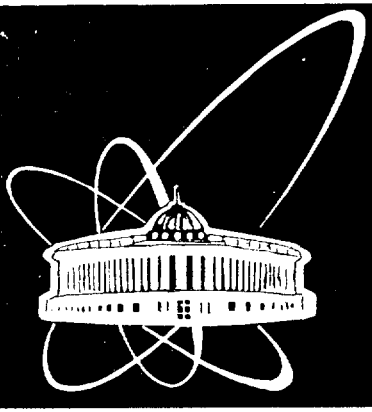

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E11-97-326

A.G.Abrashkevich*, I.V.Puzynin, S.I.Vinitsky

ASYMPT — A PROGRAM TO CALCULATE ASYMPTOTICS OF HYPERSPHERICAL POTENTIAL CURVES AND ADIABATIC POTENTIALS

Submitted to «Computer Physics Communications»

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1997

PROGRAM SUMMARY

Title of program: ASYMPT
Computer for which the program is designed and others on which it has been tested:
Computers: SGI Indigo^2, IBM RS/6000 Model 320H, 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, MS-Windows 95, Linux 1.0.9
Programming language used: FORTRAN 77
Memory required to execute with typical data: depends on the maximum values of total orbital momentum and threshold number considered. Test run requires 528 KB
No. of bits in a word: 64
Peripherals used: line printer, scratch disc store
No. of lines in distributed program, including test data, etc: 1276
External subprograms used: F02ABF [1], SPLINE and SEVAL [2]
Keywords: atomic physics, two-electron systems, hyperspherical coordinates, Schrödinger equation, adiabatic approach, potential curves, adiabatic potentials, perturbation theory, dipole asymptotics

Nature of physical problem
The purpose of this program is to calculate asymptotics of hyperspherical potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ within the hyperspherical adiabatic approach [3]. The program finds also the matching points between the numerical and asymptotic adiabatic curves within the given accuracy. The adiabatic potential asymptotics can be used for the calculation of the energy levels and radial wave functions of doubly excited states of two electron systems in the adiabatic and coupled channel approximations.

Method of solution
In order to compute the asymptotics of hyperspherical potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ it is necessary to solve the corresponding secular equation eigenvalues of which give the second order corrections in the asymptotic expansions of potential curves and effective potentials in the powers of ρ^{-1}. The matrix elements of the equivalent operator corresponding to the perturbation ρ^{-2} are calculated in the basis of the Coulomb parabolic functions in the body fixed frame. The asymptotics of potential curves and adiabatic potentials are calculated within an accuracy of $O(\rho^{-2})$ using the eigenvalues of the corresponding secular equation.

Restrictions on the complexity of the problem
The computer memory requirements depend on: a) the maximum value of the total orbital momentum considered; and b) the number of maximum threshold required. Restrictions due to dimension sizes may be easily alleviated by altering PARAMETER statements (see Long Write-Up and listing for details).

Typical Running time
The test run which accompanies this paper took 0.3 s on the DECstation 3000 Model 800.

References

[1] *NAG Fortran Library Manual, Mark 15* (The Numerical Algorithms Group Limited, Oxford, ©1991).

[2] G. E. Forsythe, M. A. Malcolm, and C. B. Moler, *Computer Methods for Mathematical Computations (Englewood Cliffs, Prentice Hall, New Jersey*, 1977).

[3] A. G. Abrashkevich, D. G. Abrashkevich, I. V. Puzynin, and S. I. Vinitsky, *J. Phys. B* **24** (1991) 1615.

LONG WRITE–UP

1 Introduction

Theoretical studies of doubly excited states of atoms and ions over the past few decades have established that the existence and properties of these states owe much to the strong electron–electron correlations [1–3]. The properties of strongly correlated doubly excited states of two–electron systems are described in a most natural way within the hyperspherical coordinate method [1–3]. The method takes advantage of the hyperspherical coordinates [1], i.e. a pair of collective variables ρ and α replacing the independent–electron radial coordinates r_1 and r_2. In these 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 most widely used adiabatic approximation, the hyperradius ρ is treated as an adiabatic parameter, analogous to the internuclear distance in the Born–Oppenheimer approximation for molecules. In this approximation, the energies and wave functions of doubly excited states are obtained as the solutions of uncoupled radial equations for the corresponding adiabatic potentials [1–3]. This approach has played a prominent role in understanding the strong electron–electron correlations in two–electron systems [1–4], description of spectra of doubly excited states [1–13], and study of one– and multi–photon ionization of He and photodissociation of H^- [14–19].

In papers [20, 21] programs designed to calculate potential curves and matrix elements of radial coupling for two-electron atoms within the hyperspherical adiabatic approach have been presented. These potentials can be used for the calculation of the energy spectrum of the doubly excited states and also scattering and photoionization cross sections using the adiabatic or coupled-channel approximations. In order to reduce the computational expenses in obtaining accurate potential curves and wave functions in the large ρ-region it is desirable to match numerical solutions at small ρ to asymptotic expansions at large ρ. Such asymptotic expansions for adiabatic potentials and wave functions for two-electron atoms have been proposed in [1,22–24] using basis sets constructed from Laguerre polynomials and bipolar harmonics in space-fixed frame. Matrix elements of the corresponding potential operators expressed in terms of products of $3J$- and $6J$-symbols require summation of oscillating series and take a rather complicated form for large values of total momentum and threshold number [22–24].

