Elastic scattering in a three-particle system with Coulomb interaction

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(Submitted 17 February 1983)
Zh. Eksp. Teor. Fiz. **85**, 434–446 (August 1983)

A method is developed for calculation of cross sections for elastic scattering in a system of three particles at low collision energies. The method consists of expansion of the wave function of the system in an adiabatic basis and reduction of the ensuing multichannel scattering problem with a large number of closed channels (about 300) to an eigenvalue problem. The possibilities of the method are demonstrated by a calculation of the cross section for elastic scattering of mesic hydrogen by the nuclei of the hydrogen isotopes.

PACS numbers: 34.10. + x, 34.40. + n, 36.10.Gv, 03.65.Nk

1. INTRODUCTION

In various problems of the physics of mesic atoms it is necessary to know the cross sections for elastic-scattering processes in a three-particle system of the type

$$(a\mu)_n + b \to (a\mu)_n + b, \tag{1}$$

where a and b are nuclei of hydrogen isotopes with masses $M_a \geqslant M_b$, μ is a meson with mass m_μ, and n is the set of quantum numbers characterizing the ground state of the $(a\mu)$ atom. Examples of such reactions are the elastic scattering of mesic deuterium atoms by protons

$$(d\mu)_{1s} + p \to (d\mu)_{1s} + p, \tag{2a}$$

or of mesic tritium atoms by deuterons

$$(t\mu)_{1s} + d \to (t\mu)_{1s} + d, \tag{2b}$$

scattering of $p\mu$ and $t\mu$ atoms in the singlet hyperfine-structure state by the nuclei p and t:

$$p\mu(\uparrow\downarrow) + p \to p\mu(\uparrow\downarrow) + p, \tag{2c}$$

$$t\mu(\uparrow\downarrow) + t \to t\mu(\uparrow\downarrow) + t, \tag{2d}$$

and so forth (see the reviews in Refs. 1–3).

At low collision energies ($\varepsilon \lesssim 100$ eV) the best means of calculating the cross sections for such processes is the adiabatic representation in the three-body problem (see the review[4]). Starting with the work of Gershteĭn[5] and Cohen *et al.*,[6] during the last quarter century several such calculations have been made and their results agree to a great extent with experiment (see the reviews[1–3]). However in some cases, for example in calculation of the cross section for reaction (2c), the results of the earlier calculations[5–7] disagree radically with the data of various experiments.[8–11] These discrepancies, as will be shown, are due to the fact that in all previous calculations the approximation of two states of the adiabatic basis was used.

In the present work we have made use of an algorithm for numerical solution of the multichannel scattering problem which arises in the adiabatic representation of the three-body problem. This algorithm permits us to go beyond the framework of the two-state approximation and to calculate as accurately as is required the cross sections for low-energy elastic-scattering processes in a system of three charged particles.

The essence of the method presented for solution of the multichannel scattering problem consists of reduction of the problem to the solution of an eigenvalue problem for a system of ordinary differential equations describing the scattering process in the adiabatic basis. This approach was used by Shore[12] in solution of the one-channel scattering problem and is close to the approach of Ref. 13. Application of the proposed approach became possible after the development of effective algorithms[14] for solution of the Sturm-Liouville problem for systems of differential equations in many dimensions, and also for calculation of the effective potentials of the three-body problem in the adiabatic representation.[15]

The method developed in the present work has been used for calculation of the cross sections for elastic scattering of mesic hydrogen atoms by nuclei of the hydrogen isotopes. Knowledge of these cross sections is necessary for description of the kinetics of muon catalysis of nuclear fusion reactions.[16]

2. FORMULATION OF THE PROBLEM

In the adiabatic representation the wave function of a system of three particles with total angular momentum J and projection m_J, $\Psi^J_{m_J}(\mathbf{r},\mathbf{R})$, where $\mathbf{r}$ is the coordinate of the μ meson and $\mathbf{R} \equiv \{R,\theta,\varphi\}$ is the radius vector joining nuclei a and b, is expanded in the complete set of solutions $\varphi_m(\mathbf{r};R)$ and $\varphi_m(\mathbf{r};k,R)$ of the discrete and continuous spectra of the two-center problem with sets of parabolic quantum numbers

$$jm = [n_1 n_2 mp],\ [n_2 mp]$$

(according to the classification of separated atoms[4,17]):

$$\Psi_{m^J_J}(\mathbf{r},\mathbf{R}) = \sum_{jm} \varphi_{jm}(\mathbf{r},R) R^{-1} \chi^J_{jm}(R) D^J_{mm_J}(\varphi,\theta,0)$$

$$+ \sum_{jm} \int_0^\infty dk \varphi_{jm}(\mathbf{r};k,R) R^{-1} \chi^J_{jm}(k,R) D^J_{mm_J}(\varphi,\theta,0). \tag{3}$$

