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DISCRETE SPECTRUM OF THE TWO-CENTER PROBLEM OF $\bar{p}He^+$ ATOMCULE

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1 Introduction

Nowadays a study of the Coulomb two-center problem attracts attention in the context of recent experimental and theoretical investigations of the metastable states of an antiprotonic helium atomcule [1]. For solving the problem under consideration some standard methods [2,3] have been applied in papers [4,5,6]. However, an exhaustive study both discrete and continuous spectra has not been done [7], while new loosely bound states supported by outer wells of some excited electron potential curves were predicted [8]. To solve the problem in both discrete and continuous spectra, the elaboration of efficient numerical methods similar [9,10] is worthwhile.

In this paper, an algorithm for solving the Coulomb two-center problem using the parametric fractional-rational transformation of the quasiradial variable to a finite interval with optimization of the parameter is proposed. The realization of the algorithm with the help of the 4th-order the finite-difference scheme and the continuous analog of Newton's method is given. The low part of the discrete spectrum of the two-center problem of $\bar{p}He^+$ system in a wide region of the quantum number values is studied. The specific behavior of the two-center wavefunctions and the potential curves in a vicinity of the united and separated atoms is discussed.

2 Coulomb 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 [3]

$$\psi \;=\; \Pi(\xi)\,\Xi(\eta)\,e^{im\varphi}/\sqrt{2\pi} \quad ,$$

where the ξ, η and φ are the prolate spheroidal coordinates. We put the charge $Z_a = -1$ in the left focus ($\xi = 1, \eta = -1$) and the charge $Z_b = 2$ in the right focus ($\xi = 1, \eta = 1$). Functions $\Pi(\xi)$ and $\Xi(\eta)$ are solutions of the eigenvalue problem for a system of equations (in atomic units, $m = e = \hbar = 1$)

$$\Big[\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi} + RZ_+\xi - \frac{m^2}{\xi^2-1} + \frac{ER^2\xi^2}{2} + A\Big]\Pi(\xi) = 0,$$

$$\Big[\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta} + RZ_-\eta - \frac{m^2}{1-\eta^2} + \frac{ER^2\eta^2}{2} - A\Big]\Xi(\eta) = 0,$$

with the boundary conditions on the intervals $1 \le \xi < +\infty$ and $-1 \le \eta \le 1$:

$$|\Pi(1)| < +\infty, \quad \Pi(\infty) = 0, \qquad |\Xi(-1)| < +\infty, \quad |\Xi(1)| < +\infty,$$

and the normalization conditions

$$\frac{R^3}{8}\int_1^{+\infty}\int_{-1}^{1}\Pi^2(\xi)\Xi^2(\eta)(\xi^2-\eta^2)d\xi d\eta = 1, \quad \int_{-1}^{1}\Xi^2(\eta)d\eta = 1.$$

Here $Z_+ = Z_a + Z_b$ and $Z_- = Z_b - Z_a$, E is an energy, A is a separation constant.

It is useful to perform the modified Jaffé transformation [2]

$$X(\mu) = (\xi^2 - 1)\Pi(\xi), \quad Y(\eta) = (1 - \eta^2)\Xi(\eta),$$
$$\mu = \frac{\xi - 1}{\xi + \alpha} \quad , \tag{1}$$

where α is a transformation parameter, $\alpha \geq 1$. In terms of the μ and η the problem transforms to the following one

$$\Phi^{(1)} = \Big[\frac{[(\alpha-1)\mu+2]\,\mu(\mu-1)^2}{\alpha+1}\frac{d^2}{d\mu^2} + \frac{2(\mu-1)\,[(\alpha-1)\mu^2+(\alpha+2)\mu+1]}{\alpha+1}\frac{d}{d\mu} +$$
$$+RZ_+\frac{\alpha\mu+1}{1-\mu} - \frac{m^2(1-\mu)^2}{[(\alpha-1)\mu+2]\,(\alpha+1)\mu} + \frac{2\,[(\alpha^2+1)\mu+2(\alpha-1)\mu+2]}{[(\alpha-1)\mu+2]\,(\alpha+1)\mu} +$$
$$+\frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2} + A\Big]X(\mu) = 0, \tag{2}$$

$$\Phi^{(2)} = \Big[(1-\eta)^2\frac{d^2}{d\eta^2} + 2\eta\frac{d}{d\eta} + RZ_-\eta - \frac{m^2}{1-\eta^2} + \frac{2(1+\eta^2)}{1-\eta^2} - \frac{ER^2\eta^2}{2} - A\Big]Y(\eta) = 0, \tag{3}$$

with the new boundary conditions on the intervals $0 \leq \mu \leq 1$ and $-1 \leq \eta \leq 1$:

$$\Phi^{(3)} = X(0) = 0, \quad \Phi^{(4)} = X(1) = 0, \quad \Phi^{(5)} = Y(-1) = 0, \quad \Phi^{(6)} = Y(1) = 0. \tag{4}$$

The normalization conditions take a form

$$\frac{R^3}{8}\int_0^1\int_{-1}^1 \frac{(1-\mu)^2X^2(\mu)}{(\alpha+1)\mu^2((\alpha-1)\mu+2)}\frac{Y^2(\eta)}{(1-\eta^2)^2}\left[\frac{(1+\alpha\mu)^2}{(1-\mu)^2} - \eta^2\right]d\mu d\eta = 1,$$

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

Due to Dirichlet boundary conditions it may be replaced by the next normalization conditions:

$$\Phi^{(7)} = \int_0^1 X^2(\mu)d\mu - 1 = 0, \quad \Phi^{(8)} = \int_{-1}^1 Y^2(\eta)d\eta - 1 = 0. \tag{5}$$

This formulation of the problem looks more convenient for solving by a numerical approach due to Dirichlet boundary conditions appearing on the finite intervals. Evidently, different values of the transformation parameter α lead to different distribution of functions $X(\mu) \equiv X(\mu, \alpha)$. Fig. 1 illustrates distributions of the quasiradial solutions $(N = 3, l = 0, m = 0)$ depending on α, and fig. 2 shows the corresponding behaviour on the initial interval. To choose an "optimal" value α^{opt} of the parameter α, we can add the following condition:

$$\Phi^{(9)} = f(\alpha) - M = 0, \tag{6}$$

where

$$f(\alpha) = \int_0^1 |X(\mu, \alpha)|d\mu, \quad M = \max_\alpha f(\alpha),$$

i.e. the value of the integral must be maximal.

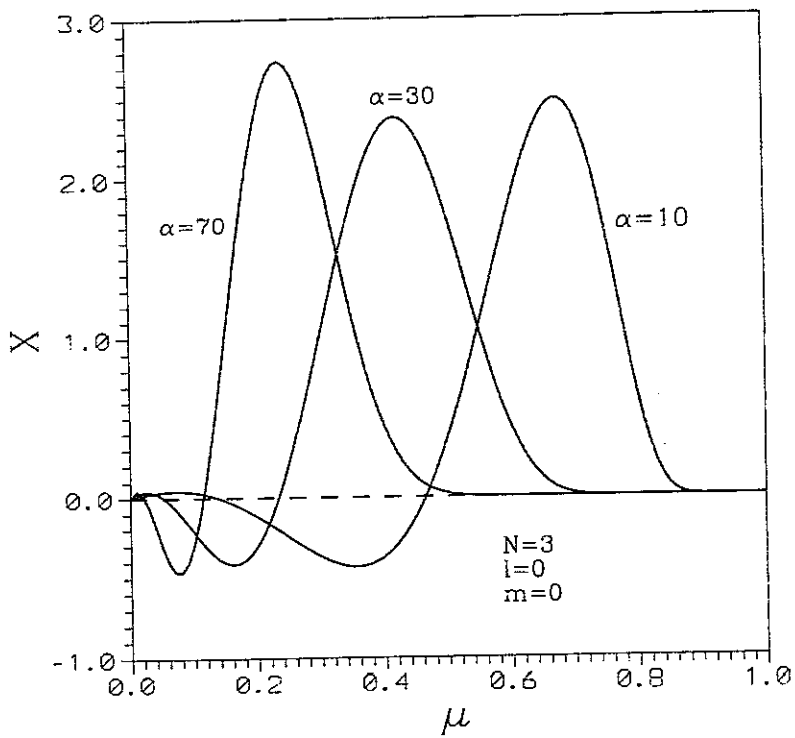

Fig.1. The distribution of the quasiradial solutions $(N = 3, l = 0, m = 0)$ on the finite interval μ at different values of transformation parameter α.

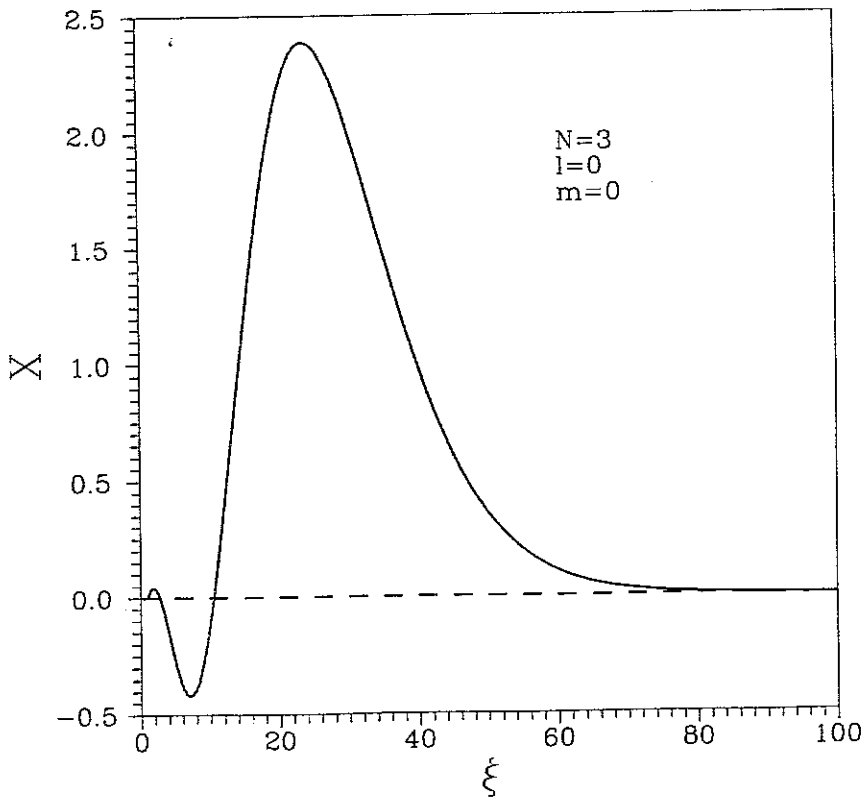

Fig.2. The quasiradial solution ($N = 3, l = 0, m = 0$) on infinite interval ξ

3 Computational scheme

The system (2-6) is solved by the multiparameter continuous analog of Newton's method [11], while we apply the modified Newton method to solve equation (6) for component $\Phi^{(9)}$.

