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D.V.Pavlov, I.V.Puzynin, B.Joulakian*, S.I.Vinitsky

WAVEFUNCTIONS OF CONTINUOUS SPECTRUM
OF THE COULOMB TWO-CENTER PROBLEM

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*Institut de Physique, Laboratoire de Physique Moléculaire
et des Collisions, Université de Metz, Technopôle 2000, 1 Rue Arago,
57078 Metz Cedex 3, France

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1 Introduction

In recent paper [1] theoretical analysis of the dissociative ionization of H_2^+ by fast electrons was carried out. As mentioned in this paper, the crucial point of calculating the cross-section of such processes is that no closed exact analytical wave functions of the continuum states exist. As consequence, the final-state wave function of the ejected electron was constructed like a product of the two Coulomb functions of the continuous spectrum of hydrogen atom that is an approximation of the scattering electron two-center wavefunction. To improve the calculation one can need to obtain these functions as the numerical solutions of the continuous spectrum of the two-center Coulomb problem. It leads to a cumbersome procedure of calculating multi-dimensional integrals with the functions presented numerically that requires huge computer facilities and may cause additional computational problems. The representation of the above integrals considered in [2] leads to the simplification of the such calculations even the numerically constructed functions are applied. Here we proposed a numerical algorithm for the calculation of such functions of separated variables based on the representation of the scattering problem as a parametric eigenvalue problem similar to [3] which is realized here with the help of the modified Newton iteration scheme [4].

The structure of this paper is following. In section 1 the formulation of the two-center problem is given briefly. In sections 2,3 the statements of the eigenvalue problems for quasiangle and quasiradial equations are presented in sections. In section 4 the method of solution and the corresponded iteration and numerical schemes are considered in details. The numerical results of the separation constants, the phase shifts together with dependence of the parameters of the grids and the wavefunctions are shown in tables and pictures.

2 Two-center problem

The wavefunction of the two-center problem with charges Z_a and Z_b separated by a distance R can be factored into the form [5].

$$\psi = \Pi(\xi) \Xi(\eta) \frac{e^{im\varphi}}{\sqrt{2\pi}}$$

where the ξ, η and φ are the prolate spheroidal coordinates. We put the charge Z_a in the left focus ($\xi = 1, \eta = -1$) and the charge Z_b in the right focus ($\xi = 1, \eta = 1$). Functions $\Pi(\xi)$ and $\Xi(\eta)$ are solutions of the eigenvalue problem for system of the equations

$$\left(\frac{d}{d\xi} (\xi^2 - 1) \frac{d}{d\xi} + RZ_+ \xi - \frac{m^2}{\xi^2 - 1} + \frac{ER^2 \xi^2}{2} + A \right) \Pi(\xi) = 0, \quad 1 \leq \xi < +\infty \quad (1)$$

$$\left(\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta} + RZ_-\eta - \frac{m^2}{1-\eta^2} - \frac{ER^2\eta^2}{2} - A\right)\Xi(\eta) = 0, \quad -1 \leq \eta \leq 1. \quad (2)$$

where $Z_+ = Z_a + Z_b$ and $Z_- = Z_b - Z_a$, E is an energy, A is a separation constant, $A = -\lambda - \frac{R^2}{2}E$, where λ is the standard separation constant. We supposed that

$$|\Pi(1)| < +\infty, \quad |\Xi(\pm 1)| < +\infty.$$

The asymptotic behaviour of the function $\Pi(\xi)$ take a form

$$\Pi(\xi) \rightarrow \frac{N_{ml}}{\xi} \sin\left(c\xi + \frac{a}{2c} \ln(2c\xi) - \frac{l\pi}{2} + \delta\right), \quad \xi \rightarrow +\infty, \quad (3)$$

where δ is the phaseshift of the radial function, N_{ml} is normalization coefficient, $c = \frac{ER^2}{2}$, $a = R(Z_a + Z_b)$ and l is the orbital quantum number.

