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NUMERICAL SOLUTION
OF THE MULTICHANNEL SCATTERING PROBLEM

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1. Introduction

The matrix Schrödinger equation can be written in the form ($\hbar = 1$)

$$\{d^2/dR^2 - 2Q(R)\,d/dR + [2M\varepsilon - \mathcal{H}(R)]\}\,\Psi(R) = 0, \tag{1}$$

where $Q(R)$ and $\mathcal{H}(R)$ are real $n \times n$ matrices of effective potentials of the problem, M is the reduced mass and ε is the total energy. The effective potentials are subject to the conditions providing self-adjointness of the differential operator: $Q(R)$ is antisymmetric and $\mathcal{H}^T(R) = \mathcal{H}(R) - 2dQ(R)/dR$ or $\mathcal{H}(R) = \mathcal{K}(R) + dQ(R)/dR$ where $\mathcal{K}(R)$ is symmetric. We will assume that potentials Q and $\mathcal{K}$ have the asymptotic form

$$\mathcal{K}(R) = \mathcal{E} + \sum_{m=1}^{M} A^{(m)} R^{-m},$$

$$Q(R) = \sum_{m=0}^{M} B^{(m)} R^{-m},$$

where $\mathcal{E}$ is diagonal matrix whose elements are the threshold energies of the different channels. Matrices $A^{(m)}$ are symmetric and $B^{(m)}$ are antisymmetric. We admit also that potential Q can be nonzero at the infinity. This assumption allows us to include into consideration the standard adiabatic PSS method [1,2] (also named as the multi-level adiabatic approach [3]) and other adiabatic approaches based, for example, on hyperspherical coordinates [4,5].

The methods being used for solving the radial Schrödinger equation, can be divided into two large groups. The first group consists of the methods based on evolutionary equations started from $R = 0$ and continuing the solution to the asymptotic region. These are, for example, the log-derivative method [6] and variable phase methods [7,8]. Another group regards Eq. (1) as a boundary inhomogeneous equation or a boundary eigenvalue problem. We mention here the matrix Numerov method [9] (it can be used only when Q is vanished), the continuous analog of the Newton method [10,11] imposing the nonlinear boundary condition in the asymptotic region with the phase shift as a parameter and, finally, the R-matrix method [12] where the eigenvalue problem is solved to obtain the R-matrix as a function of energy ε at some point beyond the interaction. The disadvantage of the major of these methods (maybe except the Numerov method) is *ab initio* nonlinearity of

the problem that complicates the application of perturbative theory when you appoximate the operator (1) by a more simple zero-order (not necessarily differential) operator.

The method proposed in this paper treats the equation (1) as a boundary inhomogeneous differential equation with a linear boundary condition in an asymptotic region. That helps us to develop an efficient computational scheme based on the variable order difference approximation [13] and the perturbative splitting of the initial operator. It was applied to calculate the scattering processes of mesoatoms of hydrogen isotopes on "bare" nuclei in the framework of the multi-level adiabatic approach [14] with the use of about 500 adiabatic states.

2. Boundary conditions

We are looking for solutions of Eq. (1) having asymptotic behaviour

$$\Psi^{(i)}(R) \simeq \vec{\phi}_i^{(-)} - \sum_{j=1} S_{ij} \vec{\phi}_j^{(+)}, \tag{2a}$$

where

$$\vec{\phi}_i^{(\pm)}(R) \simeq \bar{c}_0^{(i)} e^{\pm i(k_i R + \beta_i \ln R)}, \tag{2b}$$

and $\bar{c}_0$ is a vector scaling the asymptotic function to the unit flux [15]. Channel i is said to be open if k_i is real otherwise it is closed (we adopt the convention that k_i has a positive imaginary part for closed channels and k_i is a real positive number for open channels). The quantities S_{ij} for open channels form the S-matrix of the reaction. We deliberately omit here orbital momentum and Coulomb phase shift corrections, since the major part of adiabatic methods leads to equations having mixed asymptotic states of atomic functions. From the other side, they could be easily put into calculated S-matrix afterwords.