First, we solve the system of equations (2-5) at a fixed value of the parameter α. This problem is solved by continuous analog of Newton's method [10]

$$\Phi_u(u)\frac{du}{dt} = -\Phi(u), \quad u(0) = u_0. \tag{7}$$

Here $u(t) = \{X(t), Y(t), E(t), A(t)\}$ is a set of unknown variables, u_0 is an initial approximation from a vicinity of the solution u_*, and Φ_u is the Frechet derivative of the vector function $\Phi(u) = \{\Phi^{(1)}(u), \cdots, \Phi^{(8)}(u)\}$.

It is convenient to rewrite the equations (2-3) in the form

$$\mathbf{P}X + AX + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}X = 0, \quad \mathbf{Q}Y - AY - \frac{ER^2\eta^2}{2}Y = 0,$$

where $\mathbf{P}$ and $\mathbf{Q}$ are differential operators of the second order

$$\mathbf{P} = \frac{[(\alpha-1)\mu+2]\mu(\mu-1)^2}{\alpha+1}\frac{d^2}{d\mu^2} + \frac{2(\mu-1)[(\alpha-1)\mu^2+(\alpha+2)\mu+1]}{\alpha+1}\frac{d}{d\mu} +$$

$$+RZ_+\frac{\alpha\mu+1}{1-\mu} - \frac{m^2(1-\mu)^2}{[(\alpha-1)\mu+2](\alpha+1)\mu} + \frac{2[(\alpha^2+1)\mu+2(\alpha-1)\mu+2]}{[(\alpha-1)\mu+2](\alpha+1)\mu},$$

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

The next designations are introduced

$$v = \frac{du}{dt}, \quad \varphi = \frac{dX}{dt}, \quad \phi = \frac{dY}{dt}, \quad a = \frac{dA}{dt}, \quad e = \frac{dE}{dt}.$$

The Newton method takes a form

$$\mathbf{P}\varphi + A\varphi + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}\varphi + aX + e\frac{R^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}X =$$

$$-\left[\mathbf{P}X + AX + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}X\right],$$

$$\varphi(0) = -X(0), \quad \varphi(1) = -X(1).$$

$$\mathbf{Q}\phi - A\phi - \frac{ER^2\eta^2}{2}\phi - aY - e\frac{R^2\eta^2}{2}Y = -\left[\mathbf{Q}Y - AY - \frac{ER^2\eta^2}{2}Y\right],$$

$$\phi(-1) = -Y(-1), \quad \phi(1) = -Y(1),$$

$$\int_0^1 (2\varphi X + X^2)d\mu = 1, \quad \int_{-1}^1 (2\phi Y + Y^2)d\eta = 1.$$

We use the decomposition

$$\varphi = \varphi_1 + a\varphi_2 + e\varphi_3, \quad \phi = \phi_1 + a\phi_2 + e\phi_3.$$

To find $\varphi_1,\varphi_2,\varphi_3,\phi_1,\phi_2,\phi_3$, it is required to solve the next linear differential equations

$$\mathbf{P}\varphi_1 + A\varphi_1 + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}\varphi_1 = -\left[\mathbf{P}X + AX + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}X\right],$$

$$\varphi_1(0) = -X(0), \quad \varphi_1(1) = -X(1),$$

$$\mathbf{P}\varphi_2 + A\varphi_2 + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}\varphi_2 = -X, \quad \varphi_2(0) = 0, \quad \varphi_2(1) = 0, \tag{8}$$

$$\mathbf{P}\varphi_3 + A\varphi_3 + \frac{ER^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}\varphi_3 = -\frac{R^2}{2}\frac{(1+\alpha\mu)^2}{(1-\mu)^2}X, \quad \varphi_3(0) = 0, \quad \varphi_3(1) = 0, \tag{9}$$

$$\mathbf{Q}\phi_1 - A\phi_1 - \frac{ER^2\eta^2}{2}\phi_1 = -\left[\mathbf{Q}Y - AY - \frac{ER^2\eta^2}{2}Y\right],$$

$$\phi_1(-1) = -Y(-1), \quad \phi_1(1) = -Y(1),$$

$$\mathbf{Q}\phi_2 - A\phi_2 - \frac{ER^2\eta^2}{2}\phi_2 = Y, \quad \phi_2(-1) = 0, \quad \phi_2(1) = 0, \tag{10}$$

$$\mathbf{Q}\phi_3 - A\phi_3 - \frac{ER^2\eta^2}{2}\phi_3 = \frac{R^2\eta^2}{2}Y, \quad \phi_3(-1) = 0, \quad \phi_3(1) = 0. \tag{11}$$

Clearly, $\varphi_1 = -X, \phi_1 = -Y$. After solving (8-11), we obtain the linear system for a and e

$$2a\int_0^1 \varphi_2 X\,d\mu + 2e\int_0^1 \varphi_3 X\,d\mu = \int_0^1 X^2 d\mu + 1, \tag{12}$$

$$2a\int_{-1}^1 \phi_2 Y\,d\eta + 2e\int_{-1}^1 \phi_3 Y\,d\eta = \int_{-1}^1 Y^2 d\eta + 1. \tag{13}$$

The systems (8-11) are solved with the 4th order approximation by step h of a uniform grid ω

$$\omega = \{\mu = (i-1)h_\mu, i = \overline{1, N_\mu}, h_\mu = 1/(N_\mu - 1);$$

$$\eta = -1 + (j-1)h_\eta, j = \overline{1, N_\eta}, h_\eta = 2/(N_\eta - 1)\}$$

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 matrices of linear systems are reduced to a five-diagonal form, and we solve the above algebraic problems with the help of LU-decomposition for the band matrices. The integrals in equations (12-13) are calculated by the Simpson method.

Thus, using $X^{(k)}, Y^{(k)}, A^{(k)}, E^{(k)}$, we calculate $\varphi_2^{(k)}, \varphi_3^{(k)}, \phi_2^{(k)}, \phi_3^{(k)}$ solving (8-11). System (12-13) give us $a^{(k)}$ and $e^{(k)}$. The full increment is

$$\varphi^{(k)} = -X^{(k)} + a^{(k)}\varphi_2^{(k)} + e^{(k)}\varphi_3^{(k)}, \quad \phi^{(k)} = -Y^{(k)} + a^{(k)}\phi_2^{(k)} + e^{(k)}\phi_3^{(k)}.$$

The next approximation is calculated by the formula

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

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

where τ is the step by the parameter t calculated by

$$\tau = \frac{\delta(0)}{\delta(0) + \delta(1)}, \quad \delta(t) = \delta(u^{(k)} + tv^{(k)}) = \| \Phi(u^{(k)} + tv^{(k)}) \|_{C_2}.$$

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

Second, we solve the problem (2-5) at three values of the parameter α: $\alpha^{(k)} - \Delta\alpha$, $\alpha^{(k)}$, $\alpha^{(k)} + \Delta\alpha$, where $\Delta\alpha$ is a given value, and calculate the function

$$f(\alpha) = \int_0^1 |X(\mu, \alpha)| d\mu$$

at these points. Further, we approximate the curve $f(\alpha)$ by a parabola and will calculate a new approximation $\alpha^{(k+1)}$ as the vertex of this parabola:

$$\alpha^{(k+1)} = -\frac{B_p}{2A_p},$$

where

$$A_p = \frac{1}{2\Delta\alpha^2}\left[f(\alpha^{(k)} - \Delta\alpha) - 2f(\alpha^{(k)}) + f(\alpha^{(k)} + \Delta\alpha)\right],$$

$$B_p = \frac{1}{\Delta\alpha^2}\left[-f(\alpha^{(k)} - \Delta\alpha)(\alpha^{(k)} + \frac{\Delta\alpha}{2}) + 2f(\alpha^{(k)})\alpha^{(k)} - f(\alpha^{(k)} + \Delta\alpha)(\alpha^{(k)} - \frac{\Delta\alpha}{2})\right].$$

The search of α^{opt} is stopped if $| \alpha^{(k+1)} - \alpha^{(k)} | < \varepsilon$. Table 1 demonstrates the Runge relation σ

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

to confirm the 4th order approximation of the solution (2-5) on the uniform grid ω.

Table 1. Runge relation.R=1.$h = h_\mu = h_\eta = 0.01$

$N = 2, l = 0, m = 0, \alpha = 10 \quad N = 3, l = 0, m = 0, \alpha = 16$

f	f(h) f(h/2) f(h/4)	σ	f	f(h) f(h/2) f(h/4)	σ
X(0.2)	-0.458386316516394 -0.458368517740968 -0.458367429677101	16.3582	X(0.2)	-0.308980664390056 -0.308956559901849 -0.308955069772919	16.1761
X(0.4)	-2.029697819696383 -2.029692671579400 -2.029692354527991	16.2374	X(0.4)	0.439970315147421 0.439803405547362 0.439793077581732	16.1609
X(0.6)	-0.785438986980358 -0.785460241934896 -0.785461547346590	16.2821	X(0.6)	2.296342903348499 2.296419842476338 2.296424599775984	16.1728
X(0.8)	-0.000813278434572 -0.000813333551101 -0.000813337017038	15.9023	X(0.8)	0.032817914160072 0.032824555738012 0.032824962184904	16.3405
Y(-0.6)	0.228866565401310 0.228866584800033 0.228866586027697	15.8013	Y(-0.6)	0.229970394037188 0.229970425651006 0.229970427643412	15.8671
Y(-0.2)	0.606429673767456 0.606429720466854 0.606429723386765	15.9934	Y(-0.4)	0.609006620618948 0.609006695817933 0.609006700523754	15.9799
Y(0.2)	0.992593062684076 0.992593096844050 0.992593098976196	16.0214	Y(0.2)	0.994107571771151 0.994107622300923 0.994107625458254	16.0039
Y(0.6)	1.030005342076385 1.030005308852579 1.030005306779762	16.0283	Y(0.6)	1.027171079039612 1.027171013736271 1.027171009653483	15.9947
A	1.137873205875893 1.137872764091516 1.137872736657884	16.1037	A	1.110049329366962 1.110048580663200 1.110048533984594	16.0395
E	-0.189932204048434 -0.189930293595120 -0.189930176521154	16.3183	E	-0.073191753896325 -0.073188552155872 -0.073188353927820	16.1518

The initial values of energy E and separation constant A are given by asymptotic formula [3,14]

$$E^{asy}_{R\to 0}(R) = E^{(0)}_{Nlm} + E^{(2)}_{Nlm}R^2 + O(R^3), \quad A^{asy}_{R\to 0}(R) = A^{(0)}_{Nlm} + A^{(2)}_{Nlm}R^2 + O(R^3),$$

$$E^{(0)}_{Nlm} = -\frac{Z_+^2}{2N^2}, \quad A^{(0)}_{Nlm} = -l(l+1),$$

$$E^{(2)}_{N00} = +\frac{2Z_aZ_bZ_+^2}{3N^3}, \quad E^{(2)}_{Nlm} = -\frac{2Z_aZ_bZ_+^2}{N^3(2l-1)(2l+1)(2l+3)}\Big[1-\frac{3m^2}{l(l+1)}\Big],$$

$$A^{(2)}_{Nlm} = -\frac{E^{(0)}_{Nlm}}{4}\Big[1-\frac{m^2}{l(l+1)}\Big] - \frac{1}{8}\frac{Z_-^2}{N^2}\Big[1-\frac{3m^2}{l(l+1)}\Big].$$

Table 2 compares the calculated values of energy E and separation constant A with asymptotic values $A^{asy}_{R\to 0}$ and $E^{asy}_{R\to 0}$ of the states $(N = 9, l = 8, m = 8)$, $(N = 9, l = 7, m = 6)$ and $(N = 9, l = 6, m = 4)$.

