930300E+01 -1.8409850E+01 -1.7911520E+01 -1.7434210E+01 -1.6976820E+01 -1.6538320E+01 -1.6117680E+01
-1.5713960E+01 -1.5326260E+01 -1.4953730E+01 -1.4595590E+01 -1.4251130E+01 -1.3919670E+01 -1.3600610E+01 -1.3293380E+01
-1.2997470E+01 -1.2712420E+01 -1.2437760E+01 -1.2173100E+01 -1.1918040E+01 -1.1672200E+01 -1.1435230E+01 -1.1206770E+01
-1.0986470E+01 -1.0774000E+01 -1.0569020E+01 -1.0371210E+01 -1.0180230E+01 -9.9957700E+00 -9.8175100E+00 -9.6451500E+00
-9.4784000E+00 -9.3169700E+00 -9.1606000E+00 -9.0090100E+00 -8.8619800E+00 -8.7192700E+00 -8.5806600E+00 -8.4459400E+00
-8.3149300E+00 -8.0634500E+00 -7.8248200E+00 -7.5979500E+00 -7.3818900E+00 -7.1758300E+00 -6.9790300E+00 -6.7908600E+00
-6.6107500E+00 -6.4382000E+00 -6.2727500E+00 -6.1139600E+00 -5.9614700E+00 -5.8149100E+00 -5.6740300E+00 -5.5383900E+00
-5.4078000E+00 -5.2819700E+00 -5.1606400E+00 -5.0435400E+00 -4.9304900E+00 -4.8213100E+00 -4.7158000E+00 -4.6138000E+00
-4.5151500E+00 -4.4197100E+00 -4.3273300E+00 -4.2379200E+00 -4.1513400E+00 -4.0675100E+00 -3.9863200E+00 -3.9077000E+00
-3.8315700E+00 -3.7578600E+00 -3.6865000E+00 -3.6174400E+00 -3.5506200E+00 -3.4859800E+00 -3.4234900E+00 -3.3630900E+00
-3.3047300E+00 -3.1940600E+00 -3.0910500E+00 -2.9953500E+00 -2.9065700E+00 -2.8243300E+00 -2.7482000E+00 -2.6777600E+00
-2.6125400E+00 -2.5521400E+00 -2.4961200E+00 -2.4440200E+00 -2.3954400E+00 -2.3499800E+00 -2.3073100E+00 -2.2671600E+00
-2.2292200E+00 -2.1932500E+00 -2.1590200E+00 -2.1263500E+00 -2.0950800E+00 -2.0650600E+00 -2.0361800E+00 -2.0083400E+00
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-2.0000000E+00 -2.0000000E+00 -2.0000000E+00 -2.0000000E+00 -2.0000000E+00 -2.0000000E+00 -2.0000000E+00 -2.0000000E+00
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-2.0000000E+00

 INPUT  EE
-2.6293000E+03 -4.0744000E+02 -3.8544000E+02 -8.7030000E+01 -7.7450000E+01 -5.9479000E+01 -1.7465000E+01 -1.3916000E+01
-7.6790000E+00 -2.6393000E+00 -1.6800000E+00 -3.2800000E-01

ITER     Z    DELTA        I(DEL)  X(DEL)  I(CUT)  X(CUT)
   1    56  2.0070718E+00   441   204.700   441  204.700
   2    56  1.0035359E+00   441   204.700   305   20.380
   3    56  1.8624783E-03   305    20.380   305   20.380
   4    56  6.2118160E-04    14      .032   305   20.380


Z =  56      NCORES = 11      NVALES =  1      ION =  0


  OUTPUT FROM BRIP SUBROUTINE

  J = 0      NUMBER OF CONFIGS. =  6      NUMBER OF EXTRA RADIALS =  5      NCORES = 11

 NYCALC ARRAY  1  1  1  1  1  1  1

INPUT EE OF EXTRA RADIALS
 -1.400000E-01   -2.600000E-01   -1.300000E-01   -2.200000E-01   -9.400000E-02


 700   481    -1.21987175775E-01
 610   481    -1.87502245233E-01
 710   521    -8.98691622597E-02
 520   441    -2.72594271257E-01
 620   521    -9.62398229978E-02

  PSLOPE FOR EXCITED SPIN-ORBITALS
  3.31772072E+00    7.10806777E+01    4.10903796E+01    6.69378539E+02    1.60842089E+02

 CONFIGURATION   1      FIRST SPIN-ORBITAL IS   600   SECOND SPIN-ORBITAL IS   600

 CONFIGURATION   2      FIRST SPIN-ORBITAL IS   600   SECOND SPIN-ORBITAL IS   700

 CONFIGURATION   3      FIRST SPIN-ORBITAL IS   610   SECOND SPIN-ORBITAL IS   610

 CONFIGURATION   4      FIRST SPIN-ORBITAL IS   610   SECOND SPIN-ORBITAL IS   710

 CONFIGURATION   5      FIRST SPIN-ORBITAL IS   520   SECOND SPIN-ORBITAL IS   520

 CONFIGURATION   6      FIRST SPIN-ORBITAL IS   520   SECOND SPIN-ORBITAL IS   620

  JSL  ARRAY  FOLLOWS   100   200   300   311   400   500   600
```

```
 NET TIME NEEDED TO SET UP MATRIX IS   0.          SECONDS

MATRIX SET UP COMPLETE.BEGIN DIAGONALIZATIONS.MATRIX FOLLOWS.