 0038-5646/83/080254-08$04.00

the initial Schrödinger equation of a system of three charged particles

$$(\hat{H}-E)\Psi(\mathbf{r},\ \mathbf{R})=0 \tag{4}$$

after substitution into it of the expansion (3) and averaging over the coordinates r, θ, and φ reduces to a system of $2N$ ordinary differential equations for the function $\chi_{jlJ}(R) \equiv \chi^{J}_{jm}(R), \chi^{J}_{jm}(k,R)$:

$$\left\{\hat{I}\left(\frac{d^2}{dR^2}-\frac{J(J+1)}{R^2}\right)+\tilde{k}_i^2-U_{ii}(R)\right\}\chi_i(R)=\sum_{j\neq i}^{N}U_{ij}(R)\chi_j(R). \tag{5a}$$

Here $2N$ is the number of terms in the expansion (3),

$$\hat{I}=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad U_{ij}(R)=\begin{pmatrix}U_{ia,ja}&U_{ia,jb}\\U_{ib,ja}&U_{ib,jb}\end{pmatrix},$$

$$\chi_j(R)=\begin{pmatrix}\chi_{ja}(R)\\\chi_{jb}(R)\end{pmatrix}, \tag{5b}$$

where $\chi_{ja}(R)$ and $\chi_{jb}(R)$ are the radial wave functions of the relative motion of the nuclei and correspond in the asymptotic region $R\to\infty$ to the subsystems $(a\mu)+b$ and $(b\mu)+a$, $U_{ia,jb}(R)$, and so forth are the effective potentials constructed in Refs. 15 and 18, the asymptotic behavior of which has the form[19-21]

$$U_{ii}(R)\underset{R\to\infty}{=}0,\quad U_{ij}(R)\underset{R\to\infty}{=}(1-\delta_{ij})\left\{2q_{ij}\begin{pmatrix}1+\varkappa&0\\0&-(1-\varkappa)\end{pmatrix}\frac{d}{dR}+h_{ij}^{(*)}\begin{pmatrix}0,&0\\0,&-4\varkappa\end{pmatrix}\right\}, \tag{6a}$$

where

$$\varkappa=(M_b-M_a)/(M_b+M_a),$$

$$q_{ij}=\frac{\mathbf{R}}{R}\left\langle\psi_i\left|-\frac{1}{2}\nabla_{\mathbf{r}}\right|\psi_j\right\rangle,\quad h_{ij}^{(*)}=\left\langle\psi_i\left|-\frac{1}{2}\Delta_{\mathbf{r}}\right|\psi_j\right\rangle,$$

$$\psi_j(\mathbf{r})=\lim_{R\to\infty}\varphi_{jm}(\mathbf{r};R)$$

are the wave functions of the $(a\mu)$ mesic atom in state j.

The quantities $\tilde{k}_i^2$ are defined as follows:

$$\tilde{k}_i^2=\begin{pmatrix}\tilde{k}_{ia}^2,&0\\0,&\tilde{k}_{ib}^2\end{pmatrix}=2M\begin{pmatrix}\varepsilon+E_{1a}-E_{ib},&0\\0,&\varepsilon+E_{1a}-\bar{E}_{ib}\end{pmatrix}, \tag{7a}$$

where E_{ia} is the energy of the isolated $(a\mu)$ atom in state i,

$$\bar{E}_{ib}=E_{ia}(1+\varkappa/M)$$

is the energy of the $(b\mu)$ atom with accuracy $\sim(\varkappa/M)^2$, $\varepsilon=E-E_{ia}$ is the collision energy measured from the value E_{1a},[4,20-22] and

$$M=M_0/m_a,\ M_0^{-1}=M_a^{-1}+M_b^{-1},\ m_a^{-1}=m_\mu^{-1}+M_a^{-1}. \tag{8}$$