As an initial approximation for the quasiradial function $X(\mu)$ the radial wavefunction of the united atom is used [12]

$$R_{Nl}(r) \sim r^l\ {}_1F_1\Big(-(N-l-1), 2l+2, \frac{2r}{N}\Big), \quad r = \frac{R}{2}(\xi - 1),$$

where ${}_1F_1$ is the confluent hypergeometric function [13], having $n_r = N - l - 1$ nodes. Then the initial approximation $X^{(0)}(\xi)$ with $n_\xi = n_r$ nodes takes a form

$$X^{(0)}(\xi) = (\xi^2 - 1)R_{Nl}(\xi), \quad \xi = \frac{1+\alpha\mu}{1-\mu}.$$

The function

$$Y^{(0)}(\eta) = \cos\Big(\frac{\pi}{2}(n_\eta + 1)\eta + \frac{\pi}{2}n_\eta\Big), \quad n_\eta = l - m,$$

is applied as an initial approximation for the quasiangular wavefunction $Y(\eta)$ with n_η nodes. The examples of the solutions and initial approximations of the states with quantum numbers $(N = 5, l = 2, m = 0)$ and $(N = 7, l = 3, m = 0)$ at $R = 1$ are presented by means of solid and dashed lines correspondingly in figs.3, 4. Fig.3 demonstrates the known fact that the range of applicability of the united atom approximation is extended with increasing the value of the principal quantum number.

4 Results and Discussion

In this work a system $Z_a = -1, Z_b = 2$ corresponding to $\bar{p}He^+$ system is considered. Fig.5 shows distribution of function $f(\alpha)$ (6) for states $(N = 3, l = 0, m = 0)$, $(N = 4, l = 0, m = 0)$ and $(N = 5, l = 0, m = 0)$ at $R = 1$. It is calculated in process of the search of α^{opt}. The comparison of distributions of function $X(\mu)$ of state $(N = 4, l = 0, m = 0)$ for different values α is presented in fig.6. One can

Table 2. Comparison calculated values A and E with asymptotic value $A^{asy}_{R\to 0}$ and $E^{asy}_{R\to 0}$.

$N = 9, l = 8, m = 8.$

R	A	$A^{asy}_{R\to 0}$	E	$E^{asy}_{R\to 0}$
1.00	-71.97352815	-71.97530864	-0.00617472	-0.00617472
0.90	-71.97855682	-71.98000000	-0.00617436	-0.00617436
0.80	-71.98305654	-71.98419753	-0.00617404	-0.00617404
0.70	-71.98702719	-71.98790123	-0.00617376	-0.00617376
0.60	-71.99046866	-71.99111111	-0.00617351	-0.00617351
0.50	-71.99338084	-71.99382716	-0.00617331	-0.00617331
0.40	-71.99576364	-71.99604938	-0.00617314	-0.00617314
0.30	-71.99761701	-71.99777777	-0.00617300	-0.00617300
0.20	-71.99894088	-71.99901234	-0.00617291	-0.00617291
0.10	-71.99973521	-71.99975308	-0.00617285	-0.00617285
0.01	-71.99999735	-71.99999753	-0.00617283	-0.00617283

$N = 9, l = 7, m = 6.$

R	A	$A^{asy}_{R\to 0}$	E	$E^{asy}_{R\to 0}$
1.00	-55.98053661	-55.98555996	-0.00617437	-0.00617437
0.90	-55.98423636	-55.98830357	-0.00617408	-0.00617408
0.80	-55.98754599	-55.99075837	-0.00617382	-0.00617382
0.70	-55.99046572	-55.99292438	-0.00617359	-0.00617359
0.60	-55.99299574	-55.99480158	-0.00617339	-0.00617339
0.50	-55.99513624	-55.99638999	-0.00617322	-0.00617322
0.40	-55.99688735	-55.99768959	-0.00617308	-0.00617308
0.30	-55.99824920	-55.99870039	-0.00617297	-0.00617297
0.20	-55.99922189	-55.99942239	-0.00617290	-0.00617290
0.10	-55.99980547	-55.99985559	-0.00617285	-0.00617285
0.01	-55.99999805	-55.99999855	-0.00617283	-0.00617283

$N = 9, l = 6, m = 4.$

R	A	$A^{asy}_{R\to 0}$	E	$E^{asy}_{R\to 0}$
1.00	-41.99510240	-41.99647266	-0.00617320	-0.00617320
0.90	-41.99604025	-41.99714285	-0.00617313	-0.00617313
0.80	-41.99687647	-41.99774250	-0.00617307	-0.00617307
0.70	-41.99761204	-41.99827160	-0.00617301	-0.00617301
0.60	-41.99824780	-41.99873015	-0.00617297	-0.00617297
0.50	-41.99878450	-41.99911816	-0.00617293	-0.00617293
0.40	-41.99922276	-41.99943562	-0.00617289	-0.00617289
0.30	-41.99956310	-41.99968253	-0.00617287	-0.00617287
0.20	-41.99980592	-41.99985890	-0.00617285	-0.00617285
0.10	-41.99995149	-41.99996472	-0.00617284	-0.00617284
0.01	-41.99999951	-41.99999964	-0.00617283	-0.00617283

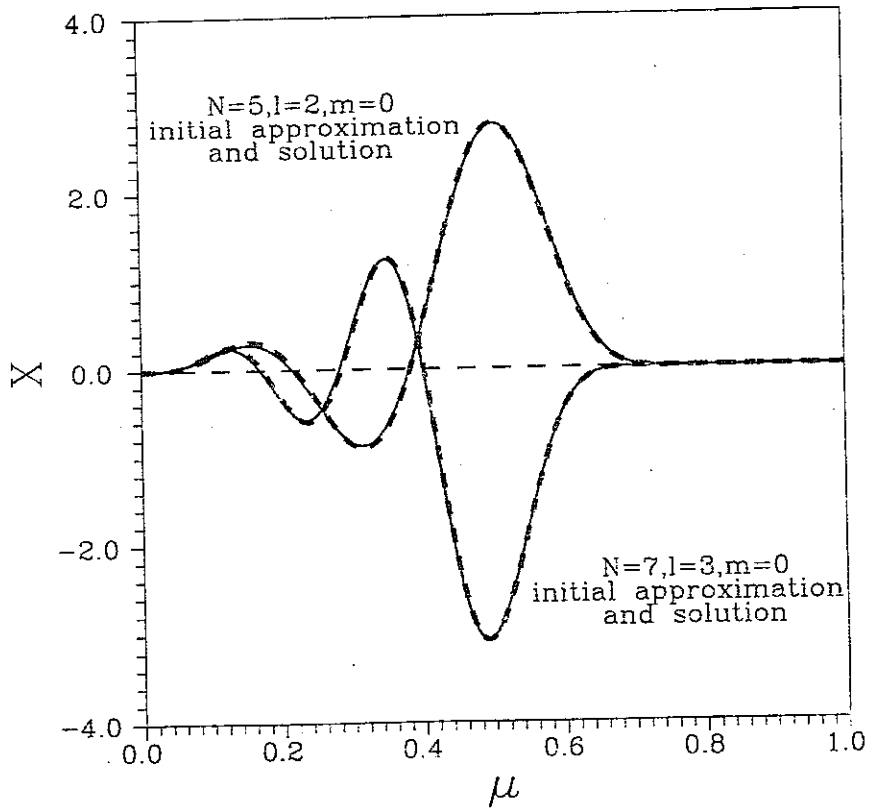

Fig 3. The initial approximation (dashed lines) and the quasiradial solution (solid lines) of the states $N = 5, l = 2, m = 0$ and $N = 7, l = 7, m = 0$ at $R = 1$.

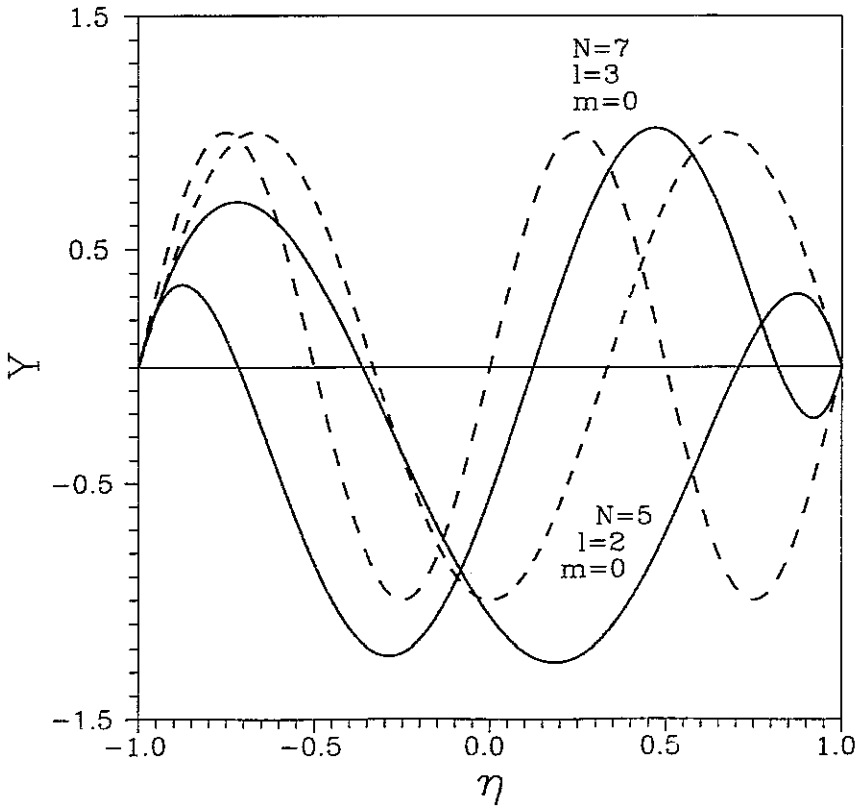

Fig 4. The initial approximation (dashed lines) and the quasiangular solution (solid lines) of the states $(N = 5, l = 2, m = 0)$ and $(N = 7, l = 7, m = 0)$ at $R = 1$.