3 Quasiangle equation

It is useful to make the next transformation [4]

$$Y(\eta) = (1 - \eta^2)\Xi(\eta).$$

The problem transforms to the following one

$$\left((1-\eta^2)\frac{d^2}{d\eta^2} + 2\eta\frac{d}{d\eta} + RZ_-\eta - \frac{m^2}{1-\eta^2} + \frac{2(1+\eta^2)}{1-\eta^2} - \frac{ER^2\eta^2}{2} - A\right)Y(\eta) = 0, \quad -1 \leq \eta \leq 1 \quad (4)$$

with the new boundary conditions

$$Y(-1) = 0, \quad Y(1) = 0. \quad (5)$$

Due to Dirichlet boundary conditions the normalization condition take a form

$$\int_{-1}^1 Y^2(\eta) d\eta - 1 = 0. \quad (6)$$

At given value of energy E we can find the value of the separated constant A . The problem (4-6) is the eigenvalue problem for the quasiangle function $Y(\eta)$ and the separated constant A . We solve it with the help of the continuous analog of Newton method and the finite-difference scheme of 4th order. The results of calculation are presented in Table 1. For convenience of comparison the dependence of the separated constant λ from the momentum of the electron k is shown. The connection λ with A and k with E take the form

$$\lambda = -A - \frac{ER^2}{2}, \quad E = \frac{k^2}{2}.$$

All calculations were performed for $Z_a = Z_b = 1$ and $R = 2$.

4 Quasiradial equation

In quasiradial equation we make the following transformation [4]

$$X(\xi) = (\xi - 1)\Pi(\xi).$$

The problem for new function $X(\xi)$ take a form

$$\left((\xi^2 - 1) \frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + RZ_+\xi - \frac{m^2}{\xi^2 - 1} + \frac{2}{\xi - 1} + \frac{ER^2\xi^2}{2} + A \right) X(\xi) = 0, \quad 1 \leq \xi < +\infty \quad (7)$$

with the new boundary condition

$$X(1) = 0 \quad (8)$$

and asymptotics

$$X(\xi) \rightarrow N_{mt} \sin\left(c\xi + \frac{a}{2c} \ln(2c\xi) - \frac{l\pi}{2} + \delta\right), \quad \xi \rightarrow +\infty. \quad (9)$$

Using modified analog of Newton method [3] we look for such ξ_{max} that $X(\xi_{max}) = 0$, $\xi_{max} \gg 1$. The phase δ is calculated by the formula

$$\delta(\xi_{max}) = \pi j - \left(c\xi_{max} + \frac{a}{2c} \ln(2c\xi_{max}) - \frac{l\pi}{2}\right),$$

where the integer number j is chosen to lead the phase δ to the interval $[0, \pi)$.

Taking into account the asymptotic correction $\Delta\delta$

$$\Delta\delta(\xi_{max}) = \sum_{i=2}^{\infty} \frac{w_i}{i-1} \left(\frac{1}{\xi_{max}}\right)^{i-1},$$

where w_i are the coefficients of the expansion of the potential $V^{\frac{1}{2}}(\xi)$ [6]

$$V(\xi) = \frac{A}{\xi^2 - 1} + \frac{RZ_+\xi}{\xi^2 - 1} + \frac{ER^2}{2} \frac{\xi^2}{\xi^2 - 1} + \frac{1 - m^2}{(\xi^2 - 1)^2}, \quad V^{\frac{1}{2}}(\xi) = \sum_{i=0}^{\infty} w_i \left(\frac{1}{\xi}\right)^i$$

in power series, we obtain the value of the phase

$$\delta = \delta(\xi_{max}) + \Delta\delta(\xi_{max}).$$

The results of calculations are presented in Table 2. Some quasiradial function $X(\xi)$ are shown in Figs.1a,1b for case $Z_a = Z_b = 1$, $R = 2$. The final value of the normalization coefficient corresponds to the normalization of the unit flow

$$N_{mt} = \frac{2}{R} \sqrt{\frac{2}{\pi}}.$$

5 Method of solution

In quasiangle equation it is convenient to rewrite the equation (4) into the form

$$\Phi^{(1)} = \mathbf{Q}Y - AY = 0,$$

where \mathbf{Q} is the differential operators of second order

$$\mathbf{Q} = (1 - \eta)^2 \frac{d^2}{d\eta^2} + 2\eta \frac{d}{d\eta} + RZ - \eta - \frac{m^2}{1 - \eta^2} + \frac{2(1 + \eta^2)}{1 - \eta^2} - \frac{ER^2\eta^2}{2}$$