We can continue the solution (2) from the infinity to some finite point R_p using the asymptotic expansion

$$\vec{\phi}_i^{(\pm)}(R) = e^{\pm i k_i R} R^{i\beta_i} \left[\bar{c}_0^{(i)} + \sum_{n=1}^{N} \bar{c}_n R^{-n} \right]. \tag{3}$$

Inserting (3) into equation (1) yields us a sequence of equations providing solutions for unknown quantities in (3)

$$[k^2 + 2i k_i B_0 + \mathcal{E} - \varepsilon]\,\bar{c}_0 = 0; \tag{4a}$$

$$\left[k_i^2 + 2ik_iB_0 + \mathcal{E} - \varepsilon\right]\bar{c}_1 + \left[2k_i\beta_i + 2i\beta_iB_0 + 2ik_iB_1 + A_1\right]\bar{c}_1 = 0; \qquad (4b)$$

$$\bullet \ldots$$

and

$$\beta_i = -\frac{(\bar{c}_0, [2ik_iB_1 + A_1]\,\bar{c}_0)}{(\bar{c}_0, [2k_i + iB_0]\,\bar{c}_0)}. \qquad (5)$$

So for a given accuracy ϵ we can find a value R_p of R such that expansion (3) differs in absolute value from the exact solution by an amount smaller than ϵ for all $R \geq R_p$.

Unfortunately, this point can appear at some large distance from the origin. In this case it will be useful to integrate the solution inward by some certain numerical technique. If all channels are open, then the given solutions can be obtained by some initial value method (like Runge-Kutta or linear multistep methods which are available in a wide choice in different Fortran package libraries). The use of these methods in a case when some channels are closed, leads to instability and poor linear independence of obtained solutions. The Fox-Goodwin technique for the solution of two-point boundary value problems allows one to avoid the instability and to build a set of solutions which has good linear independence at the given point R_m [16].

Hereafter we assume that all the necessary solutions (and their derivatives) are obtained by one or another method at a given point R_m. We denote by $\Phi^{(+)}(R)$ the $n \times n$ matrix composed of solutions having an asymptotic form $\sim \exp(ikR)$ for open channels and exponentially decaying for closed channels which we assume to be non-singular.

We look for the boundary conditions of the form

$$\Psi'(R) + G\Psi(R) = b^{(i)}, \qquad (6)$$

which selects from the common asymptotic solution functions having an asymptotic behaviour as in (2). To do that we can consider the equations

$$\Psi' = \phi_i'^{(-)} - \Phi'^{(+)}S^{(i)},$$
$$\Psi = \phi_i^{(-)} - \Phi^{(+)}S^{(i)},$$

and try to get rid of unknown parameters S_{ij} using the regularity of the matrix $\Phi^{(+)}(R)$. Extracting $S^{(i)}$ from the second equation and inserting it into the first one we obtain the necessary expressions for the matrix G:

$$G = -\Phi'^{(+)}\left[\Phi^{(+)}\right]^{-1},$$

and for the right-hand side term:

$$b^{(i)} = \phi_i'^{(-)} + G\phi_i^{(-)}.$$

For the case of the finite-difference approximation to Eq. (1) it would be better to modify the boundary condition to the form without derivatives:

$$U\Psi(R_1) + W\Psi(R_2) = \delta_{ij},$$

where R_1 and R_2 are two neighbouring nodes in the difference grid. Matrices U and W can be obtained in a similar way.