Recently, a new method for the calculation of asymptotics of hyperspherical potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ for a system of three distinguishable charged particles has been suggested [25, 26]. It allows to simplify significantly the calculation of matrix elements of potential operators using the basis constructed from linear combinations of the Coulomb parabolic functions in the rotating coordinate system. The extension of this approach onto the case of two-electron systems has been carried out in [27]. The adiabatic potentials calculated in the second-order approximation have been used [12, 13, 28] for calculation of the energy spectra of the doubly excited states of He and H^- in the adiabatic and coupled-channel approximations.

In the present paper we present a program to calculate asymptotics of hyperspherical potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ using the method developed in [25–27]. The second-order corrections to the potentials are obtained as the solutions of the corresponding secular equation. The program automatically finds matching points between numerical and asymptotic adiabatic curves with the given accuracy. These asymptotics can be used for the calculation of energy levels and radial wave functions of the doubly excited states of two-electron atoms.

The paper is organized as follows. In section 2 we give a short description of the

method. A description of the ASYMPT program is given in Section 3. Subroutine units are briefly described in Section 4. Test run is considered in Section 5.

2 Method

2.1 Hyperspherical adiabatic representation

The Schrödinger equation for a two-electron atomic system with nuclear charge Z and total energy E, expressed in the hyperspherical coordinates

$$\rho = \sqrt{r_1^2 + r_2^2}\ , \quad \alpha = \tan^{-1}(r_2/r_1), \tag{1}$$

has the following form ($\hbar = e = m_e = 1$):

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

where

$$\hat{h}(\rho) = \frac{1}{\rho^2}\hat{\Lambda}^2(\Omega) + \frac{1}{\rho}V(\alpha,\theta_{12}), \tag{3}$$

$$\hat{\Lambda}^2(\Omega) = -\frac{\partial^2}{\partial\alpha^2} + \frac{\mathbf{l}_1^2}{\cos^2\alpha} + \frac{\mathbf{l}_2^2}{\sin^2\alpha}, \tag{4}$$

and

$$V(\alpha,\theta_{12}) = -\frac{2Z}{\cos\alpha} - \frac{2Z}{\sin\alpha} + \frac{2}{\sqrt{1-\sin 2\alpha\cos\theta_{12}}}. \tag{5}$$

In the above, wave function $\Psi(\rho,\Omega)$ is connected with the total two electron wave function ψ by relation $\Psi(\rho,\Omega) = (\rho^{5/2}\sin\alpha\cos\alpha)\psi$, Ω represents the five angles $\{\alpha,\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2\}$; $\mathbf{l}_i$ is the operator of the orbital momentum of the ith electron, and $\theta_{12} = \cos^{-1}[(\mathbf{r}_1\cdot\mathbf{r}_2)/r_1r_2]$.

The hyperspherical adiabatic (HSA) states $\{\Phi_\mu(\Omega;\rho)\}_{\mu=1}^{\infty}$ 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 methods of computation of the five-dimensional channel functions $\Phi_\mu(\Omega;\rho)$ have been discussed in our previous papers [20, 21]. For large values of ρ the HSA functions take on the form of the hydrogenic wave functions perturbed by a distant charged

particle. For ρ close to the origin the HSA states resemble the hyperspherical harmonics (K-harmonics [2, 3]), defined as the eigenfunctions of $\hat{\Lambda}^2(\Omega)$, the generalized angular momentum operator.

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

$$\Psi(\rho,\Omega) = \sum_{\mu=1}^{N} F_\mu(\rho)\Phi_\mu(\Omega;\rho). \tag{7}$$

Substitution of expansion (7) into Eq. (2) and averaging over the basis functions $\Phi_\mu(\Omega;\rho)$ lead to a system of N coupled ordinary differential equations for expansion coefficients $F_\mu(\rho)$, which can be written in the explicitly Hermitian form as

$$\left(-\frac{d^2}{d\rho^2} + V_{\mu\mu}(\rho) - 2E\right) F_\mu(\rho) + \sum_{\substack{\nu=1 \\ \nu\neq\mu}}^{N} V_{\mu\nu}(\rho)F_\nu(\rho) = 0, \quad (\mu = 1,2,...,N), \tag{8}$$

where

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

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

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

2.2 Asymptotics of adiabatic potential curves at $\rho \to \infty$

As shown in [27], the general classification of states of a two electron system in the HSA representation can be uniquely built in the molecular coordinate system. The transformation of the two electron wave function, $\Psi^{LM\pi}(\mathbf{r}_1,\mathbf{r}_2)$, given in the space-fixed coordinate system XYZ with the fixed axis Z, into the molecular system xyz with the axis z directed along the vector $\mathbf{r}_2$, has the following form [27]:

$$\Psi^{LM\pi}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{\mu=(1-\sigma)/2}^{L} \Psi_m^{L\sigma}(\rho,\alpha,\theta_{12})D_{mM}^{L\pi}(\Phi,\Theta,\phi), \tag{12}$$

where $\Psi_m^{L\sigma}(\rho, \alpha, \theta_{12})$ is the wave function in the molecular coordinate system $\mathbf{e}_x = \mathbf{e}_\Theta$, $\mathbf{e}_y = \mathbf{e}_\Phi$, $\mathbf{e}_z = \mathbf{e}_{\mathbf{r}_2}$ in the total-momentum representation L, $D_{mM}^{L\pi}(\Phi, \Theta, \phi)$ is a symmetrized Wigner D-function [29], m and M are the eigenvalues of the projections L_z and L_Z of the total orbital momentum operator $\mathbf{L} = \mathbf{l}_1 + \mathbf{l}_2$ onto the molecular z and fixed Z axes, $\pi = (-1)^{l_1+l_2} = \sigma(-1)^L$ and $\sigma = \pm 1$ are the eigenvalues of the operator of total parity $P_{\rm tot}$ ($\mathbf{r}_1 \to -\mathbf{r}_1$, $\mathbf{r}_2 \to -\mathbf{r}_2$) and reflection P_{yz} in the yz plane of the molecular coordinate system: $\phi \to \pi - \phi$ (for details, see [27]), and $\mathbf{l}_i$ is the orbital momentum operator of the ith electron.