The boundary and normalization conditions of the function $Y(\eta)$ take the form

$$\Phi^{(2)} = Y(-1) = 0, \quad \Phi^{(3)} = Y(1) = 0, \quad \Phi^{(4)} = \int_{-1}^1 Y^2(\eta) d\eta - 1 = 0.$$

This eigenvalue problem is solved by the continuous analog of Newton method [4]

$$\Phi'(u) \frac{du}{dt} = -\Phi(u), \quad u(0) = u^{(0)},$$

where $u(t) = \{Y(t), A(t)\}$ the unknown variable and u_0 is initial approximation from a vicinity of the solution u_* . Φ'_u is Freshet derivative of the vector function $\Phi(u) = \{\Phi^{(1)}(u), \Phi^{(2)}(u), \Phi^{(3)}(u), \Phi^{(4)}(u)\}$.

The next designations are introduced

$$\phi = \frac{dY}{dt}, \quad a = \frac{dA}{dt}.$$

The Newton method takes a form

$$\begin{aligned} \mathbf{Q}\phi - A\phi - aY &= -(\mathbf{Q}Y - AY) \\ \phi(-1) &= -Y(-1), \quad \phi(1) = -Y(1) \\ \int_{-1}^1 (2\phi Y + Y^2) d\eta &= 1 \end{aligned}$$

We use the decomposition

$$\phi \doteq \phi_1 + a\phi_2$$

To find ϕ_1, ϕ_2 it is required to solve the next linear differential equations

$$\begin{aligned} \mathbf{Q}\phi_1 - A\phi_1 &= -(\mathbf{Q}Y - AY), \quad \phi_1(-1) = -Y(-1), \quad \phi_1(1) = -Y(1) \\ \mathbf{Q}\phi_2 - A\phi_2 &= Y, \quad \phi_2(-1) = 0, \quad \phi_2(1) = 0 \end{aligned} \tag{10}$$

It is obviously that $\phi_1 = -Y$, therefore we have

$$a = -\frac{1}{\int_{-1}^1 \phi_2 y d\eta} \quad (11)$$

Thus, using $Y^{(k)}, A^{(k)}$ we calculate $\phi_2^{(k)}$ solving (10). The relation (11) give us $a^{(k)}$. The increment for wavefunction is

$$\phi^{(k)} = -Y^{(k)} + a^{(k)}\phi_2^{(k)}$$

The next approximation calculates by the formula

$$Y^{(k+1)} = Y^{(k)} + \tau\phi^{(k)}, \quad A^{(k+1)} = A^{(k)} + \tau a$$

where τ is the step by the parameter t calculating by

$$\tau = \frac{\delta(0)}{\delta(0) + \delta(1)}$$

$$\delta(t) = \delta(Y^{(k)} + t\phi^{(k)}, A^{(k)} + ta^{(k)}) = \|\Phi(Y^{(k)} + t\phi^{(k)}, A^{(k)} + ta^{(k)})\|_{C_2}$$

The iteration process is finished when $\delta < \varepsilon$, ε is the given number.

The initial approximation of the function $Y(\eta)$ was taken

$$Y(\eta) = (1 - \eta^2)P_l^m(\eta),$$

where P_l^m is the Legendre polynomial. The examples of the solutions and initial approximations of the states with quantum numbers $m = 0, l = 6$, $m = 0, l = 8$ and $m = 0, l = 10$ at $R = 2$, $k = 1$ are presented by means of solid and dashed lines respectively on fig.2 for case $Z_a = Z_b = 1, R = 2$. The solutions and the initial approximations almost coincide. The initial values of the separated constant is calculated by the formula

$$A^{(0)} = -c^2 - l(l+1) + \frac{(l^2 - m^2)(b^2 + 4c^2l^2)}{2l(2l-1)(2l+1)} - \frac{((l+1)^2 - m^2)(b^2 + 4c^2(l+1)^2)}{2(l+1)(2l+1)(2l+3)},$$

where $b = R(Z_b - Z_a)$.