For numerical calculations it is more convenient to work with real functions and real boundary conditions. We can transfer our asymptotic solutions to get a real form:

$$\phi_i^{(1)} = \frac{1}{2i}\left(\phi_i^{(+)} - \phi_i^{(-)}\right),$$
$$\phi_i^{(2)} = \frac{1}{2}\left(\phi_i^{(+)} + \phi_i^{(-)}\right),$$

For these "standing wave" functions a common solution can be expressed in a form:

$$\hat{\Psi}^{(i)} \simeq \phi_i^{(1)} - \sum_{j=1}^{m} K_{ij}\phi_j^{(2)}, \qquad (7)$$

where K is the so-called reactance matrix:

$$K = i(I+S)^{-1}(I-S), \qquad S = (I+iK)(I-iK)^{-1},$$

that has a real symmetric form [17].

3. Solution of the boundary problem

In the case of multichannel scattering we can usually describe an appropriate zero-order problem which has a satisfactory solution to the original equation. We assume that this zero-order approximation has a block-diagonal form and Eq. (1) can be rewritten as follows:

$$\left\{d^2/dR^2 - 2Q(R)_{ii}\,d/dR + [2M\epsilon - \mathcal{H}(R)_{ii}]\right\}\Psi_i(R) =$$
$$= \sum_{j\neq i}\left\{2Q(R)_{ij}\,d/dR + \mathcal{H}(R)_{ij}\right\}\Psi_j(R),$$

where the left-hand side of the equation is a system of uncoupled differential operators and the right-hand side represents the perturbative part. Denote them as H_0 and V, respectively. So we can introduce a standard perturbative scheme of the solution of Eq. (1)

$$H_0 X_{k+1} = V X_k, \qquad k = 0, 1, \ldots \qquad (8)$$

where X_k is an iterative solution of Eq. (1) and $X_0 = 0$. We recall that Eq. (8) is inhomogeneous equation due to inhomogeneous boundary condition (6).

The existence of first derivative term in Eq. (1) makes an application of Numerov difference fourth order approximation impossible. Compact three-point difference scheme thus can only provide a second order approximation to the original differential operator. The use of higher order approximations requires increasing of the number of points for the finite difference scheme that in its turn increases the width of the band of the matrix of an approximation and respectively increases memory and computational time requirements. Lentini, Pereyra [13] proposed the method that allowed to avoid these problems. It is based on the splitting of initial high order difference scheme into its second order approximation on one side and four, six and higher order corrections on the other

$$y''(x_k) = \{\Delta_2^{(2)} + \delta_4^{(2)} + \delta_6^{(2)} + \ldots\} y(x_k),$$
$$y'(x_k) = \{\Delta_2^{(1)} + \delta_4^{(1)} + \delta_6^{(1)} + \ldots\} y(x_k),$$

where

$$\Delta_2^{(2)} y(x_k) = \frac{y(x_{k+1}) - 2y(x_k) + y(x_{k-1})}{h^2},$$
$$\Delta_2^{(1)} y(x_k) = \frac{y(x_{k+1}) - y(x_{k-1})}{2h},$$

and

$$\delta_4^{(2)} y(x_k) = \frac{-y(x_{k+2}) + 4y(x_{k+1}) - 6y(x_k) + 4y(x_{k-1}) - y(x_{k-2})}{12h^2},$$
$$\delta_4^{(1)} y(x_k) = \frac{-y(x_{k+2}) + 2y(x_{k+1}) - 2y(x_{k-1}) + y(x_{k-2})}{12h},$$

and so on.

Finally we can rewrite the main equation (1) with the new splitting of the operator

$$\left\{ \Delta_2^{(2)} - 2\mathcal{Q}(R_k)_{ii}\, \Delta_2^{(1)} + [2M\varepsilon - \mathcal{H}(R_k)_{ii}] \right\} \Psi_i(R_k) =$$

$$= \sum_{j \neq i} \left\{ 2\mathcal{Q}(R_k)_{ij}\, \Delta_2^{(1)} + \mathcal{H}(R_k)_{ij} \right\} \Psi_j(R_k) -$$
$$- \left\{ \delta_4^{(2)} - 2\mathcal{Q}(R_k)_{ii} \delta_4^{(1)} \right\} \Psi_i(R_k) - \left\{ \delta_6^{(2)} - 2\mathcal{Q}(R_k)_{ii} \delta_6^{(1)} \right\} \Psi_i(R_k) + \ldots,$$

which can be successfully solved using perturbative corrections of the solution according to iterative process (8).