Consider now asymptotic solutions for a separated atom with charge Z and electron 1 in the field of the distant electron 2, omitting all intermediate computations that can be found in papers [25–27]. The potential curves and solutions of the hyperspherical eigenvalue problem (6) are expanded in a series over inverse powers of ρ:

$$U_\mu(\rho) = U_\mu^{(0)} + U_\mu^{(1)}\rho^{-1} + U_\mu^{(2)}\rho^{-2} + O(\rho^{-3}), \tag{13}$$

$$\Phi_\mu(\Omega_{\rm as}; \rho) = \Phi_\mu^{(0)}(\Omega_{\rm as}) + \Phi_\mu^{(1)}(\Omega_{\rm as})\rho^{-1} + O(\rho^{-2}), \tag{14}$$

where $U_\mu^{(0)} = -Z^2/n^2$, $U_\mu^{(1)} = -2(Z-1)$ and $\Phi_\mu^{(0)}(\Omega_{\rm as})$ are, respectively, the zeroth and first-order energy corrections and wave function of the zeroth approximation of the hydrogen-like atom with a fixed principal quantum number n, and $\Omega_{\rm as}$ is the corresponding set of angular variables (see [26, 27]). To construct the correct functions of the zero-order approximation it is necessary [25–27] to take account of terms $\sim \rho^{-2}$ in the expansion of the surface adiabatic Hamiltonian (3) which remove the Coulomb degeneration in a layer of parabolic states $|n_1 n_2 m\rangle$ with a fixed principal quantum number $n = n_1 + n_2 + m + 1$, $m \equiv |m|$. An equivalent operator corresponding to the ρ^{-2} perturbation has the following form [27]:

$$\hat{\Lambda}^{(0)} = -3\frac{n}{Z}A_z + \frac{1}{2}(\mathbf{l}^2 - n^2) + (\mathbf{L} - \mathbf{l})^2, \tag{15}$$

where A_z is the z projection of the Runge-Lentz vector, $\mathbf{l} \equiv \mathbf{l}_1$ is the operator of electron orbital momentum, and $(\mathbf{L} - \mathbf{l})^2 = \mathbf{L}^2 + \mathbf{l}^2 - 2\mathbf{l}\cdot\mathbf{L}$. Here, $2\mathbf{l}\cdot\mathbf{L} = l_+L_- + l_-L_+ + 2L_z^2$ is the operator of Coriolis interaction, and $L_\pm$ and $l_\pm$ are spherical components (raising and lowering operators) of $\mathbf{L}$ and $\mathbf{l}$. Eigenvalues and eigenfunctions of the equivalent operator

$\hat{\Lambda}^{(0)}$ represent, respectively, the desired corrections $U_\mu^{(2)}$ in the expansion (13) and correct functions of the zeroth approximation [27]:

$$\Phi_\mu^{(0)}(\Omega_{as}) = \sum_{m=(1-\sigma)/2}^{\min(L,n-1)} \sum_{n_2=0}^{n-m-1} a_{n_2 m}^{(\mu)} \varphi_{n_1 n_2 m}(s,t) D_{mM}^{L\pi}(\Phi,\Theta,\phi). \tag{16}$$

Here, $\varphi_{n_1 n_2 m}(s,t)$ are Coulomb parabolic functions, $s = r_1 + z$, $t = r_1 - z$, of the form [30]:

$$\varphi_{n_1 n_2 m}(s,t) = C_{n_1 n_2 m} \varphi_{n_1 m}(s) \varphi_{n_2 m}(t), \quad . \tag{17}$$

$$C_{n_1 n_2 m} = 2^{1/2} \{ n_1! [(n_1 + |m|)!]^{-1} n_2! [(n_2 + |m|)!]^{-1} \}^{1/2}, \tag{18}$$

$$\varphi_{n_j m}(u_j) = [(n_j + |m|)!]^{-1} u_j^{|m|/2} \exp\left(-\frac{1}{2} u_j\right) L_{n_j+|m|}^{|m|}(u_j), \quad u_j = s,t, \quad j = 1,2, \tag{19}$$

where $L_{n_j+|m|}^{|m|}(u_j)$ are the Laguerre polynomials. The energy corrections $U_\mu^{(2)}$ and coefficients $a_{n_2 m}^{(\mu)}$ can be found from the secular equation

$$\sum_{m'=(1-\sigma)/2}^{\min(L,n-1)} \sum_{n_2'=0}^{n-m-1} \left[\left\langle n_1 n_2 m L M \pi \left| \hat{\Lambda}^{(0)} \right| n_1' n_2' m' L M \pi \right\rangle - U_\mu^{(2)} \delta_{n_2 n_2'} \delta_{m m'} \right] a_{n_2' m'}^{(\mu)} = 0. \tag{20}$$