The linear systems are solved with 4th order approximation by step of uniform grid by means of finite-difference formula

$$y_2'' = \frac{1}{12h^2}(10y_1 - 15y_2 - 4y_3 + 14y_4 - 6y_5 + y_6) + O(h^4)$$

$$y_2' = \frac{1}{12h}(-3y_1 - 10y_2 + 18y_3 - 6y_4 + y_5) + O(h^4)$$

$$y_i'' = \frac{1}{12h^2}(-y_{i-2} + 16y_{i-1} - 30y_i + 16y_{i+1} - 6y_{i+2}) + O(h^4)$$

$$y'_i = \frac{1}{12h}(y_{i-2} - 8y_{i-1} + 8y_{i+1} - y_{i+2}) + O(h^4)$$

$$y''_{n-1} = \frac{1}{12h^2}(y_{n-5} - 6y_{n-4} + 14y_{n-3} - 4y_{n-2} - 15y_{n-1} + 10y_n) + O(h^4)$$

$$y'_{n-1} = \frac{1}{12h}(-y_{n-4} + 6y_{n-3} - 18y_{n-2} + 10y_{n-1} + 3y_n) + O(h^4)$$

The matrix of linear system is reduced to five-diagonal form and we solve the above algebraic problems with the help of LU-decomposition for the band matrixes. The integrals in equation (11) is calculated by the Simpson method.

Let us rewrite the quasiradial equation into the form

$$\mathbf{P}X - E\frac{R^2\xi^2}{2}X = 0,$$

where

$$\mathbf{P} = (1 - \xi)^2 \frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + RZ + \xi - \frac{m^2}{\xi^2 - 1} + \frac{2}{\xi - 1} + A.$$

First we fixed the point $\xi_{max}^{(0)}$ and require that $X(\xi_{max}^{(0)}) = 0$ for value of the energy E which is different from the given value $E^* > 0$. Thus we obtain the system

$$\mathbf{P}X - E\frac{R^2\xi^2}{2}X = 0, \quad X(1) = 0, X(\xi_{max}) = 0. \quad (12)$$

To close the system we introduce the normalization condition

$$\int_1^{\xi_{max}} X^2(\xi) d\xi = 1. \quad (13)$$

The eigenvalue problem (12-13) is solved similarly the problem of the angle equation. When we find the value of energy E corresponded $\xi_{max}^{(0)}$ the next approximation is calculated by the formula

$$\xi_{max}^{(1)} = \xi_{max}^{(0)} + \frac{\Delta E^{(0)}}{E^*} \xi_{max}^{(0)}, \quad \xi_{max}^{(k+1)} = \frac{\xi^{(k)} \Delta E^{(k)} - \xi^{(k-1)} \Delta E^{(k-1)}}{\Delta E^{(k)} - \Delta E^{(k-1)}},$$

where $\Delta E^{(k)} = E^{(k)} - E^*$. Then the problem (12-13) is solved again. The iteration process is stopped when $|E - E^*| < \varepsilon$, ε is the given number. So we find such ξ_{max} that $X(\xi_{max}) = 0$. Using values of the phase shift at different values ξ_{max} we can find the extrapolated value of the phase δ_{ext} corresponded $\xi_{max} \rightarrow +\infty$. The example of the dependence of the phase shift from the value of ξ_{max} is presented in Table 3 for the case $k = 1, m = 0, l = 0$.

The Runge relation σ for the quasiangle equation is presented in Table 4. It is proved 4th order of the finite-difference scheme. In Tables 5a, 5b, 5c the convergence of calculating method for the quasiradial equation is shown.

