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Continuous Analog of Newton Method in the Multichannel Scattering Problem

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A method is presented for a numerical solution of the multichannel scattering problem with a large number of closed channels (~ 300). The scattering problem is reduced to a nonlinear functional equation which is subsequently solved using the continuous analog of Newton method. The efficiency of the approach is demonstrated by solving the one-channel scattering problem for which an analytic solution exists and a multichannel problem arising in the consideration of inelastic collisions in a three-body system. In particular, the scattering cross sections of tritium mesic atoms in the singlet and triplet states of the hyperfine structure including the spin–flip cross sections are calculated.

1. INTRODUCTION

Recently [1], a method has been proposed for solving the Sturm–Liouville singular problem for a large system of differential equations with the use of a continuous analog of Newton method [2–4]. Problems of this type arise in many fields of physics, in particular, in calculating the binding energies of a three-body system with Coulomb interaction [5].[1] In the description collisions of composite particles one encounters the problems of finding the states of the continuous spectrum of the Sturm–Liouville operator. Often, in such calculations presence of many coupled reaction channels and influence of the closed channels on the reaction cross section have to be taken into account [6, 7]. This leads to the necessity of solving a large number of equations and, thereby, to a significant complication of the computational procedure [8, 9].

In this paper an algorithm is developed for a numerical solution of the multichannel-scattering problem with a large number of closed channels (~ 300). The algorithm is based on the known idea [10] developed earlier for the bound states [1], according to which the initial problem is represented by a nonlinear functional equation which is subsequently solved by a continuous analog of Newton method.

[1] An example is calculation of the energy levels of a mesic molecule, the system composed of two nuclei and μ-meson [5].

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One possible way to extend this approach to the scattering states was proposed in [11], where the scattering problem was formulated as an eigenvalue problem and calculations for the two-channel case were presented.[2] In [13] a solution for a large number of closed channels (~ 300) and one open channel has been given as a solution of the Sturm–Liouville problem with zero boundary conditions. In this paper the ideas of [11, 13] are applied to the solution of the multichannel problem with an arbitrary number of open channels.

The method of finding the states of the continuous spectrum of the Schrödinger equation is expounded in Section 2 and illustrated in Section 3 on the example of the one-channel problem for which an analytic solution exists. A generalization of the method to the multichannel case is presented in Section 4. Its applicability to inelastic collisions involving three charged particles which exemplifies the basic characteristics of the multichannel scattering is demonstrated in Section 5 by calculating the inelastic cross sections for tritium mesic atoms on nuclei. These cross sections are needed for a quantitative description of the kinetics of the muon-catalyzed fusion chain [14].

2. Solution of the One-Channel Scattering Problem

For finite potentials $U(R)$ for which the eigenvalue problem is correctly posed ($\lim_{R\to 0,\infty} U(R)\, R^2 = 0$) the Schrödinger equation

$$\left[-\frac{1}{2M}\frac{d^2}{dR^2} - \frac{J(J+1)}{2MR^2} + U(R)\right] y(R) = \varepsilon y(R) \tag{1}$$

may contain a discrete (possibly infinite) set of bound states ($\varepsilon < 0$) for which the wave functions behave as

$$y_{\varepsilon J}(R) \xrightarrow[R\to 0]{} R^{J+1}, \qquad y_{\varepsilon J}(R) \xrightarrow[R\to\infty]{} e^{-\sqrt{-2M\varepsilon}\cdot R} \tag{1.a}$$

and a set of states of the continuous spectrum ($\varepsilon > 0$) with the asymptotic behavior

$$y_{\varepsilon J}(R) \xrightarrow[R\to 0]{} R^{J+1}, \qquad y_{\varepsilon J}(R) \xrightarrow[R\to\infty]{} \sin\left(kR - \frac{\pi}{2}J + \delta_J(\varepsilon)\right) \tag{1.b}$$

where $k^2 = 2M\varepsilon$, J is the angular momentum, and $\delta_J(\varepsilon)$, the scattering phase for potential $U(R)$. For bound states the problem of finding a solution $\{y_*, \varepsilon_*\}$ of Eq. (1), satisfying conditions (1.a) can be represented by the nonlinear functional equation for $z = \{y, \varepsilon\} \in C^2 \times R$

[2] The method for solving the Schrödinger radial equation for the continuous spectrum as a bound-state problem has been known for a long time (see, e.g., [12]).

$$\begin{aligned}\varphi(z)=\varphi_1=&\left[\frac{d^2}{dR^2}+2M\varepsilon+\frac{J(J+1)}{R^2}-U(R)\right]y(R)=0\\ =\varphi_2=&\quad y|_{R=0}\quad=0\\ =\varphi_3=&\left[f_1\frac{d}{dR}y+f_2\,y\right]\Big|_{R=R_m}=0\\ =\varphi_4=&\quad (y,\,y)-1\quad=0.\end{aligned}\tag{2}$$

The first of Eqs. (2) is equivalent to Eq. (1). The second and the third ones reflect the boundary condition (1.a), the latter being given by the asymptotic behavior of $y(R)$ (e.g., $f_1=1$, $f_2=\sqrt{-2M\varepsilon}$). The last equation is the normalization condition $(y,\,y)=\int_0^{R_m} y^2(R)\,dR=1$. Having stated the problem in the form of Eq. (2) it is convenient to apply the continuous analog of Newton method. (We refer here to the arguments of [15]). The root of Eq. (2), $z_*=\{y_*\varepsilon_*\}$, can be found by solving the functional evolution equation

$$\varphi'_z(z(t))\,z'(t)=-\varphi(z(t))\tag{3}$$

where a subsidiary continuous parameter $0\leqslant t<\infty$ is introduced [3] and the initial condition reads $z(0)=z_0$. Above, φ'_z is the Fresche derivative [16] of operator φ, $z_0=\{y_0,\,\varepsilon_0\}$ is the initial approximation to the solution we are looking for, and $z'(t)=\{dy/dt,\,d\varepsilon/dt\}=\{V,\,\mu\}$. It has been shown [2, 3] that if operator φ is smooth in the vicinity of the isolated solution then

$$\lim_{t\to\infty}\|z_*-z(t)\|=0.\tag{4}$$

The evolution equation (3) has been used to construct different iteration schemes for finding solutions of Eq. (2) [1, 10, 11, 17] starting from initial approximation z_0.

