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HSEIGV — A PROGRAM FOR COMPUTING ENERGY LEVELS AND RADIAL WAVE FUNCTIONS IN THE COUPLED–CHANNEL HYPERSPHERICAL ADIABATIC APPROACH

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HSEIGV — программа для расчета уровней энергии
и радиальных волновых функций в методе связанных каналов
гиперсферического адиабатического подхода

Представлена программа HSEIGV (FORTRAN 77) для расчета уровней энергии и радиальных волновых функций двухэлектронных систем в адиабатическом приближении и в приближении метода связанных каналов гиперсферического адиабатического подхода. В этом подходе решение шестимерного уравнения Шредингера, описывающее динамику двухэлектронной атомной системы, сводится к решению системы связанных дифференциальных уравнений по радиальной координате (ρ) столкновения. Система радиальных уравнений, содержащая матричные коэффициенты связи каналов при первой производной, решается методом конечных элементов с использованием аппроксимации высокого порядка точности. Приведен пример применения программы для вычисления значений энергии основного и нескольких дважды возбужденных состояний иона H^- ниже второго порога $n = 2$.

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HSEIGV — a Program for Computing Energy Levels
and Radial Wave Functions in the Coupled–Channel Hyperspherical
Adiabatic Approach

A FORTRAN 77 program is presented which calculates energy values and radial wave functions of two-electron systems in the adiabatic and coupled-channel approximations of the hyperspherical adiabatic approach. In this approach, the solution of a six-dimensional Schrödinger equation describing the dynamics of a two-electron atomic system is reduced to the solution of a system of coupled second-order ordinary differential equations in scattering (radial) coordinate ρ. The resulting system of radial equations which contains the first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method. The program is applied to the calculation of the energy values of the ground state and several doubly excited states of H^- below the $n = 2$ threshold.

PROGRAM SUMMARY

Title of program: HSEIGV

Computer for which the program is designed and others on which it has been tested:
Computers: SGI Indigo^2, IBM RS/6000, Intel Pentium Pro200 PC; *Installation*: Department of Chemistry, University of Toronto, Toronto, Canada
Computers: DECstation 3000 ALPHA AXP Model 800, IBM RS/6000 Model 320H; *Installation*: Department of Chemical Physics, The Weizmann Institute of Science, Israel
Computers: Sun–Elc, HP 715, Sgi–35D; *Installation*: Computing Center of the Weizmann Institute of Science, Israel

Operating systems under which the program has been tested: Digital UNIX v4.0, AIX 3.2.5, SunOs 4.1.3, HP/UX 9.01, Irix 6.1, Linux 1.0.9

Programming language used: FORTRAN 77

Memory required to execute with typical data: depends on (i) the number of differential equations; (ii) the number and order of finite elements; (iii) the number of hyperradial points in which the tabular values of potential curves and radial matrix elements are given; and (iv) the number of eigensolutions required. Test run requires 10 MB

No. of bits in a word: 64

No. of processors used: one

Has the code been vectorized? no

Overlay structure: none

Peripherals used: line printer, scratch disc store

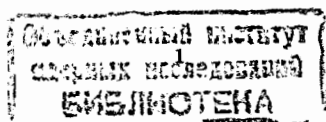*No. of lines in distributed program, including test data, etc*: 2671

Keywords: atomic, molecular, chemical physics, two-electron systems, hyperspherical coordinates, Schrödinger equation, adiabatic approximation, eigensolutions, ordinary differential equations, finite element method, high order accuracy approximations, doubly excited states

Nature of physical problem

In the hyperspherical adiabatic approach [1], the solution of a six dimensional Schrödinger equation for a two electron system is reduced after separating the scattering coordinate (hyperradius ρ) from the rest of angular variables to the solution of coupled second-order ordinary differential equations which contain the first-derivative coupling terms. The purpose of this paper is to present the finite element method procedure based on the use of high-order accuracy approximations for calculation of the approximate eigensolutions for such systems of coupled differential equations.

Method of solution

The coupled differential equations are solved by the finite element method using high-order accuracy approximations [2]. The generalized algebraic eigenvalue problem $\mathbf{A\,F} = E\,\mathbf{B\,F}$ arising after the replacement of the differential problem by the finite-element approximation of high order of accuracy is solved by the subspace iteration method [3] using the SSPACE program [3].

References

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LONG WRITE-UP

1 Introduction

Significant progress toward an understanding of two-electron correlations in atoms has resulted from a hyperspherical adiabatic (HSA) approach [1-3]. The approach is based on the use of hyperspherical coordinates as collective variables (ρ, α) replacing the independent-electron radial coordinates r_1 and r_2 and assumption about the adiabatic nature of the correlated electron motion in atoms. In the hyperspherical coordinates, the hyperradius $\rho = \sqrt{r_1^2 + r_2^2}$ represents the overall size of the electron pair and the hyperangle $\alpha = \tan^{-1}(r_2/r_1)$ represents relative distance of two electrons from the nucleus. In the adiabatic representation the motion of electrons in $\mathcal{R}^6$ space is separated into a fast rotation over the surface of the "hypersphere" $\mathcal{S}_\rho^5(\Omega \equiv \{\alpha, \hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2\})$ and a slow radial motion along hyperradius ρ treated as an adiabatic parameter.

The adiabatic approximation, in which the radial coupling between channels is neglected, has proved to be remarkably fruitful for the description and visualization of the correlation patterns of the doubly excited states of two-electron systems [2-4]. This approximation (which is analogous to the Born–Oppenheimer approximation for diatomic molecules) has been extensively used for solving a wide range of atomic problems (see, e.g., [1-12]). It has also been very useful for the study of one and multi-photon ionization of He and photodissociation of H$^-$ (see, e.g., [13-16]). The main success of the approach owes much to the conceptual and computational simplicity and effectiveness of this approximation. However, the adiabatic approximation appeared unsuitable (at least for low-lying states) for high-precision computations for which nonadiabatic affects should be accurately taken into account (see, e.g., [7,17 24]). In the recent papers [19 21], the high rate of convergence of the hyperspherical adiabatic (HSA) expansion of the total two-electron wave function for the ground and doubly excited states has been established. It was shown that the coupled channel HSA approach allows one to obtain the energy spectrum of doubly excited atoms with high accuracy using only a few equations. The high accuracy of the bound state calculations can also be obtained within the diabatic by sector approach [22, 23], while providing the slower rate of convergence of the sector diabatic expansion of the total wave function.