6 Matrix elements

If we have the solution in the case of continuous spectrum that using the solution in the case of discrete spectrum [7] it is possible to calculate the matrix elements between continuous and discrete spectrum. Don't forget that the functions of the continuous spectrum are connected with the solution $X(\xi), Y(\eta)$ by the next formula

$$\Pi_c(\xi) = \frac{X(\xi)}{\xi - 1}, \quad \Xi_c(\eta) = \frac{Y(\eta)}{\eta^2 - 1}.$$

The quasiradial function is normalized on the unit flow

$$\Pi_c(\xi) \rightarrow \frac{N_{ml}}{\xi} \sin\left(c\xi + \frac{a}{2c} \ln(2c\xi) - \frac{l\pi}{2} + \delta\right), \quad \xi \rightarrow +\infty, \quad N_{ml} = \frac{2}{R} \sqrt{\frac{2}{\pi}}.$$

The real normalization condition for quasiangle function is

$$\int_{-1}^1 \Xi_c^2(\eta) d\eta = 1.$$

Let us introduce the next designations:

$$\phi_c = \Pi_c(\xi)\Xi_c(\eta), \quad \phi_d = \Pi_d(\xi)\Xi_d(\eta),$$

where $\Pi_c(\xi), \Xi_c(\eta)$ is the solutions in the continuous spectrum corresponded to the momentum of electron $K = \sqrt{\frac{E_a}{2}}$ and the quantum numbers l_c, m_c ; $\Pi_d(\xi), \Xi_d(\eta)$ is the solutions in the discrete spectrum corresponded to the quantum numbers N_d, l_d, m_d . We calculate the matrix elements

$$H_{Kl_c m_c, N_d l_d m_d}^{(*)} = \frac{1}{R} \int \frac{d\tau}{\xi^2 - \eta^2} (Z_+ \xi + Z_- \eta) \phi_c \phi_d$$

$$D_{Kl_c m_c, N_d l_d m_d} = \frac{R}{2} \int d\tau \xi \eta \phi_c \phi_d$$

$$D_{Kl_c m_c, N_d l_d m_d \pm 1} = -\frac{R}{2\sqrt{2}} \int d\tau \sqrt{(\xi^2 - 1)(1 - \eta^2)} \phi_c \phi_d$$

$$\int d\tau = \frac{R^3}{8} \int_{-1}^{+\infty} \int_{-1}^1 (\xi^2 - \eta^2) d\xi d\eta$$

The dependences of $H_{K20,100}^{(*)}(R)$ and $Q_{K60,210}^{(-)}(R)$ are represented on Fig.3ab.

In Table 6 4th order of calculation scheme is confirmed. The values of matrix elements $H_{100,100}^{(*)}$ and $Q_{110,100}^{(-)}$ are presented.

Table 1. The separated constant λ ($Z_a = Z_b = 1, R = 2$).

k	m	l	λ	k	m	l	λ
0.1	1	1	-0.0066681477	0.1	1	1	1.9919995429
	1	2	1.9959993142		1	2	5.99428532557
	1	3	5.9952391097		1	3	11.99466680302
1.0	1	1	-0.68099994486	1.0	1	1	1.1955483554
	1	2	1.59308457997		1	2	5.4246991437
	1	3	5.5334718005		1	3	11.4679153304
4.0	1	1	-12.8279325778	4.0	1	1	-11.60040693284
	1	2	-6.1940561590		1	2	-4.0512806162
	1	3	-0.6937000038		1	3	3.4652605398

Table 2. The phase δ ($Z_a = Z_b = 1, R = 2$)

k	m	l	δ	k	m	l	δ
0.1	0	0	2.1702	0.1	1	1	1.2901
	0	1	2.2763		1	2	0.36896
	0	2	0.5832		1	3	2.07349
1.0	0	0	1.9002491	1.0	1	1	1.435894
	0	1	2.2627836		1	2	1.171195
	0	2	1.4528653		1	3	0.601453
4.0	0	0	2.4723507	4.0	1	1	2.444128
	0	1	2.655815		1	2	2.537655
	0	2	2.8655007		1	3	2.560437

7 Conclusion

In this paper the efficiency of the proposed algorithm of the calculation of the Coulomb two-center wavefunctions and the phase shifts is shown. One can see that the achieved accuracy of the calculations of the phase shifts of order 10^{-6} for the electron momentum $k \geq 1$ ($E \geq 50\text{eV}$) will be sufficient for application of such functions for numerical simulating the above mentioned problem of dissociative ionization of H_2^+ by fast electrons. The matrix elements between the continuous and discrete spectrum are calculated.

Table 3. The dependence of phase δ from the maximal value of variable ξ for the quantum numbers $m = 0, l = 0$, N_ξ is the number of points on the interval $[1, \xi_{max}]$ ($k = 1, Z_a = Z_b = 1, R = 2$).