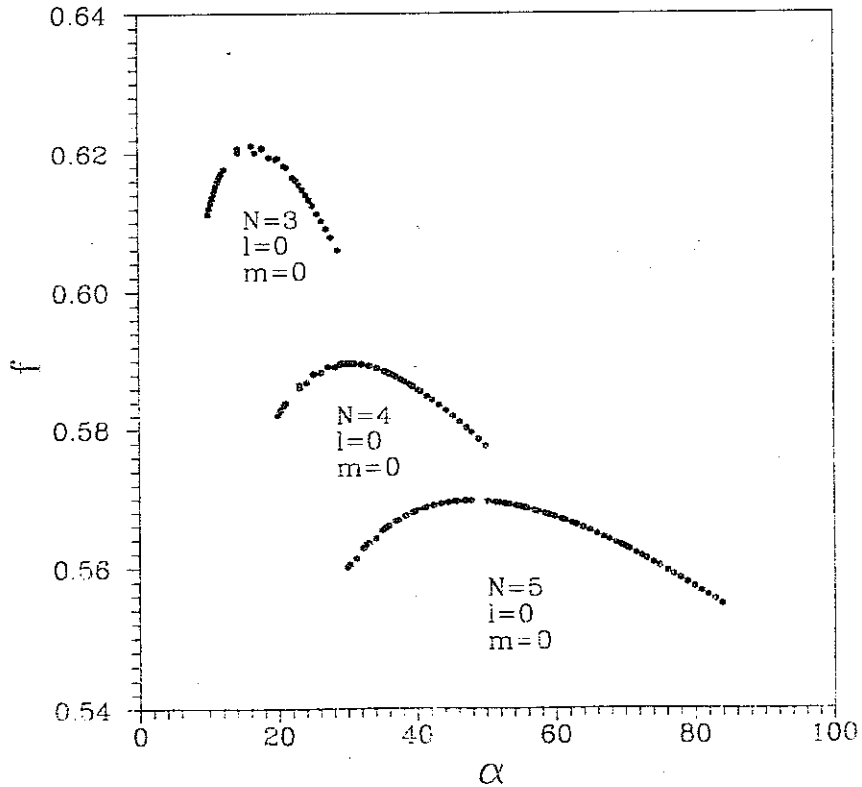

Fig.5. The distribution of function $f(\alpha)$ for states $N = 3, 4, 5, l = 0, m = 0$ at $R = 1$ calculated in the iteration process of solving equation (6). The maximum points are corresponded to the optimal value α.

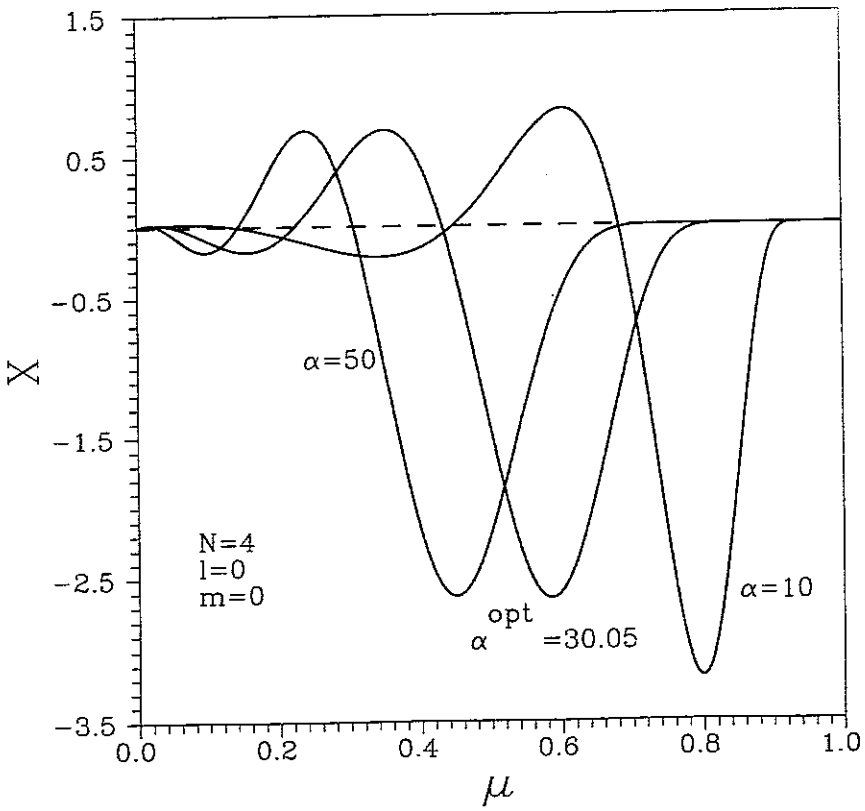

Fig.6. The distribution of the quasiradial solutions ($N = 4, l = 0, m = 0$) at $R = 1$ on the finite interval μ at different values of transformation parameter α in comparison with the quasiradial solution corresponding the optimal value α^{opt} calculated from equation (6).

see that the true choice of α provides optimal distribution of solutions around the center of the finite interval. By the way, the choice of α^{opt} allows us to find the set $\{X(\mu), Y(\eta), E, A\}$ for states with principal quantum number $N = 1, 2..., 10$ in the framework of the proposed algorithm. For example, wavefunctions of the states ($N = 9, l = 0, m = 0$) and ($N = 9, l = 8, m = 0$) are presented in figs.7, 8. Figs.9, 10 show a behaviour of potential curves $E(R)$ and separation constants $A(R)$ for n=2,3 and n=4 multiplets.

To extract the united atom Hamiltonian with the effective charge $Z_* = Z_+$,

$$h_*(\vec{r}_*) = -\frac{1}{2}\nabla^2_{\vec{r}_*} - \frac{Z_*}{r_*},$$

from the two-center Coulomb problem Hamiltonian,

$$h(R, \vec{r}_*) = h_*(\vec{r}_*) + V_*(R, \vec{r}_*), \quad V_*(R, \vec{r}_*) = \frac{Z_*}{r_*} - \frac{Z_a}{r_a} - \frac{Z_b}{r_b},$$

we will transform the "old" variables $\vec{R}, \vec{r}$ to the "new" ones $\vec{R}, \vec{r}_*$:

$$\vec{R} = \vec{R}, \quad \vec{r}_* = \vec{r} + \frac{\gamma_*}{2}\vec{R}, \quad \gamma_* = -\frac{Z_b - Z_a}{Z_b + Z_a} < 0.$$

This means that the perturbation term $V_*(\vec{r}_*, R)$ in eq. (h,V) takes the form

$$V_*(R, \vec{r}_*) = \frac{Z_*}{r_*} - \frac{Z_a}{|\vec{r}_* + R_a\vec{R}|} - \frac{Z_b}{|\vec{r}_* - R_b\vec{R}|},$$

where $R_a = Z_b/Z_*$ and $R_b = Z_a/Z_*$ are satisfied to a standard condition $R_a + R_b = 1$. It is obviously that the dipole term in the expansion $V_*(R, \vec{r}_*)$ with respect to power of R_a and R_b is disappeared, because $Z_a R_a - Z_b R_b = 0$.

Due to the perturbation theory [14], the leading terms of energy $E(R)$ are determined by the conventional relations

$$E^{(2)} = \frac{Z_a Z_b}{Z_+}\Big(\frac{1}{6}\rho_{N0,N0}(0)\Omega^{(0)}_{00,00} - \int_0^{+\infty} dr_* r_*^2 \rho_{Nl,Nl}(r_*) r_*^{-3} \Omega^{(2)}_{lm,lm}\Big),$$

$$\int_0^{+\infty} dr_* r_*^2 \rho_{Nl,Nl}(r_*) r_*^{-3} = \Big(\frac{2Z_+}{N}\Big)^3 \frac{(2l-1)!}{(2l+2)!}, \quad \rho_{Nl,Nl}(r_*) = |\psi_{Nl}(r_*)|^2,$$

$$\psi_{Nl}(r_*) = -\sqrt{\frac{(N-l-1)!}{(N+l)!2N}}\Big(\frac{2Z_+}{N}\Big)^{3/2} \exp\Big(-\frac{Z_+ r_*}{N}\Big)\Big(\frac{2Z_+ r_*}{N}\Big)^l \frac{L^{(2l+1)}_{N+l}\big(\frac{2Z_+ r_*}{N}\big)}{(N+l)!},$$

$$\Omega^{(2)}_{lm,lm} = \int_0^{+\infty} d\hat{r}_* Y^*_{lm}(\hat{r}_*) P_2(\cos\theta) Y_{lm}(\hat{r}_*) = \frac{l(l+1) - 3m^2}{(2l-1)(2l+3)},$$

that lead to the asymptotic formula of section 3. Thus, in the UA representation the above wave functions are the functions of zero approximation and the dipole

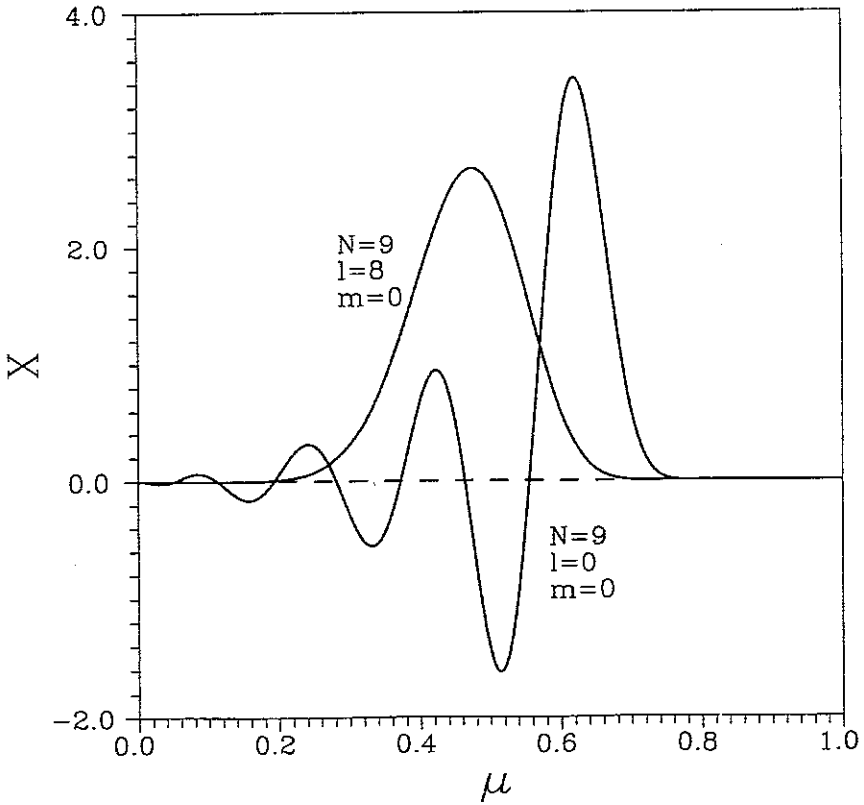

Fig.7. The distribution of the quasiradial solutions on the finite interval μ for the states $N = 9, l = 0, m = 0$ and $N = 9, l = 8, m = 0$ at $R = 1$.