4. Numerical example

In this section we apply the described procedure for investigation of the charge transfer process in $d\mu + t \rightarrow t\mu + d$ inelastic scattering. The approach is based on the decomposition of the three-body wave function $\Psi(\mathbf{R}, \mathbf{r})$ using the adiadatic basis of states of the discrete and continuous spectra of the two-center problem (see Ref. 2):

$$\Psi(\mathbf{R}, \mathbf{r}) = \sum_n \phi_n(\mathbf{r}; R) \chi_n(\mathbf{R}) + \int_k dk \phi_c(\mathbf{r}; R, k) \chi_c(\mathbf{R}; k), \qquad (9a)$$

where the functions ϕ_n and ϕ_c satisfy the stationary equations

$$\left\{ -\frac{1}{2}\Delta_\mathbf{r} - \frac{1}{r_1} - \frac{1}{r_2} \right\} \phi_n(\mathbf{r}; R) = E_n(R)\phi_n(\mathbf{r}, R),$$
$$\left\{ -\frac{1}{2}\Delta_\mathbf{r} - \frac{1}{r_1} - \frac{1}{r_2} \right\} \phi_c(\mathbf{r}; R, k) = (k^2/2)\,\phi_c(\mathbf{r}, R, k). \qquad (9b)$$

Here $\mathbf{R}$ is an internuclear position vector, $\mathbf{r}$ is a muon position vector with respect to the geometric center of nuclei, r_1 and r_2 are respective muon–nucleus distances. (We should note here that we slightly change our notation for the three-body and radial wave functions). Inserting of (9) into the three-body Schrödinger equation and averaging over angular variables leads to the system of coupled equations for the amplitudes $\chi_i(R)$ describing the relative motion of the nuclei:

$$\frac{d^2}{dR^2}\chi_i(R) + \left(2M\varepsilon - \frac{J(J+1)}{R^2} \right) \chi_i(R) - \sum_j U_{ij}(R)\chi_j(R)$$
$$- \sum_j \int_k dk\, U_{ij}(R, k)\chi_j(R, k) = 0, \qquad (10)$$

where the matrix elements $U_{ij}(R)$ are effective potentials of the problem [2], ε is the colliding energy in the body frame coordinates, J is the total orbital momentum and M is the reduced mass of the system.

Table I. Convergence of the charge transfer cross section σ_{dt} (10^{-20}cm^2) for S-wave $d\mu + t \to t\mu + d$ scattering and different incident energies (in brackets the number of channels is shown).

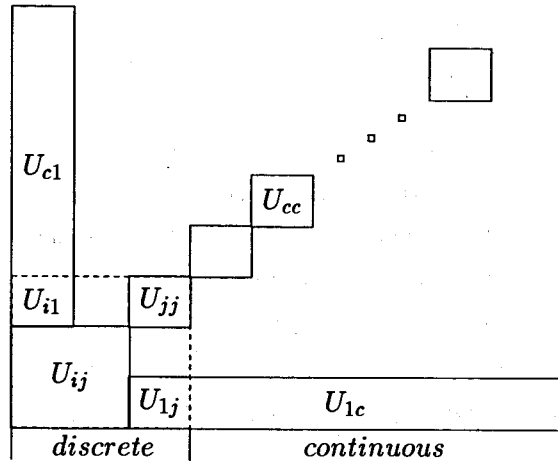| number of shells		0.01eV	0.04eV	0.1eV
discrete spectrum	continuous spectrum			
1 [2]	–	1.209	0.596	0.369
2 [6]	–	3.215	1.583	0.980
3 [12]	–	3.440	1.694	1.047
4 [20]	–	3.498	1.722	1.065
4 [20]	1 [+88]	3.998	1.965	1.217
4 [20]	2 [+176]	4.129	2.029	1.257
4 [20]	3 [+264]	4.375	2.148	1.329
4 [20]	4 [+352]	4.381	2.154	1.333
4 [20]	5 [+440]	4.376	2.150	1.329

Fig.1 The scheme of effective potentials of the multi-channel adiabatic approach taken into account in calculations.