In the above, states are characterized by the set of quantum numbers $\{LM\sigma nq\}$, where q=q(n_2, m) enumerates the roots $U_\mu^{(2)}$ as they increase in the secular equation (20) at fixed $LM\sigma n$. When $L \geq n-1$, the number of roots of Eq. (20) equals n^2, and $n(n+1)/2$ of them have the parity $\pi = +(-1)^L$, whereas $n(n-1)/2$, the parity $\pi = -(-1)^L$. The latter are degenerated with the states of opposite parity. Thus, there are $n(n+1)/2$ nondegenerate roots of Eq. (20) at fixed LMn (the standard $(2L+1)$-fold degeneracy still takes place). Solving the secular equation (20), we obtain the following expression for potential curves:

$$U_\mu(\rho) = -\frac{Z^2}{n^2} - \frac{2(Z-1)}{\rho} + \frac{U_\mu^{(2)}}{\rho^2}. \tag{21}$$

The similar expression can be obtained [27] for the adiabatic effective potentials $V_{\mu\mu}(\rho)$:

$$V_{\mu\mu}(\rho) = -\frac{Z^2}{n^2} - \frac{2(Z-1)}{\rho} + \frac{V_{\mu\mu}^{(2)}}{\rho^2}, \tag{22}$$

where $V_{\mu\mu}^{(2)}$ are the eigenvalues of the corresponding secular equation for equivalent operator

$$\hat{\Lambda} = -3\frac{n}{Z} A_z + (\mathbf{L} - \mathbf{I})^2, \tag{23}$$

which corresponds to the dipole integral of motion [31]. Matrix elements of equivalent operators $\hat{\Lambda}^{(0)}$ and $\hat{\Lambda}$ are defined on functions (16) by simple relations [26, 32]:

$$\langle n_1 n_2 m L M \pi | A_z | n_1' n_2' m' L M \pi \rangle = (n_2 - n_1)\delta_{n_2 n_2'}\delta_{m m'},$$

$$\langle n_1 n_2 m L M \pi | L^2 - 2L_z^2 | n_1' n_2' m' L M \pi \rangle = [L(L+1) - 2m^2]\delta_{n_2 n_2'}\delta_{m m'},$$

$$\begin{aligned}\langle n_1 n_2 m L M \pi | l^2 | n_1' n_2' m' L M \pi \rangle &= \delta_{m m'}\Big\{ \frac{1}{2}\left[n^2 - 1 + m^2 - (n_1 - n_2)^2\right]\delta_{n_2 n_2'} \\ &- \sqrt{(n_2+1)n_1(n_1+m)(n_2+m+1)}\,\delta_{n_2' n_2 + 1} \\ &- \sqrt{(n_1+1)n_2(n_2+m)(n_1+m+1)}\,\delta_{n_2' n_2 - 1}\Big\},\end{aligned}$$

$$\langle n_1 n_2 m L M \pi | l_+ L_- | n_1 n_2 + 1 m - 1 L M \pi \rangle = \sqrt{(n_2+1)(n_1+m)}\,\gamma_{m,m-1}^{L\pi},$$

$$\langle n_1 n_2 m L M \pi | l_+ L_- | n_1 + 1 n_2 m - 1 L M \pi \rangle = -\sqrt{(n_1+1)(n_2+m)}\,\gamma_{m,m-1}^{L\pi},$$

$$\langle n_1 n_2 m L M \pi | l_- L_+ | n_1 n_2 - 1 m + 1 L M \pi \rangle = \sqrt{n_2(n_1+m+1)}\,\gamma_{m,m+1}^{L\pi},$$

$$\langle n_1 n_2 m L M \pi | l_- L_+ | n_1 - 1 n_2 m + 1 L M \pi \rangle = -\sqrt{n_1(n_2+m+1)}\,\gamma_{m,m+1}^{L\pi},$$

$$\gamma_{m,m-1}^{L\pi} = [1 + (\sqrt{2}-1)\delta_{m1}]\sqrt{(L-m+1)(L+m)},$$

$$\gamma_{m,m+1}^{L\pi} = [1 + (\sqrt{2}-1)\delta_{m0}]\sqrt{(L+m+1)(L-m)},$$

$$\gamma_{0,0}^{L\pi} = \gamma_{0,1}^{L\pi} = \gamma_{1,0}^{L\pi} = 0 \quad \text{for} \quad \sigma = -1.$$

It is evident that these matrix elements have an extremely simple form and can be computed for very high values of the total momentum L and threshold number n without any problem. In Tables 1 and 2 we compare potential curves calculated numerically and computed according formula (21) for S and P states of He and H^- for three values of ρ: 40, 60 and 80 a.u. It is evident that these results agree very well. For instance, the five significant digits are obtained for $^1P^o$ potential curves converging to the $n = 2$ threshold of He^+ ion.

Table 1: Comparison of the numerical potential curves $U_\mu(\rho)$ with the asymptotic ones, $U_\mu^{\rm as}(\rho)$, computed using formula (46) for $^1S^e$ and $^1P^o$ states of He at $\rho = 40$, 60 and 80 a.u.

State $^{2S+1}L^\pi$	Channel number, μ	$\rho = 40$ a.u.		$\rho = 60$ a.u.		$\rho = 80$ a.u.	
		$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$	$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$	$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$
$^1S^e$	1	2.02510	2.02516	2.01664	2.01674	2.01241	2.01254
	2	0.52627	0.52620	0.51721	0.51720	0.51280	0.51280
	3	0.52413	0.52411	0.51627	0.51627	0.51228	0.51228
	4	0.25103	0.25073	0.24052	0.24045	0.23562	0.23560
	5	0.24735	0.24693	0.23888	0.23876	0.23470	0.23465
	6	0.24436	0.24447	0.23764	0.23766	0.23403	0.23403
$^1P^o$	1	2.02447	2.02453	2.01636	2.01646	2.01225	2.01238
	2	0.52588	0.52582	0.51704	0.51703	0.51271	0.51271
	3	0.52490	0.52482	0.51661	0.51659	0.51246	0.51246
	4	0.52313	0.52311	0.51583	0.51582	0.51203	0.51203

Table 2: Comparison of the numerical potential curves $U_\mu(\rho)$ with the asymptotic ones, $U_\mu^{\rm as}(\rho)$, computed using formula (46) for $^1S^e$ and $^1P^o$ states of H^- at $\rho = 40$, 60 and 80 a.u.