Let us now turn to the scattering states. Conventionally, the solution of the scattering problem consists in finding the scattering phase $\delta(k)$ at a given energy $\varepsilon=\varepsilon_*$ $(k=k_*)$. Below, we develop an approach analogous to the one presented above for the bound states. As before, let us write a nonlinear functional equation $\varphi(z)=0$ with $z=\{y,\,\varepsilon,\,\delta\}$, the root of which, $z_*=\{y_*,\,\varepsilon_*,\,\delta_*\}$ coincides with the solution of the initial problem at $\varepsilon=\varepsilon_*=k_*^2/2M$. The boundary condition $\varphi_3(z)=0$ reflects now the asymptotic behavior (1.b). Then, in analogy to Eq. (2)[3]:

$$\varphi_3(z)=\left[\sin(kR+\delta)\frac{d}{dR}y-k\cos(kR+\delta)\,y\right]_{R=R_m}=0.\tag{5}$$

[3] The boundary condition (5) contains no singularities for any $\varepsilon>0$ and, therefore, it is convenient for numerical calculation. For simplicity we restrict outselves, here, to $J=0$. For $J>0$ more accurate calculations require the replacements

$$\begin{Bmatrix}\sin(kR-(\pi/2)J)\\ \cos(kR-(\pi/2)J)\end{Bmatrix}\to\begin{Bmatrix}j_J(kR)\\ n_J(kR)\end{Bmatrix}.$$

Since the dimensionality of the space of the independent variables has now increased $z=\{y, \varepsilon\} \to \{y, \varepsilon, \delta\} \in C^2 \times R \times R$, Eq. (2) has to be supplemented with one more independent condition: $\varphi_5(z)=0$ possessing a common root with the other equations. The modified operator φ should also satisfy the smoothness requirement leading to Eq. (4). Let us take $\varphi_5(z)$ in the form[4] of a scalar product:

$$\varphi_5(z)=\left(y, \frac{d^2}{dR^2} y+(k_*^2-U(R))\, y\right)=0. \tag{6}$$

Then, the root of the nonlinear functional equation

$$\begin{aligned}
\varphi(z)=\varphi_1= &\quad \frac{d^2}{dR^2} y+(k^2-U)y &&=0\\
=\varphi_2= &\quad y|_{R=0} &&=0\\
=\varphi_3= &\quad \left[f_1 \frac{d}{dR} y+f_2 y\right]_{R=R_m} &&=0\\
=\varphi_4= &\quad (y, y)-1 &&=0\\
=\phi_5= &\quad \left(y, \frac{d^2}{dR^2} y+(k_*^2-U) y\right) &&=0
\end{aligned} \tag{7}$$

is a solution to the scattering problem (1), (1.b) at the given $k^2=k_*^2=2M\varepsilon_*$.

It should be noticed that the choice (6) of the form of condition $\varphi_5(z)=0$ is not unique. The same concerns the normalization condition of the wave function $\varphi_4(z)=0$. The influence of changing the form of φ_5 on convergence of the iteration process of finding the solution of the scattering problem will be discussed in the next section.

Let us construct the iteration scheme for solving Eq. (7) following the precedure used above for the bound states (2) [1]. The evolution equation (3) (with φ defined by (7)) will be solved using the Euler method on difference net with the step of integration $\tau_n=t_{n+1}-t_n=1$:

$$\varphi'_{z_n}(z_n)=-\varphi(z_n) \tag{8}$$

$$z_{n+1}=z_n+\tau_n \Delta z_n=\{y_n+\tau_n V_n, k_n^2+\tau_n \mu_1^n, \delta_n+\tau_n \mu_2^n\}. \tag{9}$$

Let us represent the iteration correction $V_n(R)$ to $y_n(R)$ as

$$V_n(R)=-y_n(R)+\mu_1^n v_n(R)+\mu_2^n \tilde{v}_n(R). \tag{10}$$

[4] In [18] a similar functional with the standard normalization conditions was used to obtain a bilateral convergence of the Newton iteration process for finding the discrete states of the Schrödinger equation.

Then, the boundary-value problems for $v_n(R)$ and $\tilde{v}_n(R)$ respectively read

$$\begin{gathered}\frac{d^2}{dR^2} v_n + (k_n^2 - U)v_n = -y_n \\ v_n|_{R=0} = 0 \\ \left[f_1 \frac{d}{dR} n + f_2 v_n \right]_{R=R_m} = -\left[\frac{\partial f_1}{\partial \lambda_n} \frac{d}{dR} y_n + \frac{\partial f_2}{\partial \lambda_n} y_n \right]_{R=R_m} \\ \lambda_n \equiv k_n^2\end{gathered} \tag{11.a}$$

$$\begin{gathered}\frac{d^2}{dR^2} \tilde{v}_n + (k_n^2 - U)\tilde{v}_n = 0 \\ \tilde{v}_n|_{R=0} = 0 \\ \left[d_1 \frac{d}{dR} \tilde{v}_n + f_2 \tilde{v}_n \right]_{R=R_m} = -\left[\frac{\partial f_1}{\partial \delta_n} \cdot \frac{d}{dR} y_n + \frac{\partial f_2}{\partial \delta_n} y_n \right]_{R= =R_m}.\end{gathered} \tag{11.b}$$