ξ_{max}	N_ξ	δ	δ_{ext}
199.7394749582	20001	1.900261211	1.900249131
399.4195210394	40001	1.900252114	
599.6700960262	60001	1.900250411	
800.1558628525	80001	1.900249820	
1000.7707687768	100001	1.900249553	

Table 4. Runge relation

$$\sigma = \frac{f_h - f_{h/2}}{f_{h/2} - f_{h/4}}$$

The impulse of electron $k = 1$, the distance between charges $R = 2$, the step of the uniform grid on interval $\eta \in [-1; 1]$ $h = 0.01$

f	$l = 4, m = 3$	$l = 4, m = 4$	$l = 5, m = 2$
$Y(-0.8)$	16.743221	15.866189	18.741457
$Y(-0.6)$	19.868391	15.937843	18.020318
$Y(-0.4)$	12.298477	15.959770	16.223387
$Y(-0.8)$	14.469839	15.925757	11.608296
$Y(0.0)$	12.426774	15.943446	16.875422
$Y(0.2)$	13.912054	15.946564	16.812849
$Y(0.4)$	10.841275	15.949665	15.483128
$Y(0.6)$	17.796659	15.934301	15.842029
$Y(0.8)$	16.397187	15.845237	16.732263
A	15.995529	15.969777	15.804448

Table 5a. Relation

$$\sigma = \frac{\delta_N - \delta_{2N}}{\delta_{2N} - \delta_{4N}}$$

The impulse of electron $k = 1$, the distance between charges $R = 2$, the initial value of ξ_{max} in iteration process $\xi_{max}^{(0)} = 501$, the number of grid points $N = 10001$. Using this parameters the phase shifts $\delta_N, \delta_{2N}, \delta_{4N}$ are calculated.

ml	δ_N δ_{2N} δ_{4N}	σ	ml	δ_N δ_{2N} δ_{4N}	σ
00	1.900303852846468	17.0895	11	1.435913469016245	15.7754
	1.900252079960914			1.435895298283555	
	1.900249050450859			1.435894146445816	
01	2.262824889452540	17.3793	12	1.171214283432231	15.8036
	2.262785720437930			1.171196082815751	
	2.262783466670075			1.171194931143834	
02	1.452880046424015	14.8813	13	0.6014718091072850	15.9734
	1.452865945099130			0.6014537415575438	
	1.452864997511752			0.6014526104608190	

Table 5b. $k = 4, R = 2, \xi_{max}^{(0)} = 501, N = 10001$.

ml	δ_N δ_{2N} δ_{4N}	σ	ml	δ_N δ_{2N} δ_{4N}	σ
00	2.472377922423183	16.0099	11	2.444146710509758	16.0654
	2.472352684920623			2.444129857022201	
	2.472351108559252			2.444128807968534	
01	2.655837514839573	16.3695	12	2.537672912052000	15.5390
	2.655816372711427			2.537656396425598	
	2.655815081159464			2.537655333577429	
02	2.865517109608426	15.6978	13	2.560454959120510	15.9429
	2.865501687166074			2.560438257167399	
	2.865500704711682			2.560437209558018	

Table 5c. $k = 0.1, R = 2.$

$$\xi_{max}^{(0)} = 5001, N = 10001 \quad \xi_{max}^{(0)} = 20001, N = 20001$$

ml	δ_N δ_{2N} δ_{4N}	σ	ml	δ_N δ_{2N} δ_{4N}	σ
00	2.170397206002768 2.170382727918684 2.170381890357920	17.2860	11	1.488165578085649 1.296986110214245 1.290173229380229	28.0614
01	2.286966519816308 2.277245282111599 2.276543038544585	13.8431	12	0.3575882275673924 0.3684133627865706 0.3690087260433970	18.1824
02	0.582398748351524 0.583294364469660 0.583347862324392	16.7411	13	2.080915474659997 2.074129500280666 2.073535702047295	11.4280