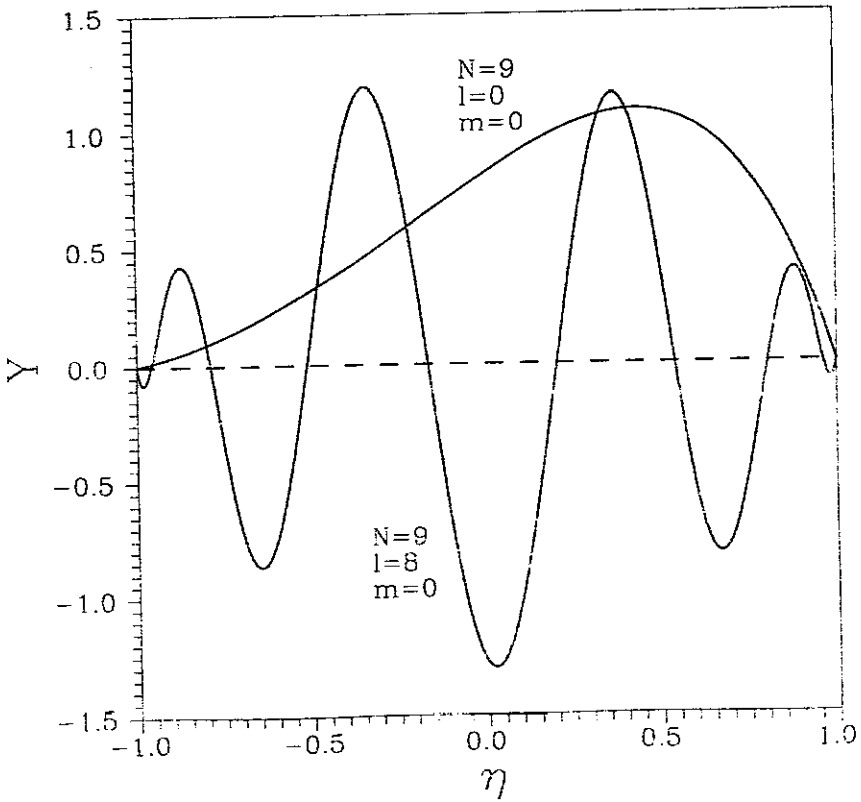

Fig.8. The behaviour of the quasiangular solutions on the finite interval μ of the states $(N = 9, l = 0, m = 0)$ and $(N = 9, l = 8, m = 0)$ at $R = 1$.

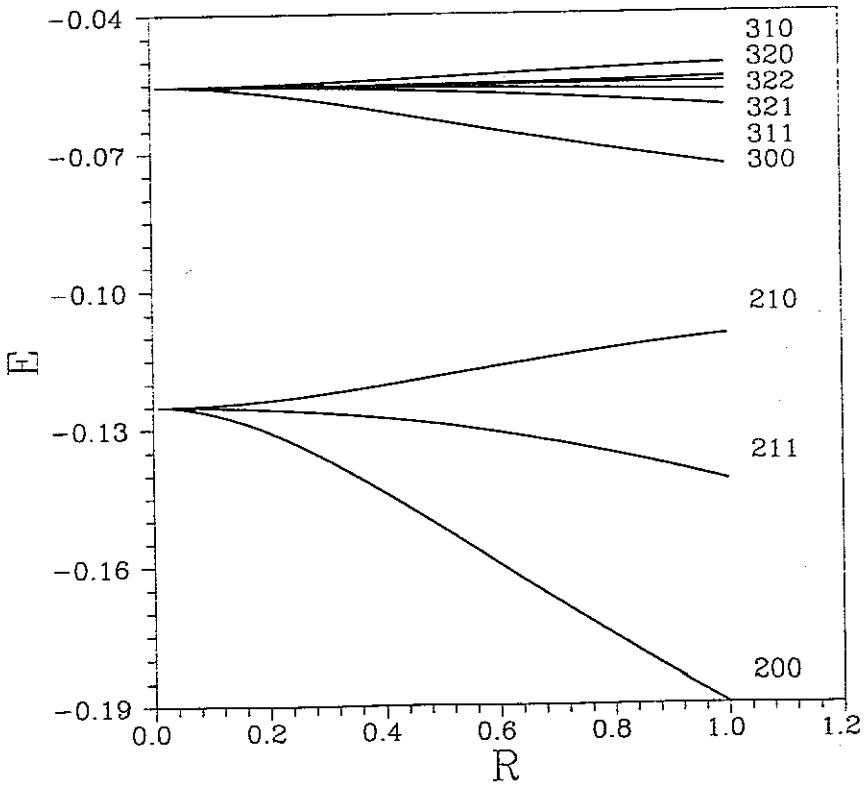

Fig.9. The behaviour of the potential curves $E(R)$ (a) and the the separation constant $A(R)$ (b) for principle numbers $N = 2, 3$.

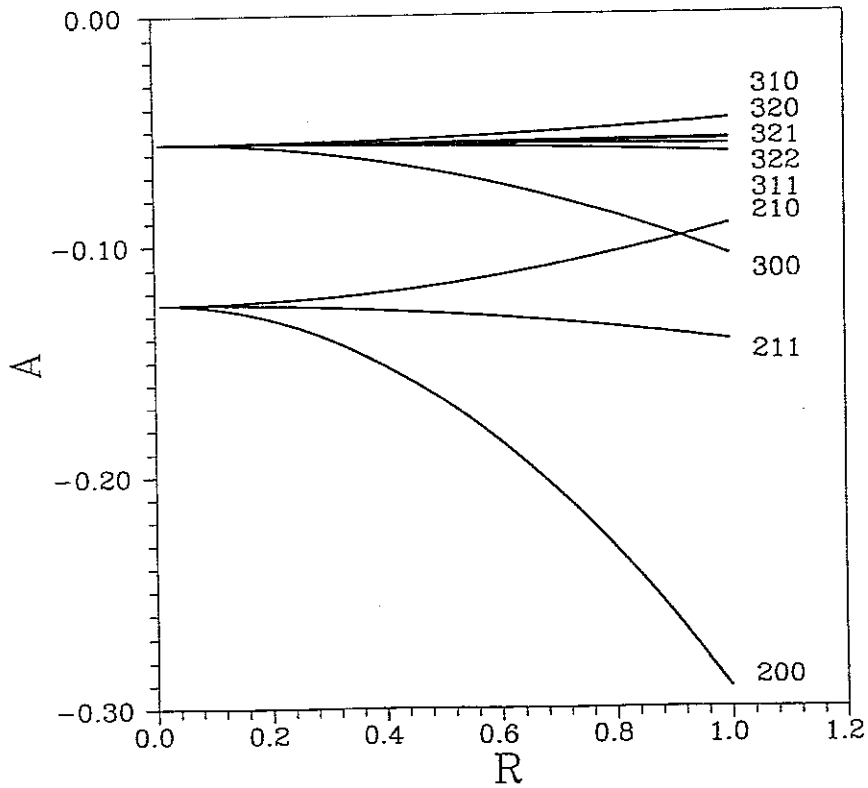

Fig.9b).

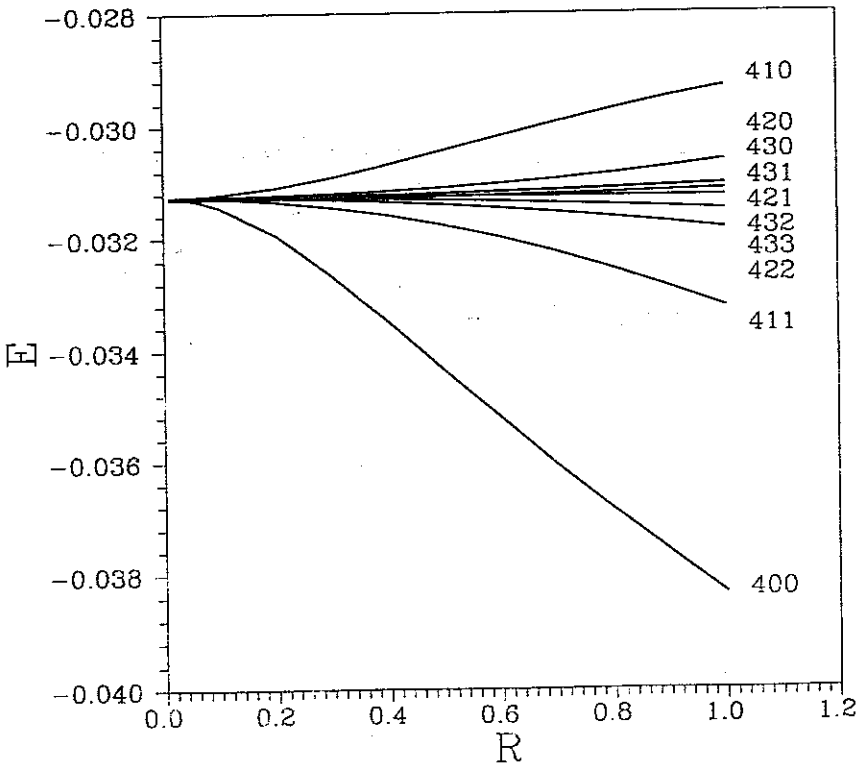

Fig.10. The behaviour of the potential curves $E(R)$ (a) and the the separation constant $A(R)$ (b) for principle number $N = 4$.