Upon substituting V_n given by (10) into the last two equations of (8)

$$\frac{\partial \varphi_4}{\partial y_n} V_n = -\varphi_4, \qquad \frac{\partial \varphi_5}{\partial y_n} V_n = -\varphi_5$$

one obtains a system of algebraic equations for iteration corrections μ_1^n and μ_2^n:

$$\begin{aligned} a_{11}^n \mu_1^n + a_{12}^n \mu_2^n &= b_1^n \\ a_{21}^n \mu_1^n + a_{22}^n \mu_2^n &= b_2^n \end{aligned} \tag{12}$$

where

$$\begin{gathered}a_{11}^n = (y_n, v_n), \qquad a_{12}^n = (y_n, \tilde{v}_n), \\ a_{21}^n = (y_n, v_n'' + (k_*^2 - U)v_n) + (v_n, y_n'' + (k_*^2 - U)y_n) \\ a_{22}^n = (y_n, \tilde{v}_n'' + (k_*^2 - U)\tilde{v}_n) + (\tilde{v}_n, y_n'' + (k_*^2 - U)y_n), \\ b_1^n = \tfrac{1}{2}(1 + (y_n, y_n)), \qquad b_2^n = (y_n, y_n'' + (k_*^2 - U)y_n).\end{gathered}$$

Formulae (9)–(12) represent the classical Newton–Kantorovich [3, 16] solution of Eq. (7).

The above approach is not unique and other ways of constructing the iteration scheme for the scattering problem (7) on basis of the evolution equation (3) can be devised. For example, the step of integration, τ_n, can be changed in the course of iteration, which may essentially extend the range of convergence of the procedure. Also, replacing $\varphi'_{z_n}(z_n)$ in (8) by $\varphi'_{z_0}(z_0)$ may significantly decrease the time of computation [1].

3. Specific Features of the Calculational Scheme

The approach described in the previous section will be illustrated by solving the Schrödinger equation for the Morse potential

$$U(R) = D \cdot [e^{-2\alpha(R-R_0)} - 2 \cdot e^{-\alpha(R-R_0)}] \tag{13}$$

for which the analytic solution reads

$$y_k(R) = \frac{e^{-\xi/2}}{2i} [e^{i\omega} \xi^{-is} F(-\delta + \tfrac{1}{2} - is, 1 - 2is, \xi) - e^{-i\omega} \cdot \xi^{is} \cdot F(-\delta + \tfrac{1}{2} + is, 1 + 2is, \xi)] \underset{R \to \infty}{\approx} \sin(kR - kR_0 - (k/\alpha) \ln 2\alpha + \omega) \tag{13.a}$$

$$\omega = \arg \Gamma(1 + 2is) + \arg \Gamma(-\delta + \tfrac{1}{2} - is), \qquad s = k/\alpha, \ \delta = \sqrt{2MD}/\alpha.$$

Table I and Fig. 1 illustrate convergence of the iteration procedure from various initial approximations for the following values of the parameters: $D = 0.104$, $\alpha = 0.67$, $R_0 = 2.09$, $M = 8.876$. Convergence was controlled by the magnitudes of $\Delta_n = \|\varphi(z_n)\|$, μ_1^n, and μ_2^n, and iteration ended when $\max\{\mu_1^n, \mu_2^n, \Delta_n\} \lesssim 10^{-6}$. The boundary-value problems (11) were solved using the finite-difference approximation of a order of accuracy of $\sim O(h^2)$ (h is a step of integrations) and applying the alternating implicit algorithm. The accuracy of calculations for the chosen difference net (see Table I) is about $10^3 - 10^{-2}$. If necessary, accuracy can be improved by extrapolating the obtained values to $h \to 0$. From the calculations performed to several difference nets it follows that the errors of the numerical solutions decrease quadratically with decreasing step of integration. As exemplified in the Table for $k = 0.08$ the method is rather stable to the choice of the initial approximation.

In the considered approach the convergence of the iteration pocedure can be improved either by choosing a better initial approximation to z_0 or by appropriately changing the form of φ_5. To illustrate this point Fig. 1 show several trajectories of z projected onto the $\{k, \delta\}$-plane. For instance, if $\varphi_5 = k^2 - k_*^2 = 0$, the problem reduces to a standard formulation in which y_* and δ_* are found for a given value of $k = k_*$. Thus, by changing the condition $\varphi_5(z) = 0$ one changes the properties of operator φ defined by Eq. (2) where, now $\varphi_1(z) = (d^2/dR^2)\, y + (k_*^2 - U)\, y$, $f_1 = \sin(k_* R_m + \delta)$, and $f_2 = -k_* \cos(k_* R_m + \delta)$. However, construction of the iteration procedure in this case is a separate problem which is outside the scope of the present consideration.

On the other hand if $\varphi_5 = \delta - \delta_* = 0$ the points Z_n move along the straight line trajectory: $\delta = \delta_*$. The scattering problem (7) is then reduced to Eq. (2), where $f_1 = \sin(kR_m + \delta_*)$, $f_2 = -k \cos(kR_m + \delta_*)$ and the solution can be found as in Section 2 using the continuous analog of Newton method. This choice for φ_5 corresponds to stating the scattering problem as an eigenvalue problem in which k^2 is found for a given $\delta = \delta_*$. Such an approach has been proposed and implemented