State $^{2S+1}L^\pi$	Channel number, μ	$\rho = 40$ a.u.		$\rho = 60$ a.u.		$\rho = 80$ a.u.	
		$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$	$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$	$-U_\mu(\rho)$	$-U_\mu^{\rm as}(\rho)$
$^1S^e$	1	0.50015	0.50016	0.50006	0.50007	0.50002	0.50004
	2	0.12709	0.12709	0.12592	0.12593	0.12552	0.12552
	3	0.12309	0.12322	0.12417	0.12421	0.12454	0.12456
	4	0.06201	0.06178	0.05823	0.05832	0.05705	0.05711
	5	0.05614	0.05514	0.05559	0.05537	0.05553	0.05545
	6	0.04882	0.05022	0.05273	0.05318	0.05403	0.05422
$^1P^o$	1	0.49952	0.49953	0.49978	0.49979	0.49987	0.49988
	2	0.12662	0.12663	0.12572	0.12572	0.12540	0.12541
	3	0.12484	0.12474	0.12491	0.12489	0.12495	0.12494
	4	0.12225	0.12238	0.12380	0.12384	0.12433	0.12435

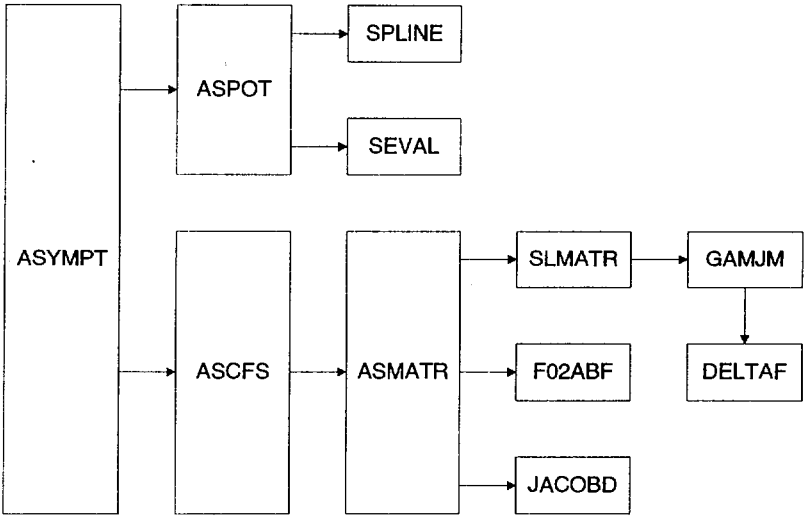
ASYMPT
ASPOT
SPLINE
SEVAL
ASCFS
ASMATR
SLMATR
GAMJM
F02ABF
DELTAF
JACOBD

Fig. 1

3 Description of the program

Fig. 1 presents a flow diagram for the ASYMPT program. The function of each subroutine is described in Section 4. The ASYMPT 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=1000,MITOT=500)
```

where MTOT and MITOT are the dimensions of the working DOUBLE PRECISION array TOT and INTEGER array ITOT, respectively. 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 ASYMPT is:

```
CALL ASYMPT  (TITLE, CHARGE, LMIN, LMAX, LSTEP, NTHRMN, NTHRMX,
              RMIN, RMAX, RSTEP, EPS, IASPOT, ICURVE, IUNITS, ID-
              FLAG, NPCMAX, NPTMAX, IPRINT, FNOUT, IOUT, FNPOT,
              IPOT, FNASP, IASP, FNPLT, IPLT, ICFS, 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.
CHARGE	REAL*8	nuclear charge.
LMIN	INTEGER	minimum value of the total orbital momentum.
LMAX	INTEGER	maximum value of the total orbital momentum.
LSTEP	INTEGER	step in total orbital momentum with which the computation is carried out.

NTHRMN	INTEGER	minimum threshold number.
NTHRMX	INTEGER	maximum threshold number.
RMIN	REAL*8	minimum value of the hyperradius ρ.
RMAX	REAL*8	maximum value of the hyperradius ρ.
RSTEP	REAL*8	step with which asymptotics of potential curves or adiabatic potentials are calculated and printed out.
EPS	REAL*8	desired accuracy with which matching points between numerical and asymptotic (given by Eqs. (21) and (22)) curves are determined. It is used only if IASPOT = 2.
IASPOT	INTEGER	flag specifying the mode of operation: = 0 – potential curves are read from the file FNPOT and the message about the number of records in the file and the last hyperradial point calculated is printed out. This mode is usually used during the computation of potential curves and radial matrix elements by the HSATOM and HSTERM programs [20, 21] to control the number of records written and to display the last hyperradial point calculated. If IPLT>0, numerical curves read from file FNPOT are written into file FNPLT; = 1 – asymptotics of potential curves and adiabatic potentials are computed using expressions (21) and (22), respectively, for a given set of hyperradial points from the interval [RMIN, RMAX] with step RSTEP. If IPLT > 0, the results of the calculation are written into file FNPLT (note that this option should be used here only if LMIN = LMAX and NTHRMN = NTHRMX, otherwise put IPLT = 0); = 2 second order (dipole) corrections $U_\mu^{(2)}$ or $V_{\mu\mu}^{(2)}$ are calculated and stored into temporary file ICFS. Numerical potential curves $U_\mu(\rho)$ or $V_{\mu\mu}(\rho)$ are read from file FNPOT and interpolated using the cubic spline interpolation on the given interval [RMIN,RMAX] with step RSTEP. The corresponding asymptotic curves are calculated using Eq. (21) or Eq. (22) on the same grid and compared with the numerical ones to determine with the given accuracy EPS matching points between these curves. The values of LMIN and LMAX should be the same for the given value of flag IASPOT.
ICURVE	INTEGER	flag specifying either potential curves or adiabatic potentials required: = 0 – asymptotics of adiabatic potentials $V_{\mu\mu}(\rho)$ are calculated; = 1 – asymptotics of potential curves $U_\mu(\rho)$ are calculated.
IUNITS	INTEGER	flag for specifying the units of measure: = 0 – the results will be given in atomic units; = 1 – the results will be given in Rydbergs.