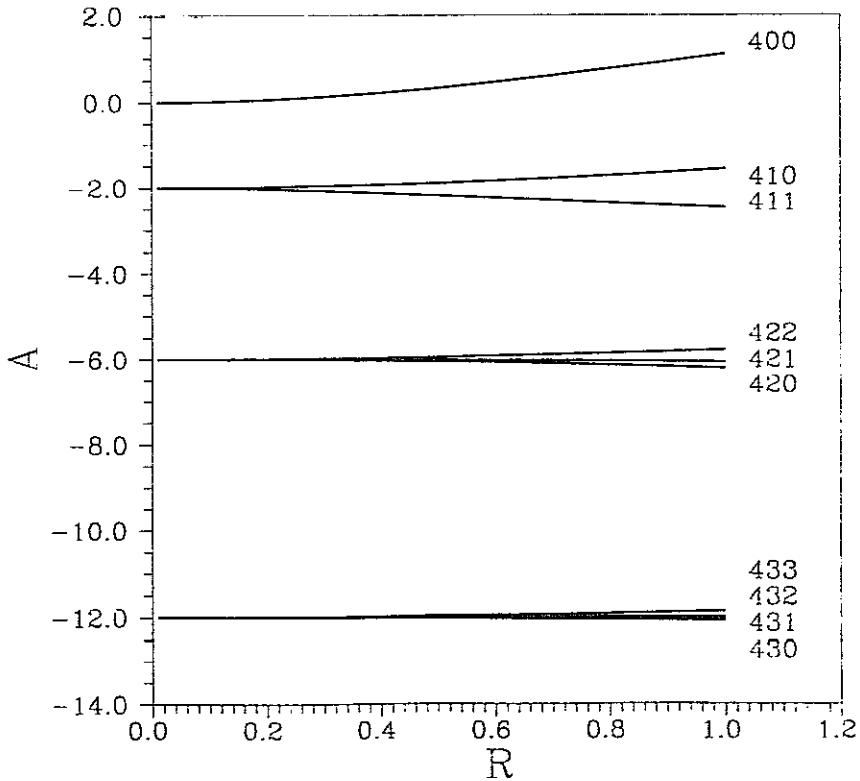

Fig.10b).

momentum operators of electron, D_e, antiproton, $D_{\bar{p}}$ and antiprotonic atomcule are determined by the following relations

$$D_e = -\vec{r}_b = -(\vec{r} + \frac{\gamma_b}{2}\vec{R}) = \frac{1}{2}\vec{R} - \vec{r}, \quad D_{\bar{p}} = \vec{R}, \quad \gamma_b = 1,$$

$$D^{tot} = D_e + D_{\bar{p}} = \frac{3}{2}\vec{R} - \vec{r} = -\vec{r}_*.$$

Such a picture of UA supports a true treatment of a behavior of the distribution of the densities of figs. 11. In Fig. 11a the set of the sections of the density of the ground state solution with respect of the reduced z' variable

$$z' = \frac{2}{R}z = \xi\eta$$

for the values $R = 0.1, 0.2, 1.0, 2.0$ is shown in comparison with the ground states of the systems $Z_a = 1, Z_b = 2$ (fig.11b) and $Z_a = 1, Z_b = 1$ (fig.11c). One can see the announced specific behaviour of localization of the density of the two-center wavefunctions in a vicinity of the united atom. Indeed, the localization of the density at small values R takes place in the opposite side of the right focus with respect to conventional H_2^+ ion (fig.11c). Moreover the localization of the density for ground states tends to separated atom limit from the same opposite side towards the right focus by such a way that $E_{100}(R)$ coincides with accuracy 0.04% with the asymptotic value

$$E_{100}^{asy}(R) = -2 + \frac{1}{R} - \frac{9}{4R^4} + O\Big(\frac{1}{R^6}\Big)$$

even at value $R = 2$.

Note that at $R \to +\infty$ the asymptotics behaviours in general case $E(R)$ and $A(R)$ take a form [15]

$$E_{R\to+\infty}^{asy}(R) = -\frac{Z_b^2}{N^2}\Big[\frac{1}{2} + \frac{1}{\tau}\lambda - \frac{1}{2\tau^2}3\lambda\Delta + \frac{1}{2\tau^3}(6\Delta^2 + 1 - N^2)\Big]$$

$$+\frac{1}{16\tau^4}(\lambda\Delta(39N^2 + 9m^2 - 109\Delta^2 - 59) + \lambda^2(17N^2 - 9m^2 - 3\Delta^2 + 19),$$

where

$$\tau = \frac{RZ_b}{N}, \quad \lambda = \frac{NZ_a}{Z_b}, \quad \Delta = n_\xi - n_\eta,$$

$$A_{R\to+\infty}^{asy}(R) = p^2 - 2p(S-\nu)\nu S + \frac{1}{2}\Big[\nu^2 + 1 - m^2\Big]$$

$$-\frac{1}{8p}\Big[(\nu^2 + 1 - m^2)\nu - (3\nu^2 + 1 - m^2)S + 2\nu S^2\Big]$$

$$-\frac{1}{64p^2}\Big[-5\nu^4 - 10\nu^2 + 6\nu^2m^2 - (1-m^2)^2 + (20\nu^2 + 20 - 12m^2)\nu S$$

$$-(24\nu^2 + 8 - 8m^2)S^2 + 8\nu S^3\Big]$$

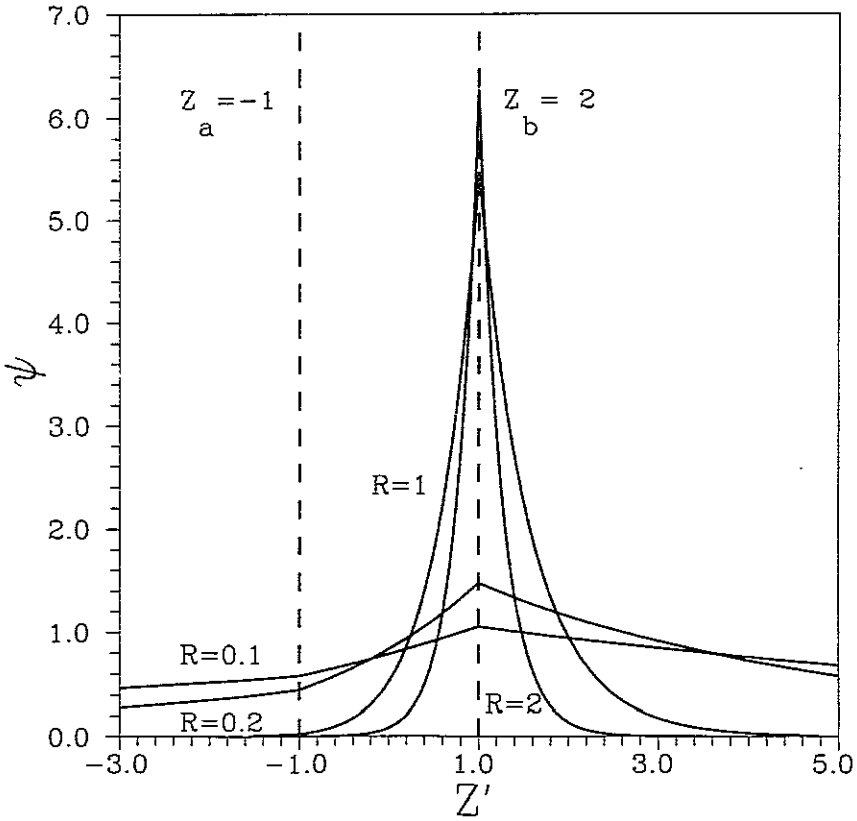

Fig.11. The evolution of the sections of the density of the ground state solution at $R = 0.1, 0.2, 1, 2$ for different charge sets: $Z_a = -1, Z_b = 2$ (a), $Z_a = 1, Z_b = 2$ (b), $Z_a = 1, Z_b = 1$ (c)

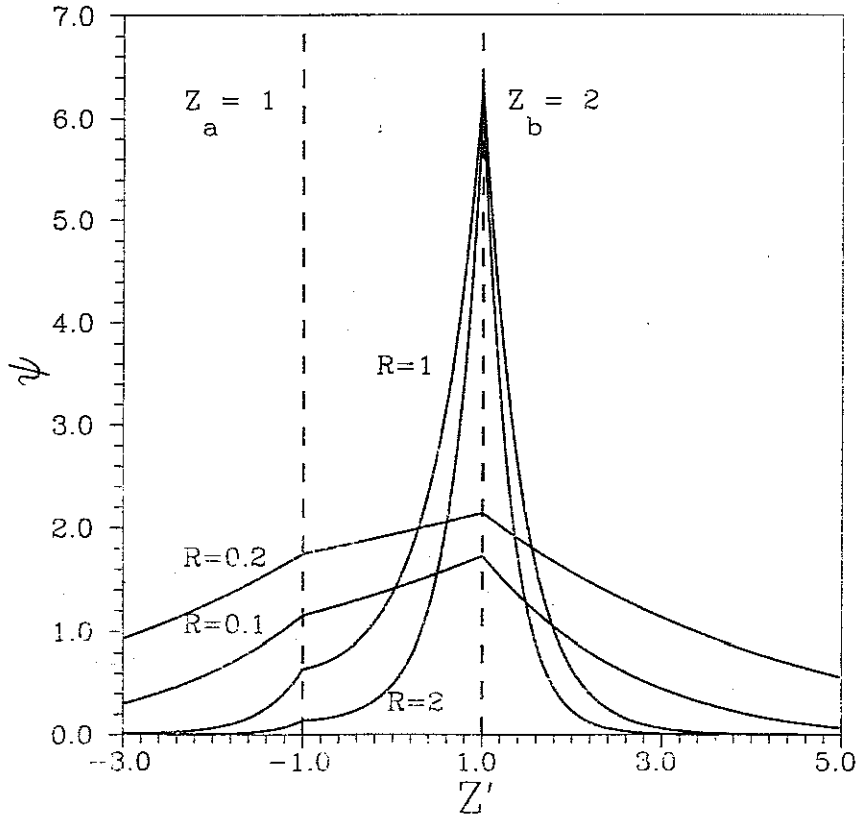

Fig.11b).

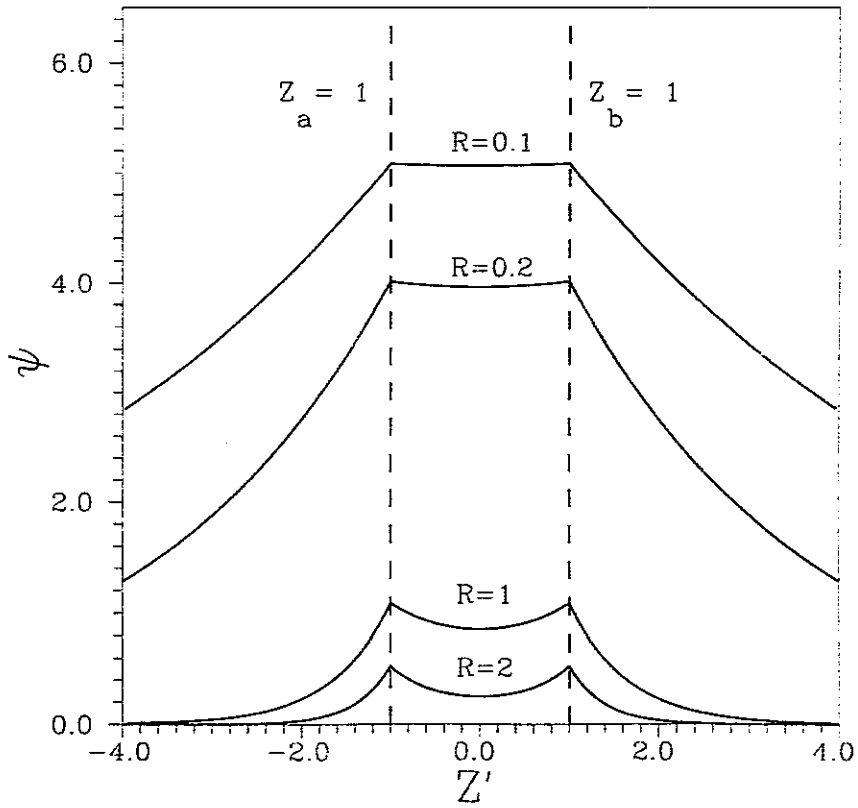

Fig.11c).