TABLE I

Convergence of the Computational Scheme (9)–(12)

k_*	n	Δ_n	μ_1^n	μ_2^n	k_n	δ_n	Δ_n	μ_1^n	μ_2^n	k_n	δ_n
0.08	0	$0.84 \cdot 10^{-2}$	$-0.824 \cdot 10^{-1}$	$0.255 \cdot 10^{2}$	0.1500	0.0500	$0.85 \cdot 10^{-2}$	$-0.824 \cdot 10^{-1}$	$0.218 \cdot 10^{2}$	0.1500	−0.0500
	11	$0.39 \cdot 10^{-12}$	$-0.29 \cdot 10^{-11}$	$0.65 \cdot 10^{-11}$	0.0800	−0.5202	$0.27 \cdot 10^{-12}$	$-0.29 \cdot 10^{-11}$	$0.54 \cdot 10^{-8}$	0.0800	−0.5202
0.14	0	$0.21 \cdot 10^{-2}$	$-0.710 \cdot 10^{-2}$	$0.680 \cdot 10^{1}$	0.1435	0.0					
	10	$0.50 \cdot 10^{-12}$	$-0.16 \cdot 10^{-9}$	$-0.58 \cdot 10^{-7}$	0.1400	−0.8897					
0.20	0	$0.32 \cdot 10^{-2}$	$-0.140 \cdot 10^{-1}$	$0.911 \cdot 10^{1}$	0.2025	0.0					
	9	$0.39 \cdot 10^{-12}$	$0.24 \cdot 10^{-11}$	$-0.52 \cdot 10^{-9}$	0.2000	−1.233					

Note. The initial approximation $y_0(R)$ to the sought wave function $y(R)$ for $k_* = 0.08$ was given by the formula $y_0(R) = 0.0035 \sin(\pi R/3.6)$, $R \leqslant 7.2$; $y_0(R) = 0.05 \sin(\pi(R - 7.2/50)$, $R > 7.2$. For $k_* = 0.14$ and $k_* = 0.2$ as the initial approximations we took $y_{11}(R)$ and $y_{10}(R)$ calculated for $k_* = 0.08$ and $k_* = 0.14$, respectively. Calculations were carried out at the mesh points with 280 nodes with step 0.1 (0.1) 20 (1) 100.

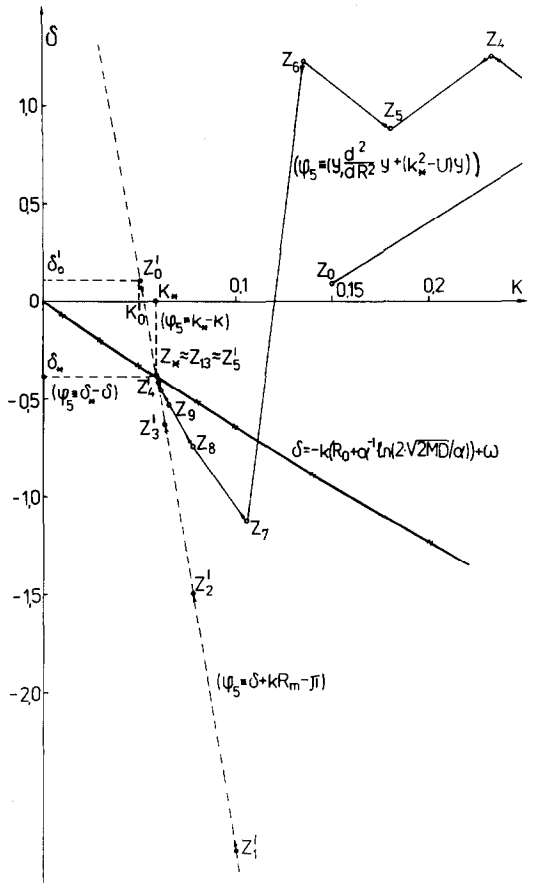

FIG. 1. Illustration for convergence of the iteration procedure of finding the solution z_* of the scattering problem (7) for different choices of φ_5.

for the two-channel case in [11], where its range of convergence has been studied and possible generalizations to the multichannel problem have been pointed out.

Yet another method for solving the scattering problem as an eigenvalue problem has been considered in [13], where the potential: $U(R)$, $R \in [0, \infty)$ has been replaced by a potential with a infinite wall at $R = R_m (y(R_m) = 0)$ giving rise to a discrete, R_m-dependent spectrum of eigenvalues k_α^2, $\alpha = 1, 2, \ldots$. The respective eigenfunctions $y_\alpha(R)$ contain information about the scattering phases δ of Eqs. (1) and (1.b). The corresponding iteration scheme can be obtained if

$$\varphi_5(z) = \delta + kR_m - \pi\alpha = 0. \tag{14}$$

Indeed, in this case the boundary condition (5) reads $\varphi_3(z) = y(R_m) = 0$, and problem (7) becomes the Sturm–Liouville problem (2), with $f_1 = 0$ and $f_2 = 1$. It is

therefore sufficient to calculate the scattering phase only once, after the procedure of solving Eq. (2) has converged ($k_n^2 \to_{n\to\infty} k_\alpha^2$) using the formula $\delta_\alpha = -k_\alpha R_m + \pi\alpha$. According to (14), in the course of iterations the points $Z'n$ can move only along the straight line, $\delta_n = -k_n R_m + \alpha\pi$ as illustrated in Fig. 1. The slope of this line, R_m which is the cut-off in integration of the Schrödinger equation determines the required value of k.[5] This approach has been applied in [13] to the multichannel scattering problem with one open and many (~ 300) closed channels.

The discussed examples indicate several possibilities of improving convergence of the proposed method and increasing its stability to the choice of the initial approximation by changing the form of φ_5. Alternatively, the properties of the operator φ can be improved by an appropriate choice of the normalization condition $\varphi_4(z) = 0$ (see, e.g., [11, 18]).

4. Solution of the Multichannel Scattering Problem

Let us now consider the multichannel problem in the approach developed in Section 2. It will be shown below that with the choice of condition $\varphi_5 = 0$ given by Eq. (6) this approach can be easily extended to the multichannel case.