IDFLAG	INTEGER	flag indicating the order in which roots of a secular equation are arranged: = 0 – roots are stored without ordering; = 1 – roots are stored in the ascending order.
NPCMAX	INTEGER	maximum number of potential curves written into file FNPOT. It is used (if IASPOT = 0 or 2) for setting dimensions of arrays to be used for storing numerical potential curves and corresponding matrix elements of radial coupling.
NPTMAX	INTEGER	maximum number of hyperradial points to be read from file FNPOT. It is used (if IASPOT = 0 or 2) to set dimensions of arrays to be used for performing the cubic spline interpolation of potential curves and effective potentials.
IPRINT	INTEGER	level of print: = 0 – minimal level of print. The second order corrections and the values of asymptotic curves on a given hyperradial grid are printed out. If IASPOT=2, the matching points between the numerical and asymptotic curves are printed out; = 1 – extended level of print. Interaction potential and mask matrices are printed out additionally.
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).
FNPOT	CHARACTER	name of the input file (up to 55 characters) containing potential curves and matrix elements of radial coupling calculated and stored by the HSATOM and HSTERM programs [20, 21]. It is used only if IASPOT=0 or 2.
IPOT	INTEGER	number of the logical device for reading data from file FNPOT.
FNASP	CHARACTER	name of the output file (up to 55 characters) for storing the second order corrections (the eigenvalues of the corresponding equivalent operator) and matching points between the relevant numerical and asymptotic curves. It is used only if IASP > 0 and IASPOT=2.
IASP	INTEGER	number of the logical device for storing data into file FNASP.
FNPLT	CHARACTER	name of the output file (up to 55 characters) for storing potential curves and adiabatic potentials (maximum 50 curves) in order to plot them lately using an available graphical package. It is used only if IPLT > 0.
IPLT	INTEGER	number of the logical device for storing data into file FNPLT.
ICFS	INTEGER	scratch working file.
TOT	INTEGER	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 the second–order corrections $U_\mu^{(2)}$ and $V_{\mu\mu}^{(2)}$ (eigenvalues of the equivalent operators (15) and (23), respectively) and matching points between the numerical and asymptotic curves with the accuracy EPS are written using unformatted segmented records into file FNASP according to the following operator:

```
WRITE (IASP) CHARGE,NROOT,(NTHRESH(I),RHOAS(I),CFAS(I),I=1,NROOT)
```

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

- CHARGE is the nuclear charge of a system.
- NROOT is the number of roots of the corresponding secular equation for a fixed value of principal quantum number n.
- array NTHRESH contains threshold numbers to which the corresponding curves are converged.
- array RHOAS contains the values of matching points at which the numerical curves are joined with the asymptotic ones.
- array CFAS contains the values of the second order corrections $U_\mu^{(2)}$ or $V_{\mu\mu}^{(2)}$ according to the given value of flag ICURVE.

Using the data stored in the file FNASP one can easily construct required asymptotic curves using expressions (21) and (22) for large values of ρ. The output data saved in the file FNASP is used as the input data in the HSATOM and HSTERM programs [20, 21] designed for the calculation of the energy levels and radial wave functions in the adiabatic and coupled-channel approximations.

If IPLT > 0, potential curves are written into the file FNPLT for each hyperradial point ρ according to the operator:

```
WRITE (IPLT,1000) RHO,(CURVES(I),I=1,NCURVES)
```

where 1000 is the label of the Fortran FORMAT operator: FORMAT(50(E14.6)). In the above, parameters presented in the WRITE statement have the following meaning:

- RHO is the value of hyperradius ρ.
- NCURVES is the number of curves to plot (maximum 50 curves).
- array CURVES contains potential curves (if ICURVE = 1) or adiabatic potentials (if ICURVE = 0). If IASPOT = 1, array CURVES will contain asymptotic curves computed using Eqs. (21) or (22) for a set of hyperradial points from the given interval [RMIN,RMAX] with step RSTEP. If IASPOT = 0, it will contain the numerical potentials taken from file FNPOT as they were originally stored there.

4 Description of subprogram units

A flow diagram for the ASYMPT 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 ASCFS controls the calculation of asymptotics of potential curves and adiabatic potentials for a fixed value of principal quantum number n. It sets the values of some flags and keys, determines sizes of working arrays, and prepares initial data for the ASMATR program.
- Subroutine ASMATR calculates matrix elements of equivalent operator corresponding to ρ^{-2} perturbation in the basis of Coulomb parabolic functions, finds the roots

of the corresponding secular equation for this operator, and calculates asymptotics of potential curves and adiabatic potentials for the given set of hyperradial points.