In our previous papers [25, 26], descriptions of the HSTERM program designed for the calculation of potential curves and matrix elements of radial coupling within the HSA approach and program ASYMPT for computing asymptotics of adiabatic potential curves with an accuracy of $O(\rho^{-2})$ have been presented (see also Ref. [27]). In this paper, we present a program for computing energy levels and radial wave functions of two-electron systems in the adiabatic and coupled channel approximations of the HSA approach using potentials prepared by the above mentioned programs. The solution of the bound state problem for a system of coupled radial equations, arising after separating the hyperradius ρ from the rest of angular variables $(\alpha, \hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ in the two-electron Schrödinger equation, is carried out using the finite element method (FEM) [28, 29]. In our recent work [30], high-order polynomial approximations for the finite-element solutions of systems of coupled ordinary differential equations have been studied in details. The effectiveness and high accuracy of such high-order approximations of the FEM have been demonstrated [30] on the basis of numerical experiments performed for a wide set of quantum-mechanical

problems. In the present paper we generalize this method to deal with the first-derivative radial coupling terms arising in the adiabatic representation. The program elaborated is a general purpose program, the use of which is not limited to two-electron systems only. The HSTERM program can be applied to the solution of a wide range of bound state problems of atomic and molecular physics reducing to the solution of a system of coupled ordinary differential equations with the first-derivative coupling terms.

The paper is organized as follows. In Section 2 we give a short description of the hyperspherical adiabatic approach. The construction of the finite-element high-order schemes is discussed in Section 3. A description of the HSEIGV program is given in Section 4. Subroutine units are briefly described in Section 5. Test run is considered in Section 6.

2 Hyperspherical adiabatic (HSA) representation

In the hyperspherical coordinates, after introducing the reduced wave function $\Psi(\rho, \Omega) = \rho^{5/2} \sin \alpha \cos \alpha \psi(\mathbf{r}_1, \mathbf{r}_2)$ ($\psi(\mathbf{r}_1, \mathbf{r}_2)$ is the whole two-electron wave function), the Schrödinger equation for a two-electron atomic system with nuclear charge Z and total energy E can be written as ($\hbar = e = m_e = 1$):

$$\left[-\frac{\partial^2}{\partial \rho^2} - \frac{1}{4\rho^2} + \hat{h}(\rho) - 2E \right] \Psi(\rho, \Omega) = 0, \tag{1}$$

where $\rho = \sqrt{r_1^2 + r_2^2}$ is the hyperradius, $\alpha = \tan^{-1}(r_2/r_1)$ is the hyperangle, and Ω denotes five angles $\{\alpha, \hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2\}$. The adiabatic Hamiltonian is

$$\hat{h}(\rho) = \frac{1}{\rho^2} \hat{\Lambda}^2(\Omega) + \frac{1}{\rho} V(\alpha, \theta_{12}), \tag{2}$$

where

$$\hat{\Lambda}^2(\Omega) = -\frac{\partial^2}{\partial \alpha^2} + \frac{l_1^2}{\cos^2 \alpha} + \frac{l_2^2}{\sin^2 \alpha} \tag{3}$$

is the generalized angular momentum operator,

$$V(\alpha, \theta_{12}) = -\frac{2Z}{\cos \alpha} - \frac{2Z}{\sin \alpha} + \frac{2}{\sqrt{1 - \sin 2\alpha \cos \theta_{12}}} \tag{4}$$

is the interaction potential, l_i is the operator of the orbital angular momentum of the ith electron, $\theta_{12} = \cos^{-1}[(\mathbf{r}_1 \cdot \mathbf{r}_2)/r_1 r_2]$, and $\hat{\mathbf{r}}_i$ is a set of the usual spherical angles (θ_i, φ_i), $i = 1, 2$.

Treating ρ as a slowly varying adiabatic parameter, the reduced wave function $\Psi(\rho, \Omega)$ can be expressed in a close-coupling expansion by a set of N adiabatic channel functions $\{\Phi_\mu(\Omega; \rho)\}_{\mu=1}^N$ at each ρ as

$$\Psi(\rho, \Omega) = \sum_{\mu=1}^N F_\mu(\rho) \Phi_\mu(\Omega; \rho). \tag{5}$$

The adiabatic channel functions $\Phi_\mu(\Omega; \rho)$ are defined as the eigensolutions of the following equation

$$\hat{h}(\rho) \Phi_\mu(\Omega; \rho) = U_\mu(\rho) \Phi_\mu(\Omega; \rho). \tag{6}$$

Eq. (6) must be solved for each value of parameter ρ to obtain the hyperspherical potential $U_\mu(\rho)$. The method of computation of the five-dimensional basis functions $\Phi_\mu(\Omega; \rho)$ has been discussed in details in our previous paper [25].

Substituting expansion (5) into the Schrödinger equation (1), one obtains the close-coupling equations for expansion coefficients $F_\mu(\rho)$, which can be written in the explicitly Hermitian form as

$$\left(-\frac{d^2}{d\rho^2} + V_{\mu\mu}(\rho) - 2E \right) F_\mu(\rho) + \sum_{\substack{\nu=1 \\ \nu \neq \mu}}^N V_{\mu\nu}(\rho) F_\nu(\rho) = 0, \quad (\mu = 1, 2, ..., N), \tag{7}$$

where

$$V_{\mu\nu}(\rho) \equiv W_{\mu\nu}(\rho) + \frac{d}{d\rho} Q_{\mu\nu}(\rho) + Q_{\mu\nu}(\rho) \frac{d}{d\rho}, \tag{8}$$

$$W_{\mu\nu}(\rho) \equiv -\frac{1}{4\rho^2} \delta_{\mu\nu} + U_\mu(\rho) \delta_{\mu\nu} + H_{\mu\nu}(\rho), \tag{9}$$

$$H_{\mu\nu}(\rho) = H_{\nu\mu}(\rho) \equiv \left\langle \frac{d}{d\rho} \Phi_\mu(\Omega; \rho) \middle| \frac{d}{d\rho} \Phi_\nu(\Omega; \rho) \right\rangle, \tag{10}$$

$$Q_{\mu\nu}(\rho) = -Q_{\nu\mu}(\rho) \equiv -\left\langle \Phi_\mu(\Omega; \rho) \middle| \frac{d}{d\rho} \Phi_\nu(\Omega; \rho) \right\rangle. \tag{11}$$