To be sure that our multichannel model is invariant under space rotations we have to use closed (with respect to the three-dimensional rotations) shells of states of continuous and discrete spectra. In calculations we have taken into account (see the Figure) the interaction of the states of the first three shells of the discrete spectrum which can be described by the quantum numbers of isolated atom: $\{1s\}, \{2s, 2p\}, \{3s, 3p, 3d\}$. And the interaction of the first shell of discrete spectrum with the fourth shell of discrete spectrum (with principal quantum number $n = 4$) and the shells of continuous spectrum: $\{l = 0, 1, m = 0\}, \{l = 2, 3, m = 0\}, \dots$ About description of quantum numbers of continuous spectrum we refer to Ref. 18. The wave number parameter of continuous spectrum k has been discretized to eliminate the integral part of Eq. (10): $k_\alpha = 0.1\,(0.1)\,3.0\,(0.5)\,10$ (44 points for every state).

The cross sections of charge transfer $\sigma_{dt}(\varepsilon)$ $(J = 0)$ while the number of states in Eq. (10) increases are shown in the Table. It is clearly seen that inclusion of continuous spectrum with a big number of states into consideration has a great effect on the accuracy of the calculation. From the other side, the computational time of the calculations taking into account continuous spectrum didn't increase significantly and grew linearly with the number of continuous spectrum shells.

This method was applied for making up the Atlas of the elastic and inelastic cross sections for mesic atomic processes [14] and for calculating muon transfer rates in hydrogen isotope mixture [19].

Acknowledgements

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Коробов В.И.   E11-92-357
Численное решение многоканальной задачи рассеяния

Предлагается вычислительный алгоритм решения многоканальной задачи упругого и неупругого рассеяния. Исходной является система радиальных уравнений Шредингера, удовлетворяющая линейному граничному условию, определенному в некоторой точке $R = R_m$ асимптотической области. Подобные граничные условия могут быть получены с помощью асимптотических решений. Для систем с большим числом открытых и закрытых каналов прямое решение исходной задачи (использующее, скажем, метод фазовых функций или логарифмической производной) представляет большую вычислительную трудность. Обсуждается, как полученное линейное уравнение может быть разбито на оператор нулевого порядка и оператор возмущения. Показано, что конечно-разностный метод переменного порядка Лентини — Перейра как нельзя лучше подходит для решения подобной задачи. Разработанная процедура применяется в рамках адиабатического подхода к задаче неупругого рассеяния $d\mu + t \rightarrow t\mu + d$.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

Korobov V.I.   E11-92-357
Numerical Solution of the Multichannel Scattering Problem

A numerical algorithm for solving the multichannel elastic and inelastic scattering problem is proposed. The starting point is the system of radial Schrödinger equations with linear boundary conditions imposed at some point $R = R_m$ placed somewhere in asymptotic region. These boundary conditions are constructed with the use of asymptotic solutions. For the systems with a great number of open and closed channels the solving of the original equation directly (with the use, for example, of phase or log-derivative methods) is a cumbersome task. We discuss how the obtained linear equation can be splitted into a zero-order operator and its perturbative part. It is shown that Lentini — Pereyra variable order finite-difference method appears to be very suitable for solving that kind of problems. The derived procedure is applied to $d\mu + t \rightarrow t\mu + d$ inelastic scattering in the framework of the adiabatic multichannel approach.

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