- Subroutine ASPOT reads potential curves and radial matrix elements stored in the file FNPOT by the programs HSATOM and HSTERM [20, 21], calculates asymptotics of potential curves and adiabatic potentials using expressions (21) and (22), respectively, compares them with the numerical ones, and finds matching points between these curves with the given accuracy EPS.

- DOUBLE PRECISION function DELTAF calculates Kroneker's delta–symbol δ_{ij}.

- DOUBLE PRECISION function GAMJM calculates the $\gamma^{L\pi}_{m,m\pm1}$ factor for the given values of total orbital momentum L and its projection m on the z axis.

- Subroutine JACOBD finds the eigenvalues and eigenvectors of a symmetric NxN matrix stored in a compact form without arranging the roots.

- DOUBLE PRECISION function SEVAL [33] evaluates the cubic spline function for a given value of x.

- Subroutine SLMATR calculates matrix elements of equivalent operator corresponding to ρ^{-2} perturbation for a given set of parabolic quantum numbers.

- Subroutine SPLINE [33] calculates coefficients for the cubic interpolating spline.

- Subroutine F02ABF from the NAG Fortran program library is described in [34].

5 Test deck

The ASYMPT program has been extensively used for the calculation of energy values of the doubly excited states [12, 13, 28, 35] and also one-photon ionization [18, 19] of He and H^-.

The test run which accompanies the ASYMPT program is designed to compute the roots of the secular equation (20). These eigenvalues are used for the calculation of the asymptotic curves for S and P states of He up to the $n = 5$ threshold for two values of hyperradius $\rho = 50$ and 80 a.u. Below we list the values of the numerical parameters and flags

used in the test run: CHARGE=2.D0, LMIN=0, LMAX=1, LSTEP=1, NTHRMN=1, NTHRMX=4, RMIN=50.D0, RMAX=80.D0, RSTEP=30.D0, EPS=0.D0, NPCMAX=1, NPTMAX=1, IASPOT=1, ICURVE=1, IUNITS=0, IDFLAG=1, IPRINT=0, IPOT=0, IASP=0, IPLT=0, ICFS=15. The results of the calculation with these parameters are presented below in the TEST RUN OUTPUT section. This test run requires 0.3 s on the DECstation 3000 Model 800.

The ASYMPT program has been tested on different models of computers and operating systems (see Program Summary) and each time the same results have been obtained. The program can also run on small computers like PC DX-386/486/Pentium under MS-DOS, MS-Windows or Linux (free UNIX-like operation system for PC).

Acknowledgments

The authors are grateful to M. B. Kadomtsev and D. G. Abrashkevich for useful discussions. This work was supported in part by the RFBR under Grant No. 96-02-17715 and also by the RFBR-INTAS under Grant No. 95-0512.

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Test run output

```
PROBLEM: Asymptotic potential curves for S and P states of He
********


        ASYMPTOTICS OF POTENTIAL CURVES AT LARGE RHO
        --------------------------------------------

     NUCLEAR CHARGE Z . . . . . . . . . . . . . (CHARGE):  2.0
     FLAG FOR SORTING (1) OR NOT (0) THE ROOTS. (IDFLAG):   1

*******************************************************************************


 NUMBER OF THRESHOLD . . . (N):   1
 TOTAL MOMENTUM. . . . . . (L):   0

 No       CFS        No       CFS        No       CFS        No       CFS
  1 -0.2500000E+00


    RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
    ---        ----------------------------------------------------
```

```
 50.000   -2.02010
 80.000   -2.01254
```

****

```
 NUMBER OF THRESHOLD . . . (N):   1
 TOTAL MOMENTUM. . . . . . (L):   1

 No       CFS        No       CFS        No       CFS        No       CFS
  1  0.7500000E+00

    RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
    ---        ----------------------------------------------------
 50.000   -2.01970
 80.000   -2.01238
```

****

```
 NUMBER OF THRESHOLD . . . (N):   2
 TOTAL MOMENTUM. . . . . . (L):   0

 No       CFS        No       CFS        No       CFS        No       CFS
  1 -0.1927051E+01    2  0.1427051E+01

    RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
    ---        ----------------------------------------------------
 50.000   -0.52077  -0.51943
 80.000   -0.51280  -0.51228
```

****

```
 NUMBER OF THRESHOLD . . . (N):   2
 TOTAL MOMENTUM. . . . . . (L):   1
```

```
No       CFS        No       CFS        No       CFS        No       CFS
 1 -0.1314297E+01    2  0.2823139E+00    3  0.3031983E+01
```

```
   RHO       VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---       ---------------------------------------------------
 50.000    -0.52053  -0.51989  -0.51879
 80.000    -0.51271  -0.51246  -0.51203
```

****

```
NUMBER OF THRESHOLD . . . (N):   3
TOTAL MOMENTUM. . . . . . (L):   0

No       CFS        No       CFS        No       CFS        No       CFS
 1 -0.5617225E+01    2  0.4601214E+00    3  0.4407104E+01

   RHO       VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---       ---------------------------------------------------
 50.000    -0.24447  -0.24204  -0.24046
 80.000    -0.23560  -0.23465  -0.23403
```