In the above, the brackets $\langle \cdot | \cdot \rangle$ mean integration over five angular variables $(\alpha, \hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$. The radial functions $F_\mu(\rho)$ satisfy the Dirichlet boundary conditions

$$F_\mu(0) = F_\mu(\infty) = 0, \quad \mu = 1, 2, ..., N. \tag{12}$$

This is the coupled–channel HSA approximation. Neglecting the coupling terms in Eq. (7), we obtain the uncoupled adiabatic approximation [31, 32]:

$$\left(-\frac{d^2}{d\rho^2} - \frac{1}{4\rho^2} + U_\mu(\rho) + H_{\mu\mu}(\rho) - 2E\right) F_\mu(\rho) = 0. \qquad (13)$$

The presence of a positively defined diagonal matrix element $H_{\mu\mu}(\rho)$ (see Eq. (10)) ensures the energy spectrum shift upwards, i.e. eigenvalues of Eq. (13) give the upper bound to the exact values of energy E. If we neglect all coupling elements in Eq. (7) including $H_{\mu\mu}(\rho)$ elements, we obtain the extreme adiabatic approximation [32]:

$$\left(-\frac{d^2}{d\rho^2} - \frac{1}{4\rho^2} + U_\mu(\rho) - 2E\right) F_\mu(\rho) = 0. \qquad (14)$$

This approximation corresponds to the Born-Oppenheimer one in molecular physics. In this approximation eigenvalues of Eq. (14) give the lower bound to exact energy E (see, e.g., [6, 8, 31, 32]).

3 High–order approximations of the finite–element method

In order to solve numerically the Sturm–Liouville problem for Eqs. (7), (13) or (14) subject to the boundary conditions (12) the high order approximations of the finite element method (FEM) [28, 29] elaborated in our previous paper [30] have been used. Such high-order approximations of the FEM have been proved [30] to be very accurate, stable, and effective for a wide set of quantum mechanical problems. The Sturm–Liouville problem (7), (12) is equivalent [28, 29] to the following variational Rayleigh-Ritz functional (prime means the differentiation in variable ρ):

$$
\begin{aligned}
R(\mathbf{F}) = & \left\{\int_0^\infty \sum_{\mu\nu}\left[F'_\mu(\rho)F'_\nu(\rho)\delta_{\mu\nu} + F_\mu(\rho)W_{\mu\nu}(\rho)F_\nu(\rho) + F_\mu(\rho)\left[Q_{\mu\nu}(\rho)F_\nu(\rho)\right]'\right.\right. \\
& \left.\left. + F_\mu(\rho)Q_{\mu\nu}(\rho)F'_\nu(\rho)\right]d\rho\right\}\left\{\int_0^\infty \sum_{\mu\nu}F_\mu(\rho)F_\nu(\rho)\delta_{\mu\nu}d\rho\right\}^{-1}.
\end{aligned}
\qquad (15)
$$

Computational schemes of the high order of accuracy are derived from the variational functional (15) on the basis of the finite element method. The general idea of the FEM in one-dimensional space is to subdivide interval $[0, \rho_{max}]$ into many small domains called elements. The size and shape of elements can be defined very freely so that physical properties can be taken into account.

In the present paper we use the isoparametric Lagrange elements $\{\phi_i^p(\eta)\}_{i=1}^p$ of order p which have been determined in [30]. For the sake of completeness, we briefly describe them here as follows. On interval [-1,1] nodes

$$\eta_i^p = -1 + 2i/p, \quad i = 0, 1, ..., p, \qquad (16)$$

are given. Functions $\phi_i^p(\eta)$ are determined from conditions

$$\phi_i^p(\eta_j^p) = \delta_{ij}, \quad i, j = 0, 1, ..., p. \qquad (17)$$

Now, we cover the interval $\Delta = [0, \rho_{max}]$ by a system of subintervals $\Delta_j = [\rho_{j-1}, \rho_j]$ in such a way that $\Delta = \bigcup_{j=1}^n \Delta_j$, where n is the number of subintervals. The finite element grid ω_ρ^p consists of mesh points $\rho_0, \rho_1, ..., \rho_n$ and nodes

$$\rho_{j,i}^p = \rho_{j-1} + 0.5(\rho_j - \rho_{j-1})(1 + \eta_i^p), \quad i = 1, 2, ..., p-1, \quad j = 1, 2, ..., n. \qquad (18)$$

In each point $\rho_{j,i}^p$ of grid ω_ρ^p we define function

$$N_l^p(\rho) = \begin{cases} \phi_{j,i}^p(\eta), & \rho = \rho_{j-1} + 0.5\,h_j(1 + \eta), \ |\eta| \leq 1 \\ 0, & \rho \in \Delta_j, \end{cases} \qquad (19)$$

$$i = 1, 2, ..., p-1, \quad l = (j-1)p+i, \quad h_j = \rho_j - \rho_{j-1}.$$

These functions have the following form in points $\rho_0, \rho_1, ..., \rho_n$:

$$N_l^p(\rho) = \begin{cases} \phi_{j,p}^p(\eta), & \rho = \rho_{j-1} + 0.5\,h_j(1+\eta), \ |\eta| \leq 1 \\ \phi_{j+1,0}^0(\eta), & \rho = \rho_j + 0.5\,h_{j+1}(1+\eta), \ |\eta| \leq 1 \ , \ l = (j-1)p. \\ 0, & \rho \in \Delta_j \bigcup \Delta_{j+1} \end{cases} \qquad (20)$$

Functions $\{N_l^p(\rho)\}_{l=0}^L$, $L = np + 1$, form a basis in the space of polynomials of the p-th order. Now, we approximate the global function $\mathbf{F}(\rho) \equiv (F_1(\rho), F_2(\rho), ..., F_N(\rho))^T$ by a finite sum of local functions $N_l^p(\rho)$

$$\mathbf{F}(\rho) = \sum_{l=0}^L F_l N_l^p(\rho) \qquad (21)$$

and substitute expansion (21) into the functional (15). From the minimum condition [28, 29] for this functional we obtain that vector–solution $\mathbf{F}^h$ is the eigenvector of generalized algebraic problem

$$\mathbf{A}^p \mathbf{F}^h = E^h \mathbf{B}^p \mathbf{F}^h. \qquad (22)$$

The following estimations for FEM eigensolutions of problem (22) are valid [28]:

$$|E_n^h - E_n| \le c_1(E_n) h^{2p}, \tag{23}$$

$$\left\| \mathbf{F}_n^h(\rho) - \mathbf{F}_n(\rho) \right\|_0 \le c_2(E_n) h^{p+1}, \tag{24}$$

where h is the maximal step of the finite–element grid, n is the number of the corresponding solution, and constants c_1 and c_2 do not depend on step h. The $\mathbf{A}^p$ and $\mathbf{B}^p$ matrices are symmetric and have a banded structure, and $\mathbf{B}^p$ matrix is also positively defined. They have the following form