$$-\frac{1}{512p^3}\Big[(33\nu^4+114\nu^2-46\nu^2m^2+37+13m^2+50m^2)\nu$$
$$-(165\nu^4+342\nu^2-138\nu^2m^2+37+13m^2-50m^2)S$$
$$+(284\nu^2+292-156m^2)\nu S^2-(192\nu^2+64-64m^2)S^3+40\nu S^4\Big]$$
$$-\frac{1}{1024p^4}\Big[-63\nu^6-340\nu^4-239\nu^2-14$$
$$+100\nu^4m^2-39\nu^2m^2+230\nu^2m^2+2m^6-18m^4+30\,m^2$$
$$+(378\nu^4+1360\nu^2-478-400\nu^2m^2-460\,m^2+78m^4)\nu S$$
$$-(845\nu^4+1810\nu^2+209-630\nu^2m^2-250\,m^2+41m^4)S^2$$
$$+(860\nu^2+900-460m^2)\nu S^3$$
$$-(384\nu^2+128-128m^2)S^4+56\nu S^5\Big],$$

where

$$p=\frac{R}{2}\sqrt{-2E^{asy}_{R\to+\infty}(R)},\quad S=\frac{R(Z_a+Z_b)}{2p},\quad \nu=2n_\xi+m+1.$$

The Table 3 demonstrates the comparison of the calculated value of separated constant A and energy E with the asymptotics values $A^{asy}_{R\to+\infty}, E^{asy}_{R\to+\infty}$ for the states $(N=3,l=2,m=2)$ and $(N=3,l=1,m=0)$. The dependence of the energy $E(R)$ and separation constant $A(R)$ in comparison with its asymptotics are presented by means of solid and dashed lines correspondingly on figs.12a and 12b.

The analysis of the asymptotics of the Born-Oppenheimer potentials

$$W(R)=-\frac{2}{R}+E(R)$$

with the accuracy $O(R^2)$ is supposed the existence of the local maximum in the states with $n_\xi=0,\quad n_\eta=N-1$ at the points $R_N\simeq\frac{3}{2}N(N-1)$. For convenience values $\Delta W(R)=W(R)-E(+\infty), E(+\infty)=-Z_b/(2N^2)$ are demonstrated in fig.13 for $N=\overline{6,10}$. As an example, the potential $W(R)$ is considered for the quantum number $(N=6,l=5,m=0)$. The local maximum is $W_{max}=-0.0629946$ at $R\simeq 47.6$ and the local minimum is $W_{min}=-0.0635974$ at $R\simeq 67.6$. In this outer well the 14th equidistant energy levels are found (Fig.14) with the help of the algorithm from Appendix. The wavefunctions without nodes of state $(N_s=1)$ and with thirteen nodes of state $(N_s=14)$ supported by the outer well in the BO potential converges to $N=6$ threshold are shown on Fig.15.

Table 3. Comparison calculated values A and E with asymptotic value $A^{asy}_{R\to+\infty}$ and $E^{asy}_{R\to+\infty}$.

$N=3,l=2,m=2.$

R	A	$A^{asy}_{R\to+\infty}$	E	$E^{asy}_{R\to+\infty}$
20.0	48.06696044	48.08497596	-0.17355795	-0.17361616
30.0	108.73009687	108.73384311	-0.18926911	-0.18927534
40.0	191.56895254	191.57024026	-0.19737836	-0.19737965
50.0	296.60781196	296.60838882	-0.20230071	-0.20230110
60.0	423.85681394	423.85711782	-0.20560039	-0.20560054
70.0	573.32079586	573.32097436	-0.20796447	-0.20796453
80.0	745.00233133	745.00244475	-0.20974081	-0.20974085
90.0	938.90290888	938.90298542	-0.21112409	-0.21112411
100.0	1155.02344706	1155.02350137	-0.21223164	-0.21223165

$N=3,l=1,m=0.$

R	A	$A^{asy}_{R\to+\infty}$	E	$E^{asy}_{R\to+\infty}$
20.0	49.99237804	50.01747437	-0.17360808	-0.17368735
30.0	110.67187623	110.67719834	-0.18928068	-0.18928940
40.0	193.52209064	193.52394795	-0.19738225	-0.19738410
50.0	298.56879662	298.56963869	-0.20230236	-0.20230292
60.0	425.82345804	425.82390594	-0.20560120	-0.20560142
70.0	575.29169106	575.29195635	-0.20796491	-0.20796501
80.0	746.97652825	746.97669820	-0.20974108	-0.20974112
90.0	940.87974044	940.87985640	-0.21112426	-0.21112428
100.0	1157.00242770	1157.00251165	-0.21223175	-0.21223176

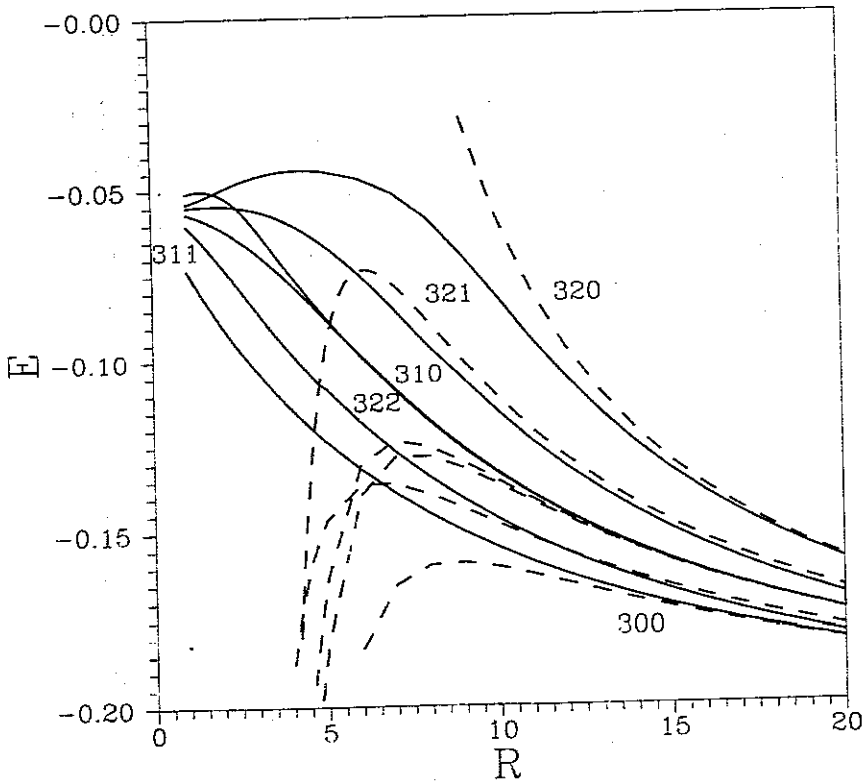

Fig.12. The comparison of numerical values (solid lines) the potential curves $E(R)$ (a) and the the separation constant $A(R)$ (b) with their asymptotic values (dashed lines).

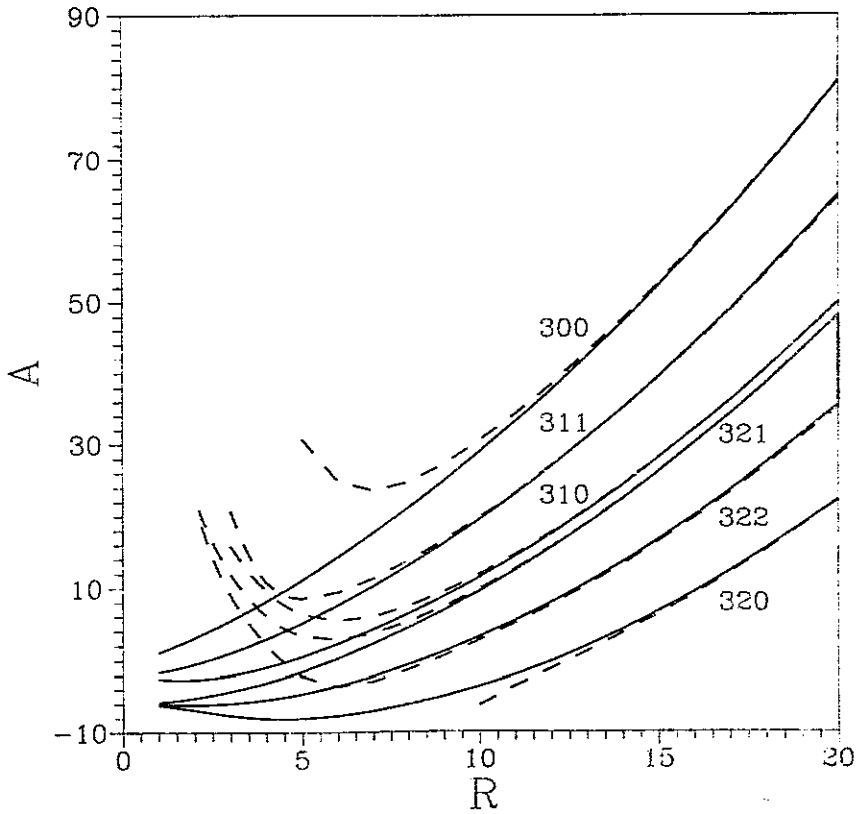

Fig.12b).