Consider an N-channel problem with s-open channels stated as follows: At a given collision energy $\varepsilon > 0$ one should find s nontrivial solutions of the system of N differential equations

$$\varphi_1(\varepsilon, y_i) = \left[\frac{d^2}{dR^2} y_i + 2M\left(\varepsilon - E_i - \frac{J(J+1)}{2MR^2}\right) y_i\right] - \sum_j^N U_{ij}\, y_j = 0 \qquad (15.a)$$

The solutions should be regular at $R = 0$,

$$\varphi_2(\varepsilon, y_i) = y_i|_{R=0} = 0 \qquad (15.b)$$

and have the asymptotic behavior at $R \to \infty$

$$\begin{aligned} \hat{y}(R) &\sim \hat{j}_J(kR) - \hat{n}_J(kR)T \qquad \text{in open channels } (i \leqslant s) \\ &\sim \exp\{-|k_i|\, R\} \qquad \text{in closed channels } (i > s). \end{aligned} \qquad (16)$$

Additionally the scattering S-matrix has to be found related to the real T matrix by

$$S = (1 + iT)(1 - iT)^{-1}$$

where $T = \lim_{R\to\infty} T(\varepsilon, R)$.[6]

[5] Naturally, $R_m \in [R_{as}, \infty)$, where the asymptotic condition $y(R_m) =_{R \geqslant R_{as}} \sin(kR + \delta)$ is valid.

[6] This formulation of the problem has been presented in [11].

In the N-channel problem (15) and (16) the complete set of solutions

$$\hat{y} = \{ y_i^{(v)} \} = \begin{pmatrix} y_1^{(1)} \cdots y_1^{(s)} \\ \vdots \quad \vdots \\ y_N^{(1)} \cdots y_N^{(s)} \end{pmatrix}$$

is an $N \times s$ matrix, in which the number of component of a vector-column (the number of the reaction channel) runs over $i = 1, 2, ..., N$, and the solution index over $v = 1, 2, ..., s$. The matrix $T = \{t_{iv}\}$ is real symmetric, whereas $S = \{S_{iv}^{(0)} + iS_{iv}^{(1)}\}$ is a complex $s \times s$ matrix. The notation used in Eqs. (15) is: M—the reduced mass, k_i—the corresponding momentum in the ith channel, $k_i^2 = 2M(\varepsilon - E_i) > 0$ in open channels ($i \leqslant s$) and $k_i^2 < 0$ in the closed ones ($i > s$), $U_{ij}(R)$—the potentials with the asymptotic behavior[7]

$$R^2 U_{ij}(R) \to \text{const.} \qquad \text{for} \quad R \to 0$$

$$U_{ij}(R) \to 0 \qquad \text{for} \quad R \to \infty.$$

Energy $\varepsilon = 0$ corresponds, here, to the threshold of the lower channel E_1. The diagonal matrices $\hat{j}_J$ and $\hat{n}_J$ are expressed in terms of the Riccati–Bessel spherical functions

$$\hat{j}_J(k_i R) = \{ j_J(k_i R)\, \delta_{iv} \}, \quad \hat{n}_J(k_i R) = \{ n_J(k_i R)\, \delta_{iv} \}.$$

The asymptotic formulae for these functions give the asymptotic behavior of the solutions of system (15.a) in open channels ($i \leqslant s$) which is

$$\hat{y} \xrightarrow[R \to \infty]{} \hat{y}_{as} = \left\{ A_i^{(v)} \sin\left(k_i R - \frac{\pi}{2} J + \delta_i^{(v)} \right) \right\} \tag{17}$$

where

$$A_i^{(v)} = \delta_{iv} + (1 - \delta_{iv}) \sqrt{k_v / k_i}\, t_{iv}(\varepsilon) \cos \delta^{(v)}(\varepsilon)$$

$$\delta_i^{(v)} = \delta^{(v)}(\varepsilon)\, \delta_{iv} + (\pi/2)(1 - \delta_{iv}), \qquad \delta^{(v)}(\varepsilon) = \operatorname{arctg} t_{vv}(\varepsilon),$$

and δ_{iv} is the Kronecker symbol.

Let us represent the multichannel scattering problem (15), (16) by s functional equations $\varphi^{(v)}(z) = 0$ analogous to Eq. (7). From the asymptotic equality for $R = R_m \to \infty$

$$\frac{d}{dR}\, y_i^{(v)} / y_i^{(v)} \big|_{R = R_m} = \frac{d}{dR}\, y_{as_i}^{(v)} / y_{as_i}^{(v)} \big|_{R = R_m}$$

[7] In the next section we consider an example differing from the standard formulation ($U_{ij}(R) \to_{R \to \infty}$ const.), admitting, nevertheless, a correct formulation of the scattering problem [13, 20]. However, in this case, taking into account strong channel coupling in the asymptotic region complicates the construction of the computational procedure.

