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NUMERICAL SOLUTION OF THE TWO CENTERS PROBLEM IN A COMPLEX PLANE[2]

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1 Introduction

The two Coulomb centers problem (the problem Z_1eZ_2) consists in a determination of wave functions of electron e, driven in a field of two fixed charges Z_1 and Z_2, which are located on a distance R from each other. It plays a fundamental role in the theory of collisions. Physical aspects of this task are covered in [1]. In the applications at account of inelastic processes (for example, passages between terms testing quasiintersection) the performances of terms in a complex plane R are required. In an outcome of direct numerical computation of terms in the complex plane R for a symmetric case were detected series of branchpoints, which allow to speak about a new type of quasiintersections. These "hidden" quasiintersections explain not only passages between bound states, but also the process of ionization [1–3].

2 Algorithm

Stationary Schrödinger equation of the two Coulomb centers supposes a separation of variables in prolated spheroidal coordinates [4], $r_i = |\mathbf{r} - \mathbf{R}_i|$:

$$\xi = \frac{r_1 + r_2}{R}; \qquad \eta = \frac{r_1 - r_2}{R}; \qquad \phi = \operatorname{arctg}\frac{x}{y}, \tag{1}$$

where $1 \le \xi < \infty$, $-1 \le \eta \le 1$, $0 \le \phi < 2\pi$. Substitution in it for the wave function as in [4,5]: $\Psi = (\xi^2-1)^{m/2} f(\xi)(1-\eta^2)^{m/2}\varphi(\eta)e^{im\phi}$ reduces in the following equations for $f(\xi)$ and $\varphi(\eta)$:

$$f''(\xi) + \frac{2\xi(m+1)}{\xi^2-1}f'(\xi) + \left[\frac{ER^2}{2} + \frac{a\xi-\lambda}{\xi^2-1} + \frac{m(m+1)}{\xi^2-1}\right] f(\xi) = 0, \tag{2}$$

$$\varphi''(\eta) - \frac{2\eta(m+1)}{1-\eta^2}\varphi'(\eta) + \left[\frac{ER^2}{2} + \frac{b\eta+\lambda}{1-\eta^2} - \frac{m(m+1)}{1-\eta^2}\right] \varphi(\eta) = 0, \tag{3}$$

where $a = (Z_1+Z_2)R$, $b = (Z_2 - Z_1)R$, λ – constant of separation.

For real values R, the problem was traditionally solved by the expansions of unknown functions f and φ on polynomials of variables ξ and η [6–11]. It leads to trinomial recurrent equations for factors of expansion. The problem Z_1eZ_2 was solved also by the finite differences [5,12,13] and by the spline-approximation [5,14] methods with use of continuous analog of the Newton's method. In the complex plane R the problem was solved by the expansions of functions [1–3]. In the present work the Newton's method applied for a solution of a nonlinear system of difference equations is considered.

To the equations (2), (3) it is necessary to add the equations circumscribing a behaviour of functions $f(\xi)$ and $\varphi(\eta)$ near the borders of a range of definition.

That the equations (2) and (3) made sense at $\xi \to 1$ and $\eta \to \pm 1$, the realization of next equalities is necessary [5]:

$$f'(1) + \left[\frac{a-\lambda}{2(m+1)} + \frac{m}{2}\right] f(1) = 0, \tag{4}$$

$$\varphi'(-1) + \left[\frac{\lambda-b}{2(m+1)} - \frac{m}{2}\right] \varphi(-1) = 0, \tag{5}$$

$$\varphi'(1) - \left[\frac{b+\lambda}{2(m+1)} + \frac{m}{2}\right] \varphi(1) = 0. \tag{6}$$

Use of an asymptotics for $f(\xi)$ in form $f(\xi) \sim \xi^\alpha \cdot e^{\beta\xi}$, $\xi \to \infty$, reduces in the following equation:

$$f'(\xi) - \left(\frac{\alpha}{\xi} + \beta\right) f(\xi) = 0, \quad \xi \to \infty. \tag{7}$$

For the factors α and β we have received relations:

$$\beta^2 + \frac{ER^2}{2} = 0, \qquad 2\alpha\beta + 2(m+1)\beta + a = 0. \tag{8}$$

The considered problem we solved for $\xi \in \langle 1, \xi_M\rangle$, where ξ_M is the large enough value, for which it is possible to assume good realization of asymptotics (8). For example, for the computation of the term $E_{3p\sigma}$ and $E_{4p\sigma}$ (spectroscopic labels [2]) at real value $R = 0.8$ we took $\xi_M \ge 25$ and $\xi_M \ge 45$, respectively.

The homogeneous boundary conditions allow to enter a normalization of the radial and angular function, for example, as:

$$\int_1^\infty |f(\xi)|^2 d\xi - 1 = 0, \qquad \int_{-1}^1 |\varphi(\eta)|^2 d\eta - 1 = 0. \tag{9}$$

For complex value R there will be complex also functions $f(\xi)$ and $\varphi(\eta)$ and also unknown quantities E, λ and parameters a and b. If we divide segment $\langle 1, \xi_M\rangle$ into N_ξ equal parts and segment $\langle -1, 1\rangle$ into N_η of equal parts and points of grids we denote ξ_i and η_i, we should determine unknowns:

$$\operatorname{Re} f(\xi_i),\ \operatorname{Im} f(\xi_i),\ i = \overline{1, N_\xi + 1}; \qquad \operatorname{Re}\varphi(\eta_i),\ \operatorname{Im}\varphi(\eta_i),\ i = \overline{1, N_\eta + 1};$$

and values $\operatorname{Re} E$, $\operatorname{Im} E$, $\operatorname{Re}\lambda$, $\operatorname{Im}\lambda$.