$$\mathbf{A}^p = \sum_{j=1}^n \mathbf{a}_j^p, \quad \mathbf{B}^p = \sum_{j=1}^n \mathbf{b}_j^p, \tag{25}$$

where the local on the element Δ_j matrices $\mathbf{a}_j^p$ and $\mathbf{b}_j^p$ are calculated by the formulae

$$
\begin{aligned}
(\mathbf{a}_j^p)_{\mu\nu}^{qr} &= \int_{-1}^{+1} \left\{ \frac{4}{h_j^2} (\phi_{j,q}^p)'(\phi_{j,r}^p)' + \left(\sum_{s=0}^p W_{\mu\nu}^s \phi_{j,s}^p \right) \phi_{j,q}^p \phi_{j,r}^p \frac{h_j}{2} \right. \\
&\left. + \sum_{s=0}^p Q_{\mu\nu}^s \phi_{j,q}^p \left[\phi_{j,s}^p (\phi_{j,r}^p)' + (\phi_{j,s}^p)' \phi_{j,r}^p \right] \right\} d\eta,
\end{aligned}
\tag{26}
$$

$$(\mathbf{b}_j^p)_{\mu\nu}^{qr} = \int_{-1}^{+1} \phi_{j,q}^p \phi_{j,r}^p \frac{h_j}{2} d\eta, \tag{27}$$

$$\rho = \rho_{j-1} + 0.5 h_j (1 + \eta), \quad q, r = 0, 1, ..., p, \quad \mu, \nu = 1, 2, ..., N.$$

In the above, $W_{\mu\nu}^s$ and $Q_{\mu\nu}^s$ are the values of matrix elements $W_{\mu\nu}(\rho)$ and $Q_{\mu\nu}(\rho)$ in the s nodes of elements Δ_j, respectively, and "$\prime$" denotes differentiation. In order to interpolate tabular matrices $\mathbf{W}$ and $\mathbf{Q}$ in the FE grid points, the same order of the interpolating polynomial as the order of the finite–element approximation is used. The integrals in Eqs.(26) and (27) are calculated using the Gauss integration rule [33] with $p + 1$ nodes.

In order to solve the generalized eigenvalue problem (22), the subspace iteration method [28, 29] elaborated by Bathe [29] for the solution of large symmetric banded matrix eigenvalue problems has been chosen. This method uses a skyline storage mode, which stores components of the matrix column vectors within the banded region of the matrix, and is ideally suited for banded finite element matrices. The procedure chooses a vector subspace of the full solution space and iterates upon the successive solutions in the subspace (for details, see [29]). The iterations continue until the desired set of solutions in the iteration subspace converges to within the specified tolerance on the Rayleigh

quotients for the eigenpairs. Generally, 10-16 iterations are required for the subspace iterations to converge the subspace to within the prescribe tolerance. If matrix $\mathbf{A}^p$ in Eq.(22) is not positively defined, problem (22) is replaced by the following problem:

$$\tilde{\mathbf{A}}^p \mathbf{F}^h = \tilde{E}^h \mathbf{B}^p \mathbf{F}^h, \tag{28}$$

,where $\tilde{\mathbf{A}}^p = \mathbf{A}^p + \alpha \mathbf{B}^p$. The number $\alpha > 0$ (the shift of the energy spectrum) is chosen in such a way that matrix $\tilde{\mathbf{A}}^p$ is positive. The eigenvectors of problems (22) and (28) are the same, and $E^h = \tilde{E}^h - \alpha$.

4 Description of the program

Fig. 1 presents a flow diagram for the HSEIGV program. The function of each subroutine is described in Section 4. The HSEIGV program is called from the main routine (supplied by a user) which sets dimensions of the arrays and is responsible for the input data. In the present code each array declarator is written in terms of the symbolic names of constants. These constants are defined in the following PARAMETER statement in the main routine:

PARAMETER (MTOT=1250000,MITOT=55000,NMESH1=11)

where

- MTOT is the dimension of the working DOUBLE PRECISION array TOT.

- MITOT is the dimension of the working INTEGER array ITOT.

- NMESH1 is the dimension of the DOUBLE PRECISION array RMESH containing the information about the subdivision of the hyperradial interval $[0, \rho_{max}]$ on subintervals and number of elements on each one of them. NMESH1 is always odd and ≥ 3.

A more concrete assignment of these dimensions is discussed below. In order to change the dimensions of the code all one has to do is to modify the single PARAMETER statement defined above in the main program unit.

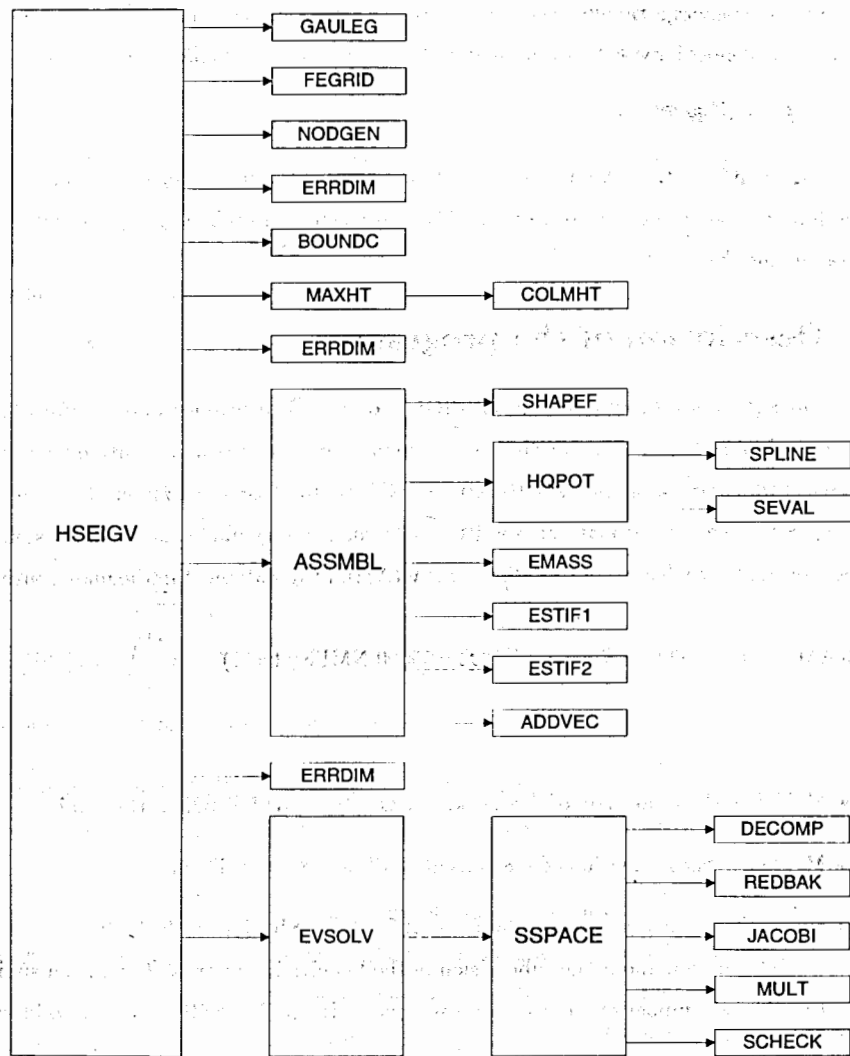The calling sequence for the subroutine HSEIGV is:

Fig.1

CALL HSEIGV (TITLE, NROOT, NDIM, MDIM, IDIM, IADT, NPOL, NMESH, RMESH, NSPL, NITEM, RTOL, SHIFT, IPRINT, IPRSTP, EGRND, FNOUT, IOUT, POTEN, IOUP, ASPOT, IASP, EVWFN, IOUF, IOUW, TOT, MTOT, ITOT, MITOT)

where the arguments have the following type and meaning:

Input data

TITLE	CHARACTER	title of the run to be printed on the output listing. The title should be no longer than 70 characters.
NROOT	INTEGER	number of eigenvalues (energy levels) and eigenvectors (radial wave functions) required.
NDIM	INTEGER	number of coupled differential equations.
MDIM	INTEGER	number of potential curves stored in file POTEN. It defines the maximum dimension of potential matrices $H_{\mu\nu}$ and $Q_{\mu\nu}$ to be read from this file (for details, see [25]). MDIM ≥ NDIM.
IDIM	INTEGER	flag specifying the number of potential curve $U_\mu(\rho)$ or adiabatic potential $W_{\mu\mu}(\rho)$ required ($\mu \equiv$ IDIM). It is used (if NDIM = 1) for computing energy levels and radial wave functions in the adiabatic approximation. IDIM ≤ MDIM.
IADT	INTEGER	flag specifying the type of adiabatic approximation (it is used only if NDIM = 1): = 0 uncoupled adiabatic approximation (see Eq. (13)); = 1 extreme adiabatic approximation (see Eq. (14)).
NPOL	INTEGER	order of finite element shape functions (interpolating Lagrange polynomials). Usually set to 6-8.
NMESH	INTEGER	dimension of array RMESH. NMESH should always be odd and ≥ 3.
RMESH	REAL*8	array RMESH contains information about subdivision of interval $[\rho_{min}, \rho_{max}]$ of hyperradius ρ on subintervals. The whole interval $[\rho_{min}, \rho_{max}]$ is divided as follows: RMESH(1) = ρ_{min}, RMESH(NMESH) = ρ_{max}, and the values of RMESH(I) set the number of elements for each subinterval [RMESH(I-1), RMESH(I+1)], where I=2, 4,..., NMESH−1.
NSPL	INTEGER	number of records written in file POTEN by the HSTERM program, i.e. number of hyperradial points from the interval $[0, \rho_{max}]$ in which potential curves $U_\mu(\rho)$ and radial matrix elements $H_{\mu\nu}(\rho)$ and $Q_{\mu\nu}(\rho)$ have been calculated and stored into file POTEN. Potential matrices read from file POTEN are interpolated using

the cubic spline interpolation. Using the spline coefficients calculated in the NSPL points the values of potential matrix elements are computed in the NGRID nodes of the finite–element grid.

NITEM	INTEGER	maximum number of subspace iterations permitted (usually set to 16).
RTOL	REAL*8	convergence tolerance on eigenvalues (1.D-06 or smaller).
SHIFT	REAL*8	shift of the energy spectrum. If SHIFT = 0 the value of the energy shift is determined automatically by the program; otherwise, the NROOT eigenvalues and eigenvectors closest to the shift given are calculated (the nonzero value of SHIFT is recommended since it significantly speeds up the calculation).
IPRINT	INTEGER	level of print: = 0 – minimal level of print. The initial data, short information about the numerical scheme parameters, main flags and keys, and energy values calculated are printed out; = 1 – radial functions calculated are printed out with step IPRSTP additionally; = 2 – potential matrix is printed out with step IPRSTP; = 3 – information about nodal point distribution is printed out; = 4 – global matrices **A** and **B** are printed out additionally; = 5 – the highest level of print. The local stiffness and mass matrices together with all current information about the course of the subspace iteration method solution of the generalized eigenvalue problem are printed out.
IPRSTP	INTEGER	step with which potential matrix and radial wave functions are printed out.
EGRND	REAL*8	ground state energy (in a.u.) of a system. It is used only if the energy values (in eV) measured relative to the ground state energy are required. Default value is zero.
FNOUT	CHARACTER	name of the output file (up to 55 characters) for printing out the results of the calculation. It is system specific and may include a complete path to the file location.
IOUT	INTEGER	number of the output logical device for printing out the results of the calculation (usually set to 7).
POTEN	CHARACTER	name of the input file (up to 55 characters) containing potential curves and matrix elements of radial coupling calculated and stored by the HSTERM program [25].
IOUP	INTEGER	number of the logical device for reading data from file POTEN.
ASPOT	CHARACTER	name of the input file (up to 55 characters) containing the second–order corrections (the eigenvalues of the corresponding equivalent operator) and matching points

between the relevant numerical and asymptotic curves calculated and stored by the ASYMPT program (for details, see [26]). It is used only if IASP > 0.

IASP	INTEGER	number of the logical device for reading data from file ASPOT.
EVWFN	CHARACTER	name of the output file (up to 55 characters) for storing the results of the calculation, namely, the energy values, finite–element grid points, and radial wave functions. It is used only if IOUF > 0.
IOUF	INTEGER	number of the logical device for storing data into file EVWFN.
IOUW	INTEGER	scratch working file.
TOT	REAL*8	working vector of the DOUBLE PRECISION type.
MTOT	INTEGER	dimension of the DOUBLE PRECISION array ITOT. The last address ILAST of array TOT is calculated and then compared with the given value of MTOT. If ILAST > MTOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MTOT of array TOT to the quantity ILAST taken from the message.
ITOT	INTEGER	working vector of the INTEGER type.
MITOT	INTEGER	dimension of the INTEGER working array ITOT. The last address ILAST of array ITOT is calculated and then compared with the given value of MITOT. If ILAST > MITOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MITOT of array ITOT to the quantity ILAST taken from the message.