****

```
NUMBER OF THRESHOLD . . . (N):   3
TOTAL MOMENTUM. . . . . . (L):   1

No       CFS        No       CFS        No       CFS        No       CFS
 1 -0.5029787E+01    2 -0.2041039E+01    3  0.1173774E+01    4  0.2944384E+01
 5  0.6702668E+01

   RHO       VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---       ---------------------------------------------------
 50.000    -0.24423  -0.24304  -0.24175  -0.24104  -0.23954
 80.000    -0.23551  -0.23504  -0.23454  -0.23426  -0.23367
```

```
**********************************************************************************

NUMBER OF THRESHOLD . . . (N):   4
TOTAL MOMENTUM. . . . . (L):   0

No       CFS        No       CFS        No       CFS        No       CFS
 1 -0.1131404E+02   2 -0.2561380E+01   3  0.4196759E+01   4  0.8678658E+01


   RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---        ---------------------------------------------------
 50.000   -0.14953  -0.14602  -0.14332  -0.14153
 80.000   -0.13927  -0.13790  -0.13684  -0.13614

**********************************************************************************

NUMBER OF THRESHOLD . . . (N):   4
TOTAL MOMENTUM. . . . . (L):   1

No       CFS        No       CFS        No       CFS        No       CFS
 1 -0.1073614E+02   2 -0.6415713E+01   3 -0.1917310E+01   4  0.1387322E+01
 5  0.5027490E+01   6  0.6907979E+01   7  0.1174637E+02


   RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---        ---------------------------------------------------
 50.000   -0.14929  -0.14757  -0.14577  -0.14445  -0.14299  -0.14224  -0.1403(
 80.000   -0.13918  -0.13850  -0.13780  -0.13728  -0.13671  -0.13642  -0.1356(

**********************************************************************************

NUMBER OF THRESHOLD . . . (N):   5
TOTAL MOMENTUM. . . . . (L):   0

No       CFS        No       CFS        No       CFS        No       CFS
```

```
 1 -0.1901274E+02   2 -0.7626983E+01   3  0.1934106E+01   4  0.9194641E+01
 5  0.1426097E+02


   RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---        ---------------------------------------------------
 50.000   -0.10761  -0.10305  -0.09923  -0.09632  -0.09430
 80.000   -0.09547  -0.09369  -0.09220  -0.09106  -0.09027
```

****

```
 NUMBER OF THRESHOLD . . . (N):   5
 TOTAL MOMENTUM. . . . . . (L):   1

 No       CFS        No       CFS        No       CFS        No       CFS
  1 -0.1843995E+02   2 -0.1280380E+02   3 -0.7008617E+01   4 -0.2306121E+01
  5  0.2635611E+01   6  0.6169365E+01   7  0.1017605E+02   8  0.1216642E+02
  9  0.1816104E+02


   RHO        VALUES OF THE ASYMPTOTIC POTENTIAL CURVES (in a.u.):
   ---        ---------------------------------------------------
 50.000   -0.10738  -0.10512  -0.10280  -0.10092  -0.09895  -0.09753  -0.09593
          -0.09513  -0.09274
 80.000   -0.09538  -0.09450  -0.09360  -0.09286  -0.09209  -0.09154  -0.09091
          -0.09060  -0.08966
```

****

Received by Publishing Department
on November 5, 1997.

SUBJECT CATEGORIES OF THE JINR PUBLICATIONS

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Абрашкевич А.Г., Пузынин И.В., Виницкий С.И. E11-97-326

ASYMPT — программа вычисления асимптотик гиперсферических адиабатических термов и потенциалов

Представлена программа ASYMPT (FORTRAN 77) для вычисления асимптотик термов и адиабатических потенциалов с точностью $O(\rho^{-2})$ в гиперсферическом адиабатическом подходе (HSA). Показано, что матричные элементы эквивалентного оператора, соответствующего возмущению ρ^{-2}, имеют простой вид в базисе кулоновских параболических функций во вращающейся системе координат и легко вычисляются для больших значений полного орбитального момента и номера порога. Поправки второго порядка к адиабатическим термам получены как решения соответствующего секулярного уравнения. Асимптотики потенциалов можно использовать для вычисления уровней энергии и радиальных волновых функций двухэлектронных систем в адиабатическом приближении и в методе связанных каналов HSA подхода.

Работа выполнена в Лаборатории вычислительной техники и автоматизации и Лаборатории теоретической физики им.Н.Н.Боголюбова ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 1997

Abrashkevich A.G., Puzynin I.V., Vinitsky S.I. E11-97-326

ASYMPT — a Program to Calculate Asymptotics of Hyperspherical Potential Curves and Adiabatic Potentials

A FORTRAN 77 program is presented which calculates asymptotics of potential curves and adiabatic potentials with an accuracy of $O(\rho^{-2})$ in the framework of the hyperspherical adiabatic (HSA) approach. It is shown that matrix elements of the equivalent operator corresponding to the perturbation ρ^{-2} have a simple form in the basis of the Coulomb parabolic functions in the body-fixed frame and can be easily computed for high values of total orbital momentum and threshold number. The second-order corrections to the adiabatic curves are obtained as the solutions of the corresponding secular equation. The asymptotic potentials obtained can be used for the calculation of the energy levels and radial wave functions of two-electron systems in the adiabatic and coupled-channel approximations of the HSA approach.

The investigation has been performed at the Laboratory of Computing Techniques and Automation and at the Bogoliubov Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna, 1997

Макет Т.Е.Попеко

Подписано в печать 01.12.97
Формат 60 × 90/16. Офсетная печать. Уч.-изд.листов 2,56
Тираж 345. Заказ 50318. Цена 3072 р.

Издательский отдел Объединенного института ядерных исследований
Дубна Московской области