(In the following we shall use the system of units $e=\hbar=m_a=1$.) In the case in which only one reaction channel is open ($\tilde{k}_{ia}^2>0$, $\tilde{k}_{ia}^2<0$, $i\neq1$, $\tilde{k}_{ib}^2<0$) it follows from the results of Refs. 4 and 22 that the asymptotic behavior of the solutions $\chi_{ia}(R)$ of the $2N$-dimensional system of equations (5) takes as $R\to\infty$, with accuracy to terms of order R^{-2}, the form

$$\chi_{1a}(R)\underset{R\gg1}{=}\{j_J(k_NR)-t_{11}(k_N)n_J(k_NR)\}\underset{R\to\infty}{\longrightarrow}\sin(k_NR-J\pi/2+\delta(k_N)), \tag{9a}$$

$$\chi_{ia}(R)=\frac{2(1+\varkappa)q_{ia}}{\tilde{k}_{ia}^2-\tilde{k}_{1a}^2}\frac{d}{dR}\chi_{1a}(R),\quad i\neq1,$$

$$k_N^2=\tilde{k}_{1a}^2\left\{1-4(1+\varkappa)^2\sum_{i=2}^{N}\frac{q_{1i}q_{i1}}{\tilde{k}_{ia}^2-\tilde{k}_{1a}^2}\right\}^{-1}=2M_N\varepsilon.$$

The leading terms of the asymptotic form of the solutions $\chi_{ib}(R)$ have the form

$$\chi_{1b}(R)=A\exp\{-\gamma_NR\},$$

$$\chi_{ib}(R)=-\frac{2(1-\varkappa)q_{i1}}{\tilde{k}_{ib}^2-\tilde{k}_{1b}^2}\frac{d}{dR}\chi_{1b}(R)-\frac{4\varkappa h_{i1}^{(*)}}{\tilde{k}_{1b}^2-\tilde{k}_{1b}^2}\chi_{1b}(R),\quad i\neq1,$$

$$\gamma_N^2=-2M\left\{1-4(1-\varkappa)^2\sum_{i=2}^{N}\frac{q_{1i}q_{i1}}{\tilde{k}_{ib}^2-\tilde{k}_{1b}^2}\right\}^{-1}(\varepsilon+E_{1a}-\bar{E}_{1b}), \tag{9b}$$

$$\bar{E}_{1b}=E_{1a}\left(1+\frac{\varkappa}{M}+\frac{16\varkappa^2}{M}\sum_{i=2}^{N}\frac{h_{1i}^{(*)}h_{i1}^{(*)}}{\tilde{k}_{ib}^2-\tilde{k}_{1b}^2}\right).$$

[In the Appendix it is shown that terms proportional to R^{-1} in the nondiagonal potentials $U_{ij}(R)$ do not change the asymptotic behavior of the solutions (9).]

The asymptotic expressions (9) for the solutions $\chi_{ia}(R)$ and $\chi_{ib}(RT)$ of the system of equations (5) have been matched to the boundary conditions of the scattering problem (4) for processes (2a)–(2e)[4,22]:

$$\Psi(\mathbf{r},\mathbf{R})\underset{R\to\infty}{\sim}\psi_n(\mathbf{r}_a)\left\{e^{i\mathbf{k}_a\mathbf{R}_a}+\frac{f(\theta)}{R_a}e^{ik_aR_a}\right\}, \tag{10}$$

where $\psi_n(\mathbf{r}a)$ is the wave function of the isolated $(a\mu)$ atom in the ground state, $\mathbf{R}_a$ is the vector connecting nucleus b and the center of mass of the $(a\mu)$ atom, and k_a is the momentum of their relative motion:

$$k_a^2=2\mathcal{M}_a\varepsilon,\quad \mathcal{M}_a^{-1}=(M_a+m_\mu)^{-1}+M_b^{-1}. \tag{11a}$$

The partial elastic-scattering cross sections σ_N^J calculated from the system of N pairs of equations (5) with the boundary conditions (9) are:

$$\sigma_N{}^J=\frac{4\pi(2J+1)}{k_N^2}\frac{t_N^2}{1+t_N^2},\qquad t_N\equiv t_{11}{}^J(k_N). \tag{12}$$

In the limit $N\to\infty$ the following relations are valid[4,21]:

$$\lim_{N\to\infty}4\sum_{i=2}^{N}\frac{q_{1i}q_{i1}}{E_1-E_i}={}^1/_2,\qquad \lim_{N\to\infty}4\sum_{i=2}^{N}\frac{h_{1i}^{(*)}h_{i1}^{(*)}}{E_1-E_i}=E_1,$$

$$M_N\to\mathcal{M}_a=M\left(1-\frac{(1+\varkappa)^2}{4M}\right)^{-1},\qquad k_N^2\to k_{1a}^2=2\mathcal{M}_a\varepsilon.$$

$$\gamma_N^2\to\gamma_{1b}^2=-2\mathcal{M}_b(\varepsilon+E_{1a}-E_{1b}),\ \mathcal{M}_b^{-1}=(M_b+m_\mu)^{-1}+M_a^{-1}. \tag{11b}$$