Output data

The results of the calculation of energy values and radial wave functions are written using unformatted segmented records into file EVWFN according to the following operator:

```
WRITE (IOUF) NDIM,NN,NROOT,(EIGV(II),II=1,NROOT),
             (RGRID(JJ),JJ=1,NGRID),
             ((WFN(I,J),I=1,NN),J=1,NROOT)
```

In the above, parameters presented in the WRITE statement have the following meaning:

- NDIM is the number of radial equations.

- NGRID is the number of finite–element grid points.

- NN = NGRID * NDIM.

- NROOT is the number of roots (energy levels).

- Array EIGV contains the energy values calculated.

- Array RGRID contains the values of the finite–element grid points.

- Two-dimensional array WFN contains NROOT eigenfunctions each per NN = NDIM * NGRID elements in length stored by the following way: for each of the NGRID mesh points per NDIM elements of eigenfunction (see scheme below):

1-st root	2-nd root	. . .	last root

1	1	1
2	2	2
1-st point	1-st point	1-st point .
.	.	.
.	.	.
NDIM	NDIM	NDIM
1	1	1
2	2	2
2-nd point .	2-nd point	2-nd point .
.	.	.
.	.	.
NDIM	NDIM	NDIM

1	1	1
2	2	2
last point .	last point .	. . . last point .
.	.	.
NDIM	NDIM	NDIM

5 Description of subprogram units

A flow diagram for the HSEIGV program is presented in Fig. 1. The function of each subroutine is briefly described below. Additional details may be found in COMMENT cards within the program.

- Subroutine ADDVEC assembles the element vector STIFF into the corresponding global vector using a compact storage form.

- Subroutine ASSMBL controls the calculation of element stiffness and mass matrices and assembles them into the corresponding global matrices.

- Subroutine BOUNDC sets the Dirichlet or Neumann boundary conditions.

- Subroutine COLMHT calculates column heights in banded matrix.

- Subroutine DECOMP calculates $L(D)L^T$ factorization of stiffness matrix. This factorization is used in subroutine REDBAK to reduce and back-substitute the iteration vectors.

- Subroutine EMASS calculates a diagonal part of the local on element mass matrix.

- Subroutine ERRDIM prints error messages when high-speed storage requested by a user is exceeded and stops the execution of program HSEIGV.

- Subroutine ESTIF1 calculates a diagonal part of the local on element stiffness matrix.

- Subroutine ESTIF2 calculates a non-diagonal part of the local on element stiffness matrix.

- Subroutine EVSOLV prepares all input data for the SSPACE program, prints out the calculated eigensolutions, and writes them into the file EVWFN if necessary.

- Subroutine FEGRID calculates nodal points for the finite–element grid.

- Subroutine GAULEG [34] calculates nodes and weights of the Gauss-Legendre quadrature.

- Subroutine HQPOT reads potential curves and matrix elements of radial coupling at the NSPL points from file POTEN and interpolate them using the cubic spline interpolation in the NGRID points of the finite–element mesh.

- Subroutine JACOBI solves the generalized eigenproblem in subspace using the generalized Jacobi iteration.

- Subroutine MAXHT calculates addresses of diagonal elements in banded matrix.

- Subroutine MULT evaluates product of the two vectors stored in compact form.

- Subroutine NODGEN generates a nodal point distribution for the finite–element grid.

- Subroutine SCHECK evaluates shift for Sturm sequence check (called only if SHIFT=0).

- DOUBLE PRECISION function SEVAL [35] evaluates the cubic spline function for a given value of x.

- Subroutine SHAPEF calculates shape functions of the given order and their derivatives with respect to the master element coordinate η at a specified value of x.

- Subroutine SPLINE [35] calculates coefficients for the cubic interpolating spline.

- Subroutine SSPACE [28] finds the smallest eigenvalues and corresponding eigenvectors in the generalized eigenproblem using the subspace iteration method [28]. We have added to this program the possibility of finding the eigensolutions closest to the energy spectrum shift given and also the possibility of using the previously calculated eigenvectors as the starting vectors for inverse iterations. The list of arguments for this program is adequately commented in the routine, so, the interested

reader is referred to the program listing for further details. Warning messages will be issued if the requested accuracy RTOL is not obtained after NITEM iterations or if the stiffness matrix **A** is not positively defined.

6   Test deck

The HSEIGV program has been used [11,19–21] for the calculation of the energy values of the doubly excited states of He and H$^-$ in both the adiabatic and coupled–channel approximations of the hyperspherical adiabatic approach.

The test run which accompanies the HSEIGV program is devoted to the computation of the ground state energy in the coupled–channel approximation and energy values of the first four $^1S^e$ doubly excited states of H$^-$ (below the $n = 2$ threshold) in the adiabatic approximation of the HSA approach. It consists of the following three steps: (i)calculation of the potential curves and matrix elements of radial coupling using the HSTERM program [25]; (ii) computation of the adiabatic potential curve asymptotics and matching points between the calculated and asymptotic curves using the ASYMPT program [26]; (iii) ten–channel calculation of the ground state energy of H$^-$ and one–channel computation of the energies of the first several $^1S^e$ doubly excited states below the $n = 2$ threshold using the HSEIGV program.

File 'hsterm.dat' containing the initial data for the calculation of the first ten potential curves and corresponding radial matrix elements for the $^1S^e$ state of H$^-$ using the HSTERM program is given below:

```
Hyperspherical potential curves for 1Se state of H-
&RMESH    IREAD=0,IRBEG=1,IREND=250,
          NGRID=11,RVALUE=0.D0,
          RGRID=0.1D0,0.1D0,15.1D0,0.25D0,30.1D0,
             1.D0,45.1D0,5.D0,90.1D0,10.D0,200.1D0,
                                                &END
&FLAGS    ISTATE=1,ISECTR=0,IDIPOL=0,INTGRL=2,
          NGAUSS=0,IPRINT=0,IPRSTP=1,
          IAS=0,RAS=0.D0,
                                                &END
```

```
&STATE1   JTOT1=0,MTOT1=0,ISPIN1=0,IPI1=0,LMAX1=5,
          KMAX1=7,NCH1=10,SHIFT1=0.6500D0,Z=1.D0,
          NPOL1=7,NELEM1=40,NITEM=16,RTOL=1.D-6,
                                                        &END
&STATE2                                                 &END
&FILES    IOUT=7,FNOUT='hsterm.out',ST1FN1='hm1se.matrix',
          ST1FN2='hm1se.ovlapm',ST1FN3='hm1se.asympt',
          ST1FN4='hm1se.fncrnt',ST1FN5='hm1se.wavefn',
          ST1FN6='hm1se.acoeff',ST1FN7='hm1se.fnsurf',
          ST1NT1=11,ST1NT2=12,ST1NT3=13,ST1NT4=14,
          ST1NT5=15,ST1NT6=16,ST1NT7=17,NTWRK1=31,
          NTWRK2=32,NTWRK3=33,NTWRK4=34,NTWRK5=35,
                                                        &END
```