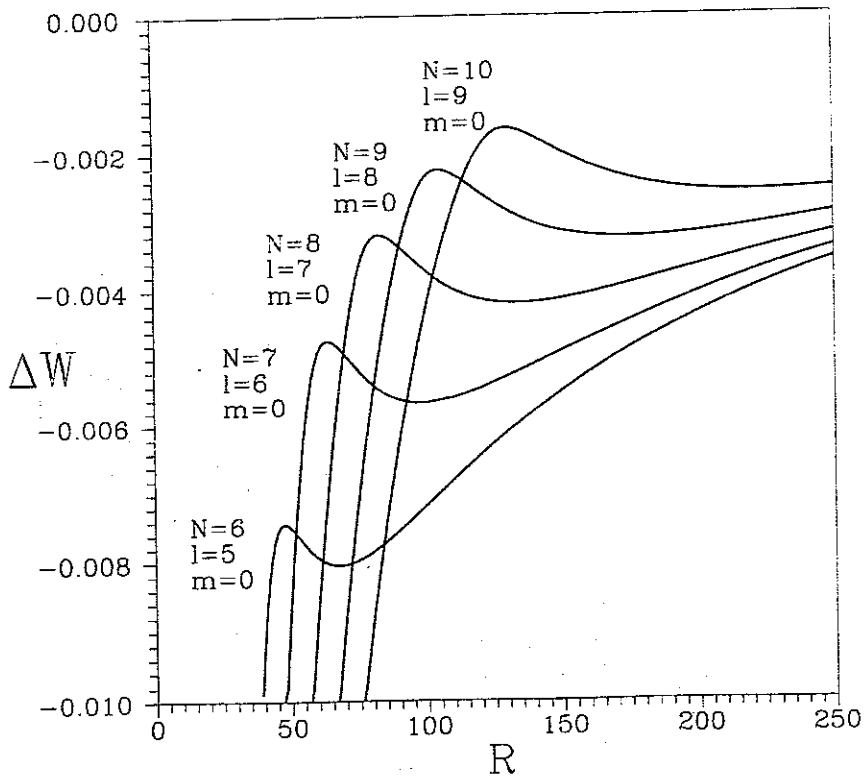

Fig.13. The behavior of the BO potentials ΔW counted off from the corresponding threshold for the states with quantum numbers $(N = n, l = n - 1, m = 0)$, $n = 6, 7, 8, 9, 10$

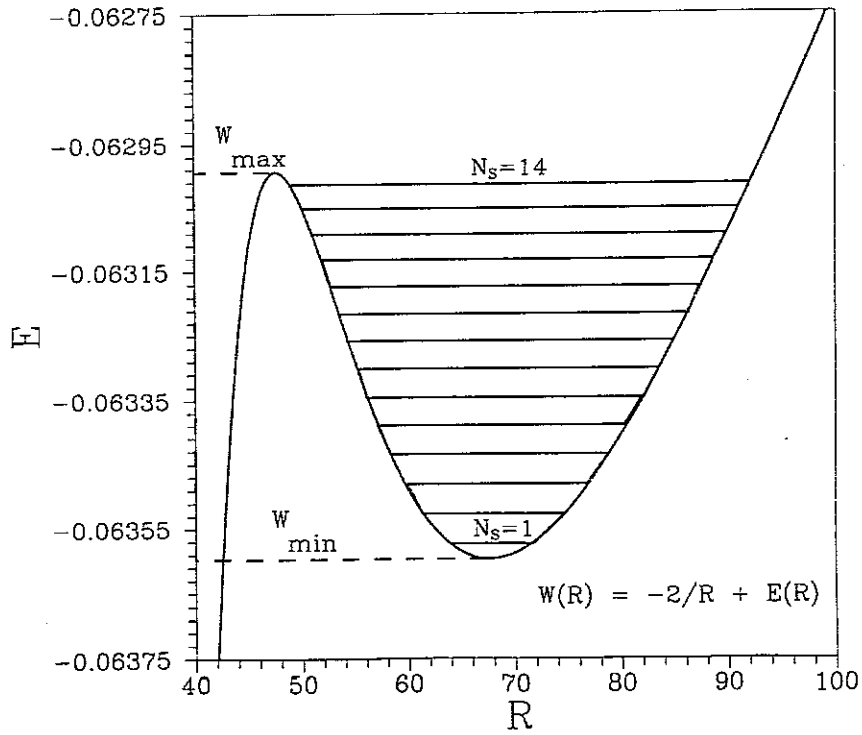

Fig.14. The energy levels $N_s = 1, ..., 14$ in the outer well for the BO potential $W(R)$ for the state $(N = 6, l = 5, m = 0)$ of the system $\bar{p}\,{}^4He^+$.

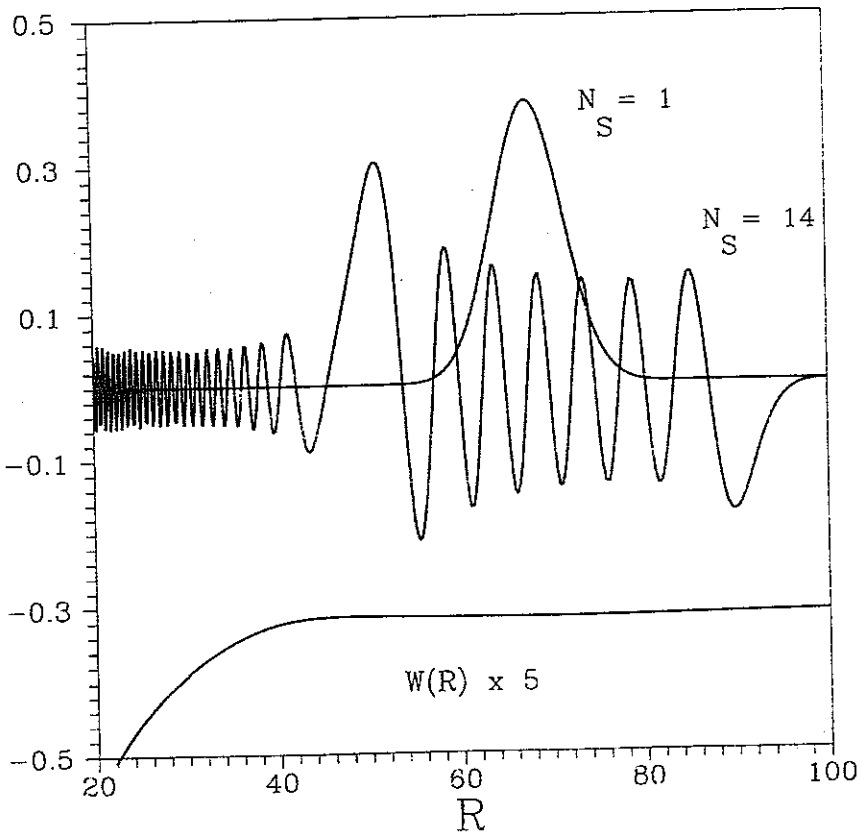

Fig.15. The radial wavefunctions with $N_s = 1$ and $N_s = 14$ for system $\bar{p}\,{}^4He^+$ in the BO potential $W(R)$ for the state $N = 6, l = 5, m = 0$.

5 Conclusion

The essential part of the proposed algorithm connected with finding an optimal value of the parameter α responded for a reduction of the initial problem to a finite interval can be applied also to solve other problems, where such a parameter is ordinary used without an optimization procedure. In general, the additional condition (6) using for this aim follows from the virial theorem which will be satisfied by an approximate solution varied under a scale transformation [16]. In further we will develop an algorithm for calculation of the continuous spectrum of the two-center problem and the matrix elements of nonadiabatic coupling [17] to support a more detail study of the metastable states of the $\bar{p}He^+$ system with the help of pulse laser fields [18,19].

6 Acknowledgement.

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7 Appendix

To find the energy E and the wavefunction $\psi(R)$ of the outer well, it is needed to solve the equation (in atomic units, $m = e = \hbar = 1$)

$$\frac{1}{2M_0}\left(\frac{d^2}{dR^2} + \frac{2}{R}\frac{d}{dR}\right)\psi(R) + (E - W(R))\psi(R) = 0,$$

where $M_0 = M_{He}m_{\bar{p}}/(M_{He} + m_{\bar{p}})$ is the reduced mass, $W(R)$ is the full potential energy. The boundary and normalization conditions take a form

$$|\psi(0)| < +\infty, \quad \psi(+\infty) = 0, \qquad \int_0^{+\infty} R^2\psi^2(R)dR = 1.$$

We carry out the transformation of the independent variable R to reduce the problem from the infinite interval $[0; +\infty]$ to the finite interval $[0; 1]$

$$\zeta = \frac{R}{R+\alpha}, \quad R = \frac{\alpha\zeta}{1-\zeta}, \quad 0 \le \zeta \le 1,$$

where α is a transformation parameter, $\alpha \ge 1$. To receive the Dirichlet boundary condition, we introduced a new function $y(\zeta) = \zeta\psi(\zeta)$. With respect to the function $y(\zeta)$ we have the equation

$$\Phi^{(1)} = \frac{1}{2M_0}\frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2}y(\zeta) + (E - W(\zeta))y(\zeta) = 0$$

with the boundary conditions

$$\Phi^{(2)} = y(0) = 0, \quad \Phi^{(3)} = y(1) = 0,$$

and the normalization condition

$$\int_0^1 \frac{\alpha}{\zeta^2(1-\zeta)^2} y^2(\zeta) d\zeta = 1.$$

Due to Dirichlet boundary conditions we can use the unit normalization condition

$$\Phi^{(4)} = \int_0^1 y^2(\zeta) d\zeta - 1 = 0.$$

This problems is solved by continuous analog of Newton's method [10,11]

$$\Phi_z(z)\frac{dz}{dt} = -\Phi(z), \quad z(0) = z_0,$$

where $\Phi(z) = \{\Phi^{(1)}(z), \Phi^{(2)}(z), \Phi^{(3)}(z), \Phi^{(4)}(z)\}$, $z = \{y(\zeta,t), E(t)\}$, $\Phi_z(z)$ is the Frechet derivative, and t is the continuous parameter $t \in [0,\infty)$. We introduce the next designations

$$v = \frac{dy}{dt}, \quad e = \frac{dE}{dt}$$

and perform the decomposition $v = v_1 + ev_2$. For unknown functions v_1 and v_2 we have the equations

$$\frac{1}{2M_0}\frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2}v_1 + (E - W(\zeta))v_1 = -\Big[\frac{1}{2M_0}\frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2}y + (E - W(\zeta))y\Big],$$

$$v_1(0) = -y(0), \quad v_1(1) = -y(1),$$

$$\frac{1}{2M_0}\frac{(1-\zeta)^4}{\alpha^2}\frac{d^2}{d\zeta^2}v_2 + (E - W(\zeta))v_2 = -Ey, \quad v_2(0) = 0, \quad v_2(1) = 0. \qquad (14)$$

Clearly, $v_1 = -y$, therefore from the unit boundary condition we obtain

$$e = -\left(\int_0^1 v_2 y d\zeta\right)^{-1}. \qquad (15)$$

Thus, using $y^{(k)}, E^{(k)}$ we calculate $v_2^{(k)}$ solving (14). The relation (15) give us $e^{(k)}$. The increment for wavefunction is

$$v^{(k)} = -y^{(k)} + e^{(k)}v_2^{(k)}.$$

The next approximation is recalculated by the formula

$$y^{(k+1)} = y^{(k)} + \tau v^{(k)}, \quad E^{(k+1)} = E^{(k)} + \tau e,$$

where τ is the step by the parameter t calculating by

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

$$\delta(t) = \delta(y^{(k)} + tv^{(k)}, E^{(k)} + te^{(k)}) = \| \Phi(y^{(k)} + tv^{(k)}, E^{(k)} + te^{(k)}) \|_{C_2}.$$

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

The choice of the transformation parameter α makes possible to have a needed number of grid points in a vicinity of the local minimum of the potential $W(R)$, where we search the weakly bound states.

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