where functions $\{y_{as_i}^{(v)}\}$ are defined by (17) one obtains the boundary condition for the scattering problem in the following form

$$\varphi_3^{(v)}(\varepsilon, \delta^{(v)}) = \left[\hat{f}_1^{(v)} \frac{d}{dR}\mathbf{y}^{(v)} + \hat{f}_2^{(v)}\mathbf{y}^{(v)}\right]_{R=R_m} \tag{15.c}$$

where a matrix notation is introduced

$$\begin{aligned}
\hat{f}_1^{(v)}(\varepsilon, \delta^{(v)}) &= \{f_1^{(v)}\}_{ij} = \{\theta(i-s)[\delta_{iv}\sin(k_i R - (\pi/2)J + \delta^{(i)}) \\
&\quad + (1-\delta_{ij})\cos(k_i R - (\pi/2)J)] + (1-\theta(i-s))\}\,\delta_{ij} \\
\hat{f}_2^{(v)}(\varepsilon, \delta^{(v)}) &= \{f_2^{(v)}\}_{ij} = \{\theta(i-s)[-\delta_{iv}\cos(k_i R - (\pi/2)J + \delta^{(i)}) \\
&\quad + (1-\delta_{iv})\cdot\sin(k_i R - (\pi/2)J)]k_i + (1-\theta(i-s))|k_i|\}\,\delta_{ij}
\end{aligned} \tag{18}$$

and where

$$\begin{aligned}
\theta(i-s) &= 1, \qquad i \leqslant s \\
&= 0, \qquad i > s.
\end{aligned}$$

In this formulation the boundary condition $\varphi_3^{(v)}(\varepsilon, \delta^{(v)}) = 0$ for the vth vector-column of solutions of Eq. (15)

$$\mathbf{y}^{(v)} = \begin{pmatrix} y_1^{(v)} \\ \vdots \\ y_N^{(v)} \end{pmatrix}$$

contains in an explicit form only one parameter $\delta^{(v)}(\varepsilon) = \operatorname{arctg} t_{vv}(\varepsilon)$ for the sought matrix $T(\varepsilon)$. This allows one to formulate the multichannel scattering problem in terms of s functional equations $\varphi^{(v)}(z) = 0$ analogous to (7) for unknowns $Z = \{\mathbf{y}^{(v)}, \varepsilon, \delta^{(v)}\}$. Indeed, if one defines in analogy to Section 2:

$$\varphi_4^{(v)}(\mathbf{y}) = (\mathbf{y}, \mathbf{y}) - 1 = 0 \tag{15.d}$$

$$\varphi_5^{(v)}(\varepsilon, \mathbf{y}) = \left(\mathbf{y}, \frac{d^2}{dR^2}\mathbf{y} + \left(k_*^2 - \frac{J(J+1)}{R^2} - \hat{U}\right)\mathbf{y}\right) = 0 \tag{15.e}$$

one obtains s nonlinear functional equations $\varphi^{(v)}(z) = 0$, $v = 1, 2, \ldots s$, in which the components $\varphi_l^{(v)}$ $(l = 1, 2, \ldots, 5)$ are given by Eqs. (15). Here $\hat{U} = \{U_{ij}(R)\}$ is the matrix of potentials in (15.a), $k_*^2 = \{2M\cdot(\varepsilon_* - E_i)\,\delta_{ij}\}$, is a fixed diagonal matrix (the same for all v), and the scalar product is defined by $(\mathbf{y}, \mathbf{y}) = \sum_{i=1}^{N}\int_0^{R_m}[y_i^{(v)}(R)]^2\,dR$. The equations can be considered separately because they are not coupled except for the requirement that parameter ε_* (common energy in all channels) is the same for all v.

It can be easily seen, that by determining the roots of these equations, $z_* = \{\mathbf{y}_*^{(v)}, \varepsilon_*, \delta_*^{(v)}\}$, solves, at the same time, the multichannel scattering problem for a

given collision energy $\varepsilon = \varepsilon_*$, fixed by conditions (15.e). I.e., one obtains the corresponding eigenfunctions $\hat{y}_*(\varepsilon_*, R)$ and scattering parameters $\delta_*^{(v)}(\varepsilon_*)$.

Then, using the asymptotic formulae (17) the T-matrix at $\varepsilon = \varepsilon_*$ is given by

$$T = \{t_{iv}(\varepsilon)\}$$
$$t_{vv} = \operatorname{tg} \delta^{(v)}, \qquad t_{iv} = \sqrt{\frac{k_i}{k_v}} \frac{y_i^{(v)}(R_m) \sin(k_v R_m + \delta^{(v)} - (\pi/2)J)}{y_v^{(v)}(R_m) \cos \delta^{(v)} \cos(k_i R_m - (\pi/2)J)}, \qquad i \neq v \tag{19}$$

where $k_i = \sqrt{2M \cdot |\varepsilon_* - E_i|}$.

The solution of equations $\varphi^{(v)}(z) = 0$, follows immediately from the scheme presented in Section 2; formulae (9)–(12) should be used with the following replacements:

$$U \to \hat{U},\ f_1 \to \hat{f}_1^{(v)},\ f_2 \to \hat{f}_2^{(v)},\ y_n \to \mathbf{y}_n^{(v)}.\ v_n \to \mathbf{v}_n^{(v)},\ \tilde{v}_n \to \tilde{\mathbf{v}}_n^{(v)}$$

where the matrices $\hat{U}$, $\hat{f}_1^{(v)}$, and $\hat{f}_2^{(v)}$ have been determined above and $\mathbf{y}_n^{(v)}$, $\mathbf{v}_n^{(v)}$, and $\tilde{\mathbf{v}}_n^{(v)}$ are now N-dimensional vector functions.

Having calculated the S-matrix $S = (1 + iT)(1 - iT)^{-1}$ one can determine the physical characteristics of the considered collision process:

$$\sigma_{iv}(k_i) = (4\pi/k_i^2)(2J + 1)(1 - |S_{iv}|^2). \tag{20}$$

Here, $\sigma_{ii}(k_i)$ is the elastic cross section in the ith channel, $k_i = \sqrt{2M \cdot |\varepsilon - E_i|}$ and $\varepsilon - E_i$ are the corresponding momentum and collision energy respectively and $\sigma_{iv}(k_i)$ for $i \neq v$ are the cross sections for transitions from the ith to the vth channel.