In order to carry out this calculation, dimensions of several arrays listed in the PA-RAMETER statement of the HSTERM program should be changed. These dimensions are: MTOTAL=31000, MITOT=5000, NRTMAX=7, NSTMAX=281, NCLMAX=6, and NCHMAX=10. As a result, we obtain potential matrix elements calculated for 246 values of hyperradius ρ taken (with a nonuniform step) on interval [0.1,200.1]. This part of the calculation requires 13.6 min on DECstation 3000 Model 800. The results of the computation are written into file 'hm1se.matrix'.

The initial data for the ASYMPT program are given (using the Fortran operator DATA) as follows:

```
DATA FNPOT /'hm1se.matrix'/,  FNASP /'hm1se.aspot'/
DATA FNOUT /'asympt.out'/,    EPS/2.D-6/,   CHARGE/1.D0/
DATA RMIN/20.D0/,RMAX/200.D0/,RSTEP/0.001D0/,ICFS/15/
DATA LMIN  /0/, LMAX  /0/,   LSTEP /1/,    IPRINT/0/
DATA NTHRMN/1/, NTHRMX/4/,   NPCMAX/10/,   NPTMAX/246/
DATA IASPOT/2/, ICURVE/0/,   IDFLAG/1/,    IUNITS/1/
DATA IOUT  /7/, IPLT  /0/,   IPOT /10/,    IASP  /11/
```

In order to carry out the calculation, dimensions of working arrays TOT and ITOT in the PARAMETER statement of the main routine of the ASYMPT program should be set as follows: MTOT = 5000 and MITOT = 900. This part of the test run requires 1.1 s. The results of the computation of the second-order (dipole) corrections $V_{\mu\mu}^{(2)}$ (in Ry) and matching points between the calculated adiabatic potentials and asymptotic ones (for details, see [26]) are written into file 'hm1se.aspot'.

For the final part of the test run, the initial data for the HSEIGV program are given as foolows:

```
DATA FNOUT /'hseigv.out'/, POTEN /'hm1se.matrix'/
DATA ASPOT /'hm1se.aspot'/,RTOL/1.D-10/,SHIFT/0.528D0/
DATA EGRND /0.D0/,RMESH/0.16D0,200.D0,30.D0/
DATA NMESH/3/, IOUT/7/,  IOUF/0/,   IOUW/20/,
DATA IOUP/10/, IASP/0/,  NSPL/246/, NITEM/16/
DATA NDIM/10/, MDIM/10/, IDIM/1/,   IADT/1/
DATA NROOT/1/, NPOL/6/,  IPRINT/0/, IPRSTP/135/
```

The ten-channel calculation of the ground state energy of H⁻ gives the value $E = -0.527737$ a.u. which is in excellent agreement with the variational calculation $E_{var} = -0.527751$ a.u. [36]. Comparison with the energy value $E_{MCHF} = -0.527542$ a.u. obtained [37] by the multiconfigurational Hartree-Fock method using 32 configurations shows that our value calculated using only 10 states of the HSA basis is more accurate.

The second part of the test run is designed to show how to use the HSEIGV program for computing the energies of high lying states. Consider, as an example, the calculation of the first four doubly excited $^1S^e$ states of H⁻ below the $n = 2$ threshold. In order to perform such calculation the values of several parameters and flags should be changed. These parameters can be chosen, as follows: NROOT = 4, NDIM = 1, IDIM = 2, IADT = 0, IASP = 2, IPRINT = 1, EGRND = -0.527751D0, SHIFT = 0.132D0, NMESH = 5, RMESH(1) = 0.16D0, RMESH(2) = 120.D0, RMESH(3) = 30.D0, RMESH(4) = 580.D0, RMESH(1) = 200.D0, RTOL = 1.D-7. The results of this calculation are presented in Table 1 where they are compared with results obtained by several other methods. It is evident that our adiabatic energies agree very well with other calculations. If the higher accuracy is desired, the adiabatic energies obtained can be used for the calculation of the energy values of doubly excited states in the coupled-channel approximation as the energy spectrum shifts for the HSEIGV program. This test run (for the combined computation

Table 1: Energy values $-E$ (in a.u.) of the $^1S^e$ doubly excited states of H$^-$ below the second threshold.

Method	E_1	E_2	E_3	E_4
HSA[a]	0.148911	0.125995	0.124976	0.124399
POM[b]	0.148782			
TDM[c]	0.147896	0.125973	0.125012	
CRM[d]	0.148777			
FPM[e]	0.148695	0.126015	0.124662	

[a]HSA, present HSA calculation in the adiabatic approximation
[b]POM, Projection–operator method using a Hylleraas basis functions [38]
[c]TDM, Truncated diagonalization method with hydrogenic basis functions [39]
[d]CRM, Complex rotation method with Hylleraas–type functions [40]
[e]FPM, Feshbach–projected method using a Slater–type basis [41]

of the energy values of the ground state and four doubly excited states) requires 11.8 s on the DECstation 3000 Model 800.