If we put to zeros real and imaginary parts of the complex equations (2), (3) in interior points $\xi = \xi_2, \dots, \xi_{N_\xi}$ and $\eta = \eta_2, \dots, \eta_{N_\eta}$, respectively, and equations (4–7) and if to these equations we shall add the equations (9), we shall receive a system of $2N_\xi + 2N_\eta + 6$ nonlinear equations. The number of unknowns is equal $2N_\xi + 2N_\eta + 8$. For complex functions $f(\xi)$ and $\varphi(\eta)$ it is possible (and it is necessary) to add two conditions of a normalization, for example:

$$\operatorname{Im} f(\xi_M) = 0, \qquad \operatorname{Im} \varphi(1) = 0. \tag{10}$$

The problem (2–7), (9), (10) we solved by a Newton's method. The system matrix is sparse. It has nonzero columns corresponding to derivatives with respect to the variables $\operatorname{Re} E$, $\operatorname{Im} E$, $\operatorname{Re}\lambda$, $\operatorname{Im}\lambda$ and also nonzero rows corresponding to derivatives of the equations of a normalization with respect to the variables $\operatorname{Re} f_i$, $\operatorname{Im} f_i$, $\operatorname{Re}\varphi_i$, $\operatorname{Im}\varphi_i$. We solved this system by the LU-decomposition of the system matrix. With the purpose of saving memory, we produced direct LU-decomposition, without of creation of a system matrix itself.

3 Numerical results

The problem $Z_1 e Z_2$ we solved for $Z_1 = Z_2 = 1$ and $m = 0$, with the purpose to compare outcomes with outcomes of works [1–3], which are obtained by other method. The computation in the complex plane we began always on a real axes R. On a real axes as initial values $\operatorname{Re} E$ we used values from a table from [5]. As initial approximations of wave functions $f(\xi)$ and $\varphi(\eta)$ we used either constant, or linear function with one zero, or cos function with appropriate number of zeros – all renormalized with respect to (9).

The problem is ill-conditioned, during a solution there appear very small values of the module of the diagonal elements l_{ii}. Therefore we applied a regularization, using idea of work [15]. The renormalization of unknown functions f and φ on each step of Newton's method promoted to improving and acceleration of convergence.

First and second derivatives in the equations (2–6) we approximated with the second order accuracy, in the asymptotic equation (7) we used both first, and second order accuracy. According to Runge's rule it is possible by results of the computation to conclude, that all difference scheme has in these cases first and the second order accuracy, respectively.

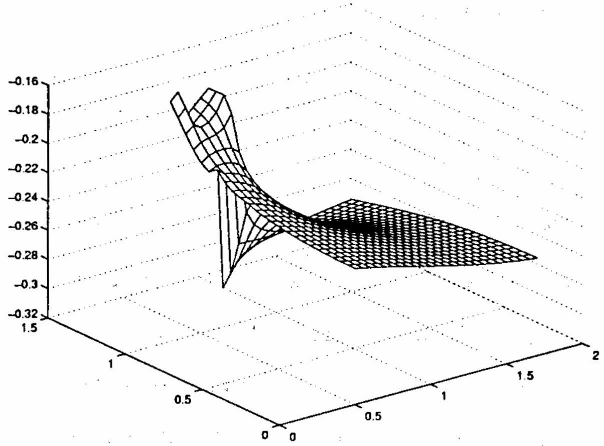

Fig. 1

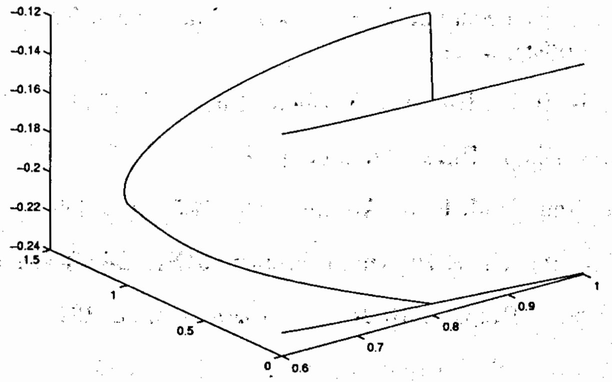

Fig. 2

Figure 1 shows surface $\operatorname{Re} E$ of a term $3p\sigma$. This surface was obtained by calculation along rays parallel to imaginary axes $\operatorname{Im} R$, beginning always on real axes $\operatorname{Re} R$. The similar figure is indicated in [2]. On Figure 2 the passage of a term $3p\sigma$ in a term $4p\sigma$ in an outcome of one round movement along the closed trajectory enveloping a branchpoint is shown.

The work shows, that the method of finite differences can be used for a solution of the two centers problem in complex area also, as well as method based on recurrent equations for factors of expansions of wave functions.

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Численное решение задачи двух центров
в комплексной плоскости

Задача двух кулоновских центров в комплексной плоскости межъядерного расстояния R рассматривается как система нелинейных уравнений. Система, которая получается в результате применения метода конечных разностей, решается методом Ньютона с использованием LU-разложения матрицы системы. При вычислении LU-разложения и решении системы применяется регуляризация.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Numerical Solution of the Two Centers Problem
in a Complex Plane

The two Coulomb centers problem in a complex plane of an internuclear distance R is considered as a system of the nonlinear equations. The system, which arises at use of a finite-differences method, is solved by the Newton's method with use of LU-decomposition of the system matrix. At an evaluation of the LU-decomposition and solution of the system the regularization was applied.

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

Preprint of the Joint Institute for Nuclear Research. Dubna, 1998