5. Numerical Example

Let us demonstrate the performance of the proposed method using as example the problem of slow collisions in a three-body system. Such collisions reflect the basic characteristics of the multichannel scattering [21]. This problem arises, for instance, in the description of various mesoatomic processes [5, 22] occurring in mixtures of hydrogen isotopes. In particular, the kinetic formulae describing the μ-catalysis of nuclear fusion in such mixtures contain as parameters the cross sections for collisions of tritium mesic atoms in various states of the hyperfine structure with tritium nuclei. Both elastic and spin–flip collisions are important. Let us introduce the following notation for the respective cross sections $\sigma_{ij}(\varepsilon)$:

$$\begin{array}{ccc} t\mu(\uparrow\uparrow) + t & \xrightarrow{\sigma_{bb}} & t\mu(\uparrow\uparrow) + t \\ & \searrow^{\sigma_{ab}} \quad \nearrow_{\sigma_{ba}} & \\ t\mu(\uparrow\downarrow) + t & \xrightarrow[\sigma_{aa}]{} & t\mu(\uparrow\downarrow) + t. \end{array} \tag{21}$$

In the adiabatic representation of the three-body problem [5] reactions (21) are described by the system of Eqs. (15.a), with the effective potentials

$$U_{ij}(R) = \begin{pmatrix} U_{iaja}, & U_{iajb} \\ U_{ibja}, & U_{ibjb} \end{pmatrix}$$

defined in [23, 13], and with the wave functions of the relative motion of nuclei $y_{ia}(R)$ and $y_{ib}(R)$, which in the asymptotic region $R \to \infty$ correspond respectively to the subsystems $t\mu(\uparrow\downarrow) + t$ (a) and $t\mu(\uparrow\uparrow) + t$ (b).

The problem is characterized by strong coupling of channels in the limit

$$R \to \infty: U_{ij}(R) \xrightarrow[R \to \infty]{} \begin{pmatrix} \Delta E_{iaja} & 0 \\ 0 & \Delta E_{ibjb} \end{pmatrix}.$$

Its presence does not prevent a correct formulation of the scattering problem [13], it leads, however, to a rather complicated boundary condition at $R = R_m$. Let us consider the region of low collision energies ($\varepsilon < E2a$) where only $t\mu_{1s}(\uparrow\downarrow) \rightleftarrows t\mu_{1s}(\uparrow\uparrow)$ spin–flip transitions are allowed. In this case ($s = 1, 2$) the boundary conditions $\varphi_3^{(v)} = 0$ are given by Eq. (15.b), and matrices of coefficients $\hat{f}_1^{(v)}$ and $\hat{f}_2^{(v)}$ assume the form

$s = 1$

$$\begin{aligned} \{f_1^{(v)}(\varepsilon, \delta^{(v)})\}_{ij} &= F_{ii}^{(v)} \delta_{ij}, && i = 1a, 2a, \ldots, N-1 \text{ and } v = 1a \\ &= \delta_{ij}, && i = 1b, 2b, \ldots, N \\ \{f_2^{(v)}(\varepsilon, \delta^{(v)})\}_{ij} &= -\frac{d}{dR} F_{ii}^{(v)} \delta_{ij}, && i = 1a, 2a, \ldots, N-1 \text{ and } v = 1a \\ &= |k_i| \delta_{ij}, && i = 1b, 2b, \ldots, N \end{aligned} \tag{22}$$

where

$$\begin{aligned} F_{ii}^{(v)} = {} & \theta(i-s)[\delta_{iv} \sin(k_i R - (\pi/2)J + \delta^{(i)}) + (1-\delta_{iv}) \cos(k_i R - (\pi/2)J)] \\ & + (1 - \theta(i-s))[\delta_{iv} \cos(k_i R - (\pi/2)J + \delta^{(i)}) - (1-\delta_{iv}) \sin(k_i R - (\pi/2)J)] \end{aligned}$$

$s = 2$

$$\{f_1^{(v)}(\varepsilon, \delta^{(v)})\}_{ij} = F_{ii}^{(v)} \delta_{ij}; \{f_2^{(v)}(\varepsilon, \delta^{(v)})\}_{ij} = -\frac{d}{dR} F_{ii}^{(v)} \delta_{ij}$$

where $i = 1a, 1b, 2a, \ldots, N$ and $v = 1a, 1b$.

In the derivation of these formulae only the leading terms of the asymptotic expansions of $y_{ia}(R)$ and $y_{ib}(R)$ [20] were retained. However, to increase accuracy, in the actual numerical calculations, terms proportional to $1/R$ have been also included.

Another feature is the necessity of taking into account a large number of closed channels (~ 300) which significantly influence the magnitude of the cross sections (21) [13].

Figure 2 presents the calculated S-wave cross sections (21) and Fig. 3 the corresponding T-matrix elements and demonstrates the dependence on the number of solved equations N of the system (15.a). Number $N=2$ corresponds to inclusion of one shell of the discrete spectrum of the adiabatic basis, $N=20$ to three such shells and $N=N_{\max}=260$ to three shell of discrete and four shells of the continuous spectrum. The structure of the matrix of potentials in Eq. (15.a) used in the calculations is as in [1]. Equation (15) for $N=20$ was solved using the calculational procedure given by Eqs. (9)–(12). As the numerical method is sufficiently stable to the choice of the initial approximation, the latter has been taken in a simple form $y_{i0}=y_0\cdot\delta_{i1}$, where $y_0(R)$ corresponds to the one-channel case (Sect. 3). The solution of (15) at $N=20$ was used as an initial approximation for $N=N_{\max}$. In this case, $\varphi'_{z_n}(z_n)$ in Eq. (8) was replaced by $\varphi'_{z_0}(z_0)$ which, as mentioned in Section 2, led to significant shortening of computation time.