Table 6. Relation

$$\sigma = \frac{f(N, h) - f(2N, h/2)}{f(2N, h/2) - f(4N, h/4)}$$

The impulse of electron $k = 1$; the distance between charges $R = 2$; the initial value of ξ_{max} is $\xi_{max}^{(0)} = 501$; the number of points on interval $[1; \xi_{max}]$ is $N = 10001$; step of uniform grids for μ, η is $h = h_\mu = h_\eta = 0.05$. The values $H_{100,100}^{(*)}$ and $Q_{110,100}^{(-)}$ are calculated.

$$H_{100,100}^{(*)} \quad Q_{110,100}^{(-)}$$

$f(N, h)$ $f(2N, h/2)$ $f(4N, h/4)$	σ	$f(N, h)$ $f(2N, h/2)$ $f(4N, h/4)$	σ
0.1678882687538151 0.1683145983625204 0.1683412035313158	16.0243	-0.02861528026087824 -0.02822615078494821 -0.02820174267099179	15.9426

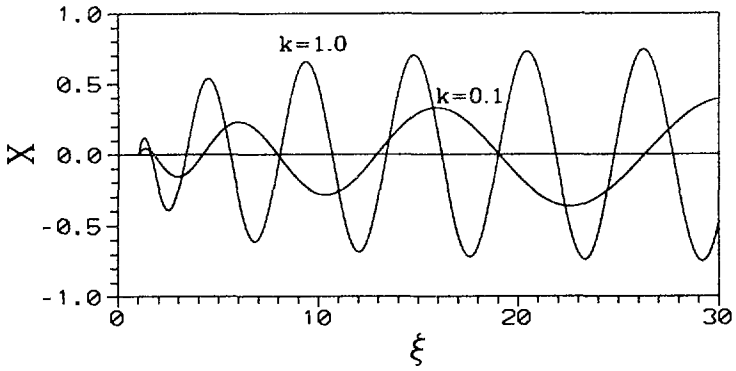


Fig.1a. The distribution of the quasiradial solution, $R = 2$.

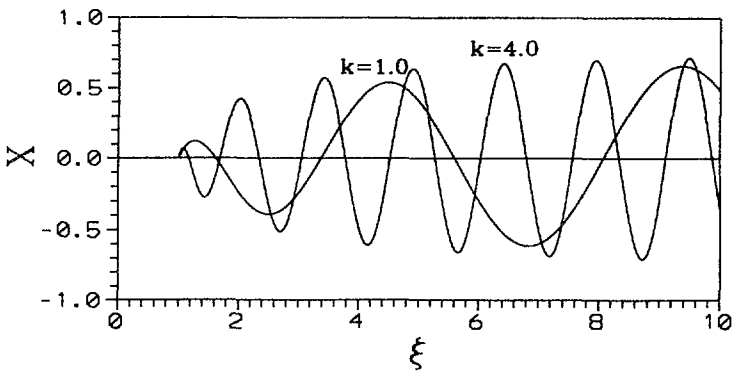


Fig.1b. The distribution of the quasiradial solution, $R = 2$.

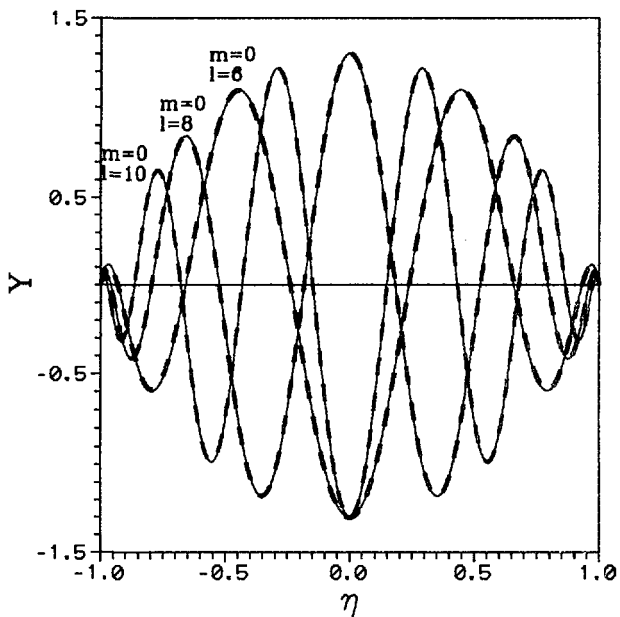


Fig.2. The distribution of the quasisingle solutions and the initial approximations, $R = 2$.