The elastic-scattering cross section is

$$\sigma^J(\varepsilon)=\lim_{N\to\infty}\sigma_N{}^J. \tag{13}$$

3. METHOD OF SOLUTION

To find the T-matrix parameters $t_{11}(k_N)$ or the phase shifts $\delta(k_N)$ corresponding to them one usually solves the Cauchy problem for the $2N$-dimensional system of Equations (5) and then determines the values of t_{11}, comparing the asymptotic solutions (9) with the numerical solution of the system (5). However, numerical solution of the Cauchy problem in the presence of closed channels involves certain difficulties[23] since such problems have simultaneously the features of scattering problems and of eigenvalue problems, for the solution of which one usually uses fundamentally different calculation schemes.

In Ref. 13 the scattering problem was discussed as an eigenvalue problem. In this approach the collision energy ϵ is found as the eigenvalue of the Sturm–Liouville problem for a given value of t_{11} with boundary conditions (9a) and (9b) for $R = R_m \gg 1$ and $\chi_j(0) = 0$.

Using the asymptotic form of the solutions (9) of the system of equations (5), the problem can be further simplified by choosing the boundary conditions at some point $R = R_m$ in a form which does not require specifying t_{11}:

$$\begin{aligned} &\chi_{1a}(R_m)=0, \\ &\frac{d}{dR}\chi_{ia}(R_m)=0, \quad i=2,\ldots,N. \\ &\left[\frac{d}{dR}\chi_{ib}(R)+\gamma_N\chi_{ib}(R)\right]_{R=R_m}=0, \quad i=1,2,\ldots,N. \end{aligned} \tag{14}$$

The condition $\chi_{ia}(R_m) = 0$ is equivalent to replacement of the true potential in the first channel by a potential with an infinite wall at[2] $R = R_m$, which is well known to correspond to the discrete spectrum of eigenvalues $\varepsilon^{(\alpha)}(R_m)$, $\alpha = 1,2,\ldots$, which depends on the choice of R_m (see Fig. 1). The eigenfunctions of the Sturm–Liouville problem (5) and (14) contain information on the scattering phase shifts of the problem (5) and (9). (Usually at low collision energies it is sufficient to consider just the first eigenvalue with $\alpha = 1$.) After solving the problem (5) and (14), we determine from relation (9a) the value t_N:

$$t_N = j_J(k_N R_m)/n_J(k_N R_m), \tag{15a}$$

$$\delta_N = \delta(k_N) = \operatorname{arctg}(t_N) \approx \pi(\alpha + J/2) - k_N R_m. \tag{15b}$$

In the case $J = 0$ Eqs. (15a) and (15b) are equally suitable for determination of the phase shifts δ, and the error in calculation of the phase shifts due to the finite integration interval $[0, R_m]$ does not exceed the value

$$\sim (kR_m)^{-1} R_m^{-2} \approx 1/\pi R_m^2$$

(see Ref. 25). For $J \neq 0$ the error in calculation of δ by means of Eq. (15b) is

$$\approx J(J+1)/(kR_m) \approx J(J+1)/\pi,$$

and therefore Eq. (15a) is preferable since it takes into account exactly the phase shift of the long-range centrifugal potential.

With the exception of the resonance energy region, the scattering phase shifts are small ($\delta \ll 1$), and therefore from Eq. (15b) one obtains the useful relation

$$R_m = \pi(\alpha + J/2)\, k_N, \tag{16}$$

which permits an approximate choice of R_m corresponding to a given collision energy ε. From Eq. (15b) it also follows that for calculation of the phase shifts δ_N with accuracy of $\sim 10^{-2}$ the momenta k_N must be found with high accuracy $\sim 10^{-4}$–10^{-5}, since they are multiplied by the large quantity $R_m \gtrsim 100$.