The achieved accuracy of the calculations which is about $\sim 5\%$ is determined by the approximation order of the difference net, by the cut-off value of R (R_m), and by the neglected contributions from the higher states of the adiabatic basic. In the

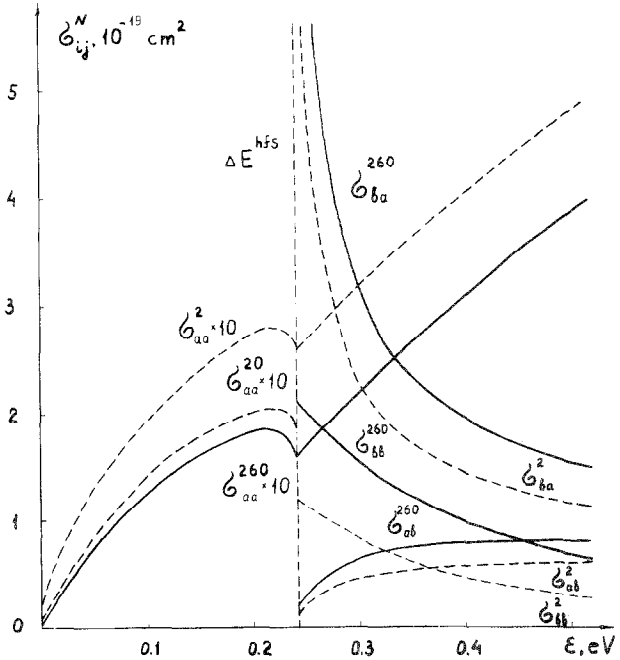

FIG. 2. Calculated cross sections for reactions (21), σ^N_{ij}, $J=0$. The curves correspond to taking into account $N=2$, 20 and 260 equations in the system of equations (15.a). Calculations were carried out on difference net with 330 nodes with step: 0.1 (0.1) 20 (1) 150.

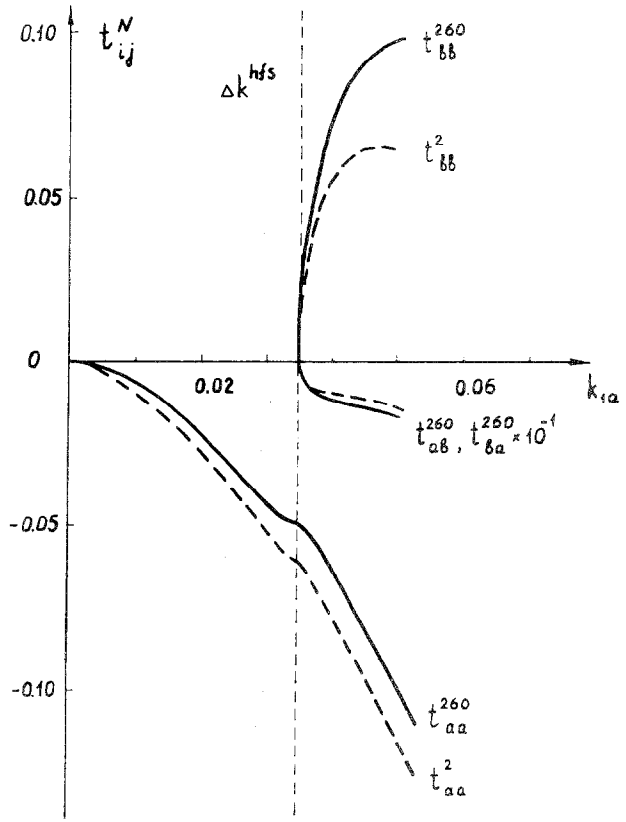

FIG. 3. Calculated elements of T-matrix, t_{ij}^N, N defined as in Fig. 2.

calculations finite difference approximation of the order $\|\varphi_h^{(\nu)} - \varphi^{(\nu)}\| \sim O(h^2)$ was used, however, if necessary the algorithm can be modified to admit accuracy up to $\sim O(h^4)$ [24]. The contribution from the neglected states of the adiabatic basis ($N \to \infty$) can be estimated as in [25]. The results for $N = 2$ coincide within a relative accuracy $10^{-3} - 10^{-4}$, throughout the whole energy region under consideration, with the results obtained using the phase-function method [26] and, for energies below threshold $\varepsilon < \Delta E^{hfs}$, with the results of [13], where $s = 1$ and $N \sim 300$.

As is seen in Fig. 2, the cross sections $\sigma_{ij}(\varepsilon)$ vary significantly with energy at $\varepsilon \leqslant 0.3$ eV. We note also the threshold singularity at $\varepsilon = \Delta E^{\text{hfs}} = 0.241$ eV; that is, clearly pronounced and surviving as $N \to \infty$.

6. CONCLUSION

The method developed above enables one to solve the multichannel scattering problem with a large number of closed channels (~ 300). The scattering problem is

represented in the form of a nonlinear equation which can be solved using the continuous analog of Newton method. The latter has been verified in many applications, and conditions of its local convergence have been theoretically examined [3].

An important peculiarity of the given approach is, in our opinion, that it allows us to solve the multichannel scattering problem with a strong, possibly long-range, coupling of channels without transforming the initial system of equations into a form suitable for numerical integration [6, 8]. It also does not require a particular organization of calculation in the asymptotic region near singularity $R_m \to \infty$ [26], unlike the standard straightforward integration technique. All this is essential for numerical solution of the multichennel scattering problem with a large number of closed channels and long-range potentials.

The method provides a common description of different phenomena (resonances, threshold behaviour, Ramsauer effect, etc.) in a wide range of energy and opens a possibility of examining the influence of the closed channels on their physical characteristics. It can be used most effectively at low collision energies where only a few partial waves contribute. The calculations performed for inelastic collisions involving three charged particles demonstrate the applicability of the method.

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