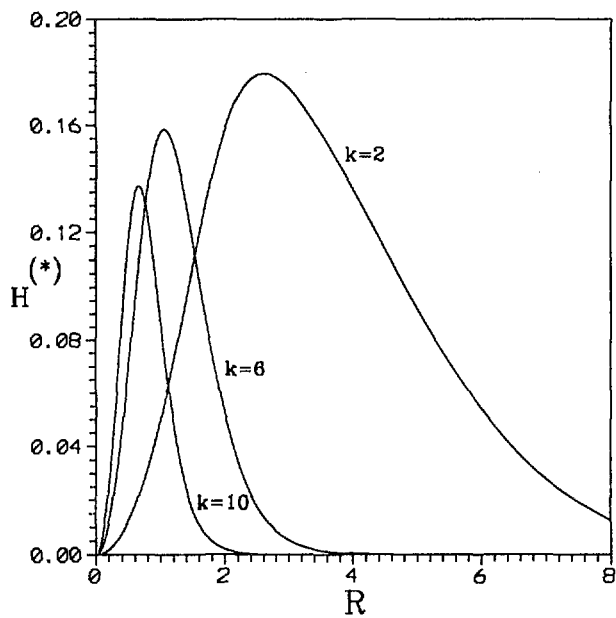


Fig.3a. The dependence $H_{K20,100}^{(*)}(R)$ for different K .

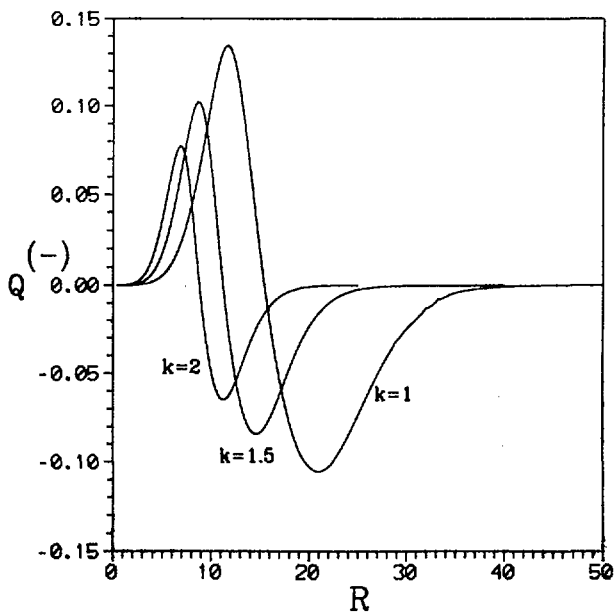


Fig.3b. The dependence $Q_{K60,210}^{(-)}(R)$. for different K .

References

- [1] B.Joulakian, J.Hassen, R.Rivarola, and A.Motassim, Phys. Rev. A, **54**, 1473 (1996)
- [2] V.V.Serov, V.L.Derbov, B.Joulakian, S.I.Vinitsky, Wave packet evolution approach to ionization of hydrogen molecular ion by fast electrons, Draft (2000) (to be published)
- [3] S.I.Vinitsky, I.V.Puzynin, Yu.S.Smirnov. Yad.Fiz. 1990, v. 52, N 4(10), p. 1176.
- [4] T.Zhanlav, D.V.Pavlov, I.V.Puzynin. A Numerical Solution of the Two-Center Problem. JINR, E11-91-138, Dubna, 1991.
- [5] I.V.Komarov, L.I.Ponomarev, S.Yu.Slavyanov, Spheroidal and Coulomb Spheroidal Functions, Moscow, Nauka, 1976.
- [6] Puzynin V.I., The Miln Equation for the Calculation the Phases and Norms of Wave Functions for Continuum Spectrum of Coulomb Two-Center Problem, IHEPh, Preprint 92-119, Protvino, 1992.
- [7] D.V.Pavlov, I.V.Puzynin, S.I.Vinitsky, Discrete Spectrum of the Two-Center Problem of $\bar{p}He^+$ Atomcule, JINR, E4-99-141, Dubna, 1999.

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