Acknowledgments

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TEST RUN OUTPUT

PROBLEM: Ground state energy of H-
****

C O N T R O L   I N F O R M A T I O N

```
NUMBER OF DIFFERENTIAL EQUATIONS. . . . . (NDIM ) =      10
NUMBER OF ENERGY LEVELS REQUIRED. . . . . (NROOT ) =       1
NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =     200
NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =    1201
NUMBER OF INTERPOLATION POINTS. . . . . . (NSPL ) =      246
ORDER   OF SHAPE FUNCTIONS . . . . . . . . (NPOL ) =       6
ORDER   OF GAUSS-LEGENDRE QUADRATURE . . . (NGQ  ) =       7
ADIABATIC CURVE NUMBER (IF NDIM=1). . . . (IDIM ) =       1
UPPER (0) OR LOWER (1) BOUND (IF NDIM=1). (IADT ) =       1
SHIFT   OF ENERGY SPECTRUM . . . . . . . . (SHIFT ) =  0.528000
```

SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
****

NO OF GROUP	NUMBER OF ELEMENTS	BEGIN OF INTERVAL	LENGTH OF ELEMENT	GRID STEP	END OF INTERVAL
1	200	0.16000	0.14920	0.024867	30.000

T O T A L   S Y S T E M   D A T A

```
TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     11990
TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =    484745
MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =        70
MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =        40
```

THERE ARE   0 ROOTS LOWER THEN SHIFT
CONVERGENCE REACHED FOR RTOL 0.1000E-09

I T E R A T I O N   N U M B E R   4
RELATIVE TOLERANCE REACHED ON EIGENVALUES
0.6332E-11

****

LEVEL NUMBER	ENERGY (A.U.)	ENERGY (RY)
1	-0.52773741D+00	-0.10554748D+01

****

PROBLEM: Doubly excited states of H- below the n=2 threshold
****

C O N T R O L   I N F O R M A T I O N

```
NUMBER OF DIFFERENTIAL EQUATIONS. . . . . (NDIM ) =       1
NUMBER OF ENERGY LEVELS REQUIRED. . . . . (NROOT ) =       4
NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =     700
NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =    4201
NUMBER OF INTERPOLATION POINTS. . . . . . (NSPL ) =      246
ORDER   OF SHAPE FUNCTIONS . . . . . . . . (NPOL ) =       6
ORDER   OF GAUSS-LEGENDRE QUADRATURE . . . (NGQ  ) =       7
ADIABATIC CURVE NUMBER (IF NDIM=1). . . . (IDIM ) =       2
UPPER (0) OR LOWER (1) BOUND (IF NDIM=1). (IADT ) =       0
SHIFT   OF ENERGY SPECTRUM . . . . . . . . (SHIFT ) =  0.132000
```

SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
****

NO OF GROUP	NUMBER OF ELEMENTS	BEGIN OF INTERVAL	LENGTH OF ELEMENT	GRID STEP	END OF INTERVAL
1	120	0.16000	0.24867	0.041444	30.000
2	580	30.00000	0.29310	0.048851	200.000

TOTAL SYSTEM DATA

TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN) =   4199
TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =   18887
MAXIMUM HALF BANDWIDTH . . . . (MK) =   7
MEAN   HALF BANDWIDTH . . . . (MMK) =   4

DIPOLE ASYMPTOTICS OF ADIABATIC POTENTIALS:
****

| CHANNEL | THRESHOLD | MATCHING | DIPOLE |
NUMBER	NUMBER	RHO-POINT	COEFFICIENT
2	2	88.80800	-5.082763

THERE ARE   1 ROOTS LOWER THEN SHIFT
CONVERGENCE REACHED FOR RTOL 0.1000E-06
I T E R A T I O N   N U M B E R 17
RELATIVE TOLERANCE REACHED ON EIGENVALUES
 0.6116E-11 0.1761E-11 0.8361E-08 0.3249E-07

****

LEVEL NUMBER	ENERGY (a.u.)	ENERGY (Ry)	ENERGY (eV)
1	-.14891133D+00	-.29782265D+00	0.10308837D+02
2	-.12599542D+00	-.25199084D+00	0.10932415D+02
3	-.12497592D+00	-.24995183D+00	0.10960158D+02
4	-.12439947D+00	-.24879893D+00	0.10975844D+02

****

R   R A D I A L   E I G E N F U N C T I O N S
-       --

| 0.201444 | 0.2452D-06 | 0.5785D-07 | 0.2328D-07 | 0.3132D-07 |
| 5.796444 | 0.1726D+00 | 0.3689D-01 | 0.1478D-01 | 0.1983D-01 |

11.391444	0.3389D+00	0.3470D-01	0.1332D-01	0.1744D-01
16.986444	0.1553D+00	-.5919D-01	-.2440D-01	-.3322D-01
22.581444	0.5320D-01	-.1240D+00	-.4848D-01	-.6407D-01
28.176444	0.1722D-01	-.1572D+00	-.5720D-01	-.7238D-01
34.445402	0.4705D-02	-.1666D+00	-.5260D-01	-.6051D-01
41.040230	0.1175D-02	-.1575D+00	-.3722D-01	-.3299D-01
47.635057	0.2872D-03	-.1391D+00	-.1632D-01	0.1143D-02
54.229885	0.6754D-04	-.1179D+0Q	0.6453D-02	0.3528D-01
60.824713	0.1549D-04	-.9725D-01	0.2877D-01	0.6485D-01
67.419540	0.5029D-05	-.7862D-01	0.4921D-01	0.8697D-01
74.014368	0.3373D-05	-.6263D-01	0.6700D-01	0.1001D+00
80.609195	0.2040D-05	-.4931D-01	0.8175D-01	0.1036D+00
87.204023	-.5504D-07	-.3847D-01	0.9338D-01	0.9806D-01
93.798851	-.1793D-05	-.2981D-01	0.1020D+00	0.8449D-01
100.393678	-.2147D-05	-.2299D-01	0.1079D+00	0.6442D-01
106.988506	-.1080D-05	-.1765D-01	0.1112D+00	0.3960D-01
113.583333	0.5827D-06	-.1351D-01	0.1121D+00	0.1196D-01
120.178161	0.1807D-05	-.1030D-01	0.1109D+00	-.1652D-01
126.772989	0.1959D-05	-.7838D-02	0.1078D+00	-.4391D-01
133.367816	0.1066D-05	-.5947D-02	0.1029D+00	-.6843D-01
139.962644	-.3265D-06	-.4499D-02	0.9649D-01	-.8856D-01
146.557471	-.1500D-05	-.3392D-02	0.8882D-01	-.1031D+00
153.152299	-.1926D-05	-.2545D-02	0.8005D-01	-.1112D+00
159.747126	-.1467D-05	-.1896D-02	0.7037D-01	-.1125D+00
166.341954	-.3777D-06	-.1395D-02	0.5993D-01	-.1069D+00
172.936782	0.8449D-06	-.1005D-02	0.4888D-01	-.9500D-01
179.531609	0.1689D-05	-.6950D-03	0.3737D-01	-.7741D-01
186.126437	0.1826D-05	-.4405D-03	0.2552D-01	-.5528D-01
192.721264	0.1220D-05	-.2215D-03	0.1345D-01	-.2992D-01
199.316092	0.1247D-06	-.2048D-04	0.1266D-02	-.2845D-02

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