( 1, 1) =   -1.00931561O5E+00   ( 2, 1) =   -1.3563472180E-02   ( 3, 1) =   -9.6221940802E-02   ( 4, 1) =   -2.2899411665E-07
( 5, 1) =   -4.8857657661E-02   ( 6, 1) =    5.0997761004E-02   ( 7, 1) =   -7.8457909524E-03   ( 2, 2) =   -7.9005287624E-01
( 3, 2) =    1.6834075824E-02   ( 4, 2) =   -1.0347499216E-07   ( 5, 2) =   -3.3444387292E-02   ( 6, 2) =    2.2749991389E-02
( 7, 2) =    1.1816848633E-02   ( 3, 3) =   -6.6654428166E-01   ( 4, 3) =   -5.7793464233E-03   ( 5, 3) =   -1.5544013632E-02
( 6, 3) =   -4.6191825230E-02   ( 7, 3) =    3.6596426054E-02   ( 4, 4) =   -7.4985355594E-01   ( 5, 4) =   -2.3622303329E-03
( 6, 4) =    3.0663544179E-08   ( 7, 4) =   -9.4322057340E-09   ( 5, 5) =   -5.4824631916E-01   ( 6, 5) =   -2.8905222606E-02
( 7, 5) =   -2.3781998203E-03   ( 6, 6) =   -5.6513811095E-01   ( 7, 6) =    9.6237286505E-02   ( 7, 7) =   -6.8955679819E-01

EIGENVALUES OF  7 X  7 MATRIX FOLLOW.
-4.833725066494E-01  -5.550340949621E-01  -6.186191123333E-01  -7.497203003876E-01  -7.694291414975E-01  -7.992909948950E-01
-1.043241401960E+00

 EIGENVECTOR STORED IN COLUMN   1  OF VEC
 1.391911324180E-01   1.087299519866E-01  -1.492877993683E-01   7.513261096478E-03  -4.823316379407E-01   7.730761507433E-01
 3.408368909874E-01

 EIGENVECTOR STORED IN COLUMN   2  OF VEC
-3.417487491222E-03   8.876732559463E-02   2.370584896736E-01   3.309696195003E-03  -8.529461860886E-01  -4.081578254422E-01
-2.044284575052E-01

 EIGENVECTOR STORED IN COLUMN   3  OF VEC
 2.254298251520E-01  -1.157603187749E-01  -8.189392198671E-01   3.798474016937E-02  -1.066824719867E-01  -2.828064807753E-02
-5.014934808369E-01

 EIGENVECTOR STORED IN COLUMN   4  OF VEC
-6.811262171163E-03  -8.236155713330E-03  -2.254430714765E-02   9.911499754063E-01  -7.558380698202E-04  -6.251602690130E-02
 1.144134083202E-01

 EIGENVECTOR STORED IN COLUMN   5  OF VEC
 6.930741830333E-02  -2.527586735550E-01  -3.820281206468E-01  -1.249691192358E-01  -1.009559553694E-01  -4.432975717918E-01
 7.503611976257E-01

 EIGENVECTOR STORED IN COLUMN   6  OF VEC
-2.604652366423E-02   9.486061847044E-01  -2.208175042665E-01  -2.154853824751E-02   8.922832234417E-02  -1.678538739029E-01
 1.187710350292E-01

 EIGENVECTOR STORED IN COLUMN   7  OF VEC
 9.613881684565E-01   5.558086961563E-02   2.358831885842E-01   5.464642905581E-03   1.015060349193E-01  -7.977935739410E-02
 1.745263632289E-02

 TRACE =  -5.018707552685E+00    SUM OF EIGENVALUES =  -5.018707552685E+00

 COMPONENTS OF H X PSI/E FOR EIGENVECTOR STORED IN COLUMN   7  OF VEC  FOLLOW
 9.613882E-01   5.558087E-02   2.358832E-01   5.464643E-03   1.015060E-01  -7.977936E-02   1.745264E-02

 AVERAGE RELATIVE ERROR IN COEFFICIENTS OF IMPVEC EIGEN VECTOR IS   4.811557E-14

ORBITALS        ZARI          ZARA          BTHI(1)       BTHI(2)       BTHI(3)       BTHA(1)       BTHA(2)       BTHA(3)
 600, 600   -2.57334E+01   2.50818E+01  -1.17483E+03   6.82312E+02   0.            2.12708E-04   0.            1.24592E-04
 700, 600   -5.15221E+00   5.11072E+00  -5.58347E+02   3.24261E+02   0.            1.01071E-04   0.            5.90715E-05
 700, 700   -1.13500E+01   1.10486E+01  -2.65360E+02   1.54102E+02   0.            4.80258E-05   0.            2.80101E-05
 610, 610   -1.83546E+01   1.78757E+01  -9.77020E+01   0.            2.45482E+02   5.21015E-05   8.11990E-04   1.55698E-04

 710, 610   -4.14126E+00   4.08860E+00  -5.64842E+01   0.            1.41771E+02   3.01124E-05   4.62511E-04   8.99940E-05
 710, 710   -9.10044E+00   8.85992E+00  -3.26556E+01   0.            0.            1.74038E-05   0.            5.20173E-05
 520, 520   -4.25173E+01   4.18965E+01  -2.31690E+02   0.            0.            2.35194E-04   0.            7.44119E-04
 620, 520   -5.74986E+00   5.74116E+00  -5.56812E+01   0.            0.            5.64126E-05   0.            1.77994E-04
 620, 620   -1.06541E+01   1.03881E+01  -1.33837E+01   0.            0.            1.35331E-05   0.            4.26031E-05
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