In particular, it is impossible to neglect the difference $\sim (2M)^{-1}$ between $\tilde{k}_{1a}$ and k_N [see Eqs. (7) and (9)], since the difference

$$\begin{aligned} &\delta(\tilde{k}_{1a}) - \delta(k_N) = (k_N - \tilde{k}_{1a}) R_m \\ &= 2(1+\varkappa)^2 \sum_{i=2}^{N} \frac{q_{1i} q_{i1}}{\tilde{k}_{1a}^2 - \tilde{k}_{ia}^2} k_N R_m \\ &\approx \frac{(1+\varkappa)^2}{8M} \pi \left(\alpha + \frac{J}{2}\right) \sim 10^{-1} - 10^{-2} \end{aligned} \tag{17}$$

at low collision energies ε is comparable in order of magnitude with the scattering phase shift $\delta(k_N)$. In addition, in the calculation of the phase shifts from Eq. (15) for $\varepsilon = 0$ the necessary relation $t_{11}(k_N) = 0$ is satisfied, whereas $t_{11}(\tilde{k}_{ia}) \neq 0$.

For solution of the system of equations (5) with boundary conditions (14) we used the program VAAR[14] which permits the eigenvalues for the Sturm-Liouville problem to be found for a system of about 300 equations with absolute accuracy $\sim 10^{-4}$–10^{-5}. All subsequent calculations were carried out with $N = 1,3,6$ and $N = N_B$, i.e., with inclusion of 2, 6, and 12 states of the discrete spectrum of the adiabatic basis in the expansion (3) for the wave function $\Psi^J_{mJ}(\mathbf{r},R)$, and also with inclusion of the continuous spectrum of the two-center problem for $N_B = (6 + 75)$ and $N_B = (9 + 119)$ respectively for the cases $J = 0$ and $J = 1$. The value $N_B = 128$ corresponds to inclusion of the states $1s\sigma$, $2p\sigma,\ldots,4f\pi$, $5g\pi$ of the discrete spectrum ($N = 9$) and of the states $|s\rangle = |1\rangle\ldots|6\rangle$ of the continuum (see Ref. 4).

The effective potentials $U_{ij}(R)$ of the system of equations (5) have been calculated in Refs. 15 with absolute accuracy 10^{-7}–10^{-5}.

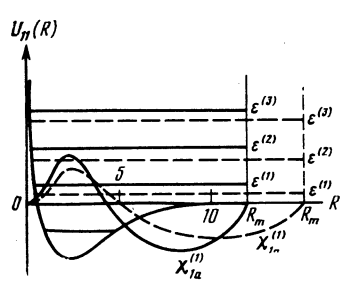

FIG. 1. Diagram of energy levels $\varepsilon^{(\alpha)}$ and wave functions of the problem (5) and (14). Variation of the spectrum $\varepsilon^{(\alpha)}$ is achieved by shifting the integration limit R_m

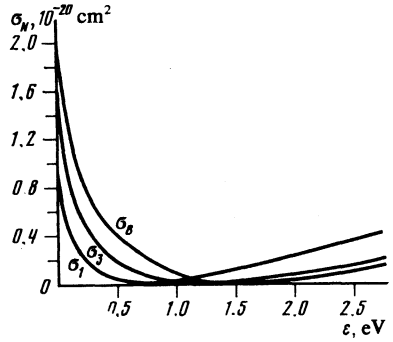

FIG. 2. Cross section for elastic scattering $\sigma_N(\varepsilon)$ in the reaction $d\mu + p \to d\mu + p$ with $J = 0$; N is the number of pairs of equations in the system (5). For $\varepsilon = 0$ we have $\sigma_B(0) = 4\pi a^2 = 2\pi \cdot 10^{-20}$ cm^2.

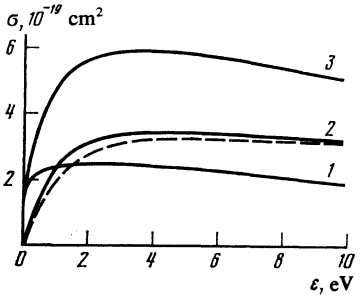

FIG. 4. Partial and total cross sections for the scattering $t\mu + d \to t\mu + d$. Partial cross section $\sigma_B = \sigma_B(J = 0)$—curve 1, $\sigma_B(J = 1)$—curve 2, total cross section $\sigma = \sigma_B(J = 0) + \sigma_B(J = 1)$—curve 3. The dashed line shows the p-wave cross section $\sigma_{\text{eff}}(J = 1)$ calculated with $N = 4$, $M = 11.1$, $\varkappa = -0.197$.

4. ELASTIC SCATTERING OF MESIC ATOMS OF THE HYDROGEN ISOTOPES

The proposed method of solution of the scattering problem has been used for calculation of the phase shifts and cross sections for elastic scattering in reaction (2).

In Fig. 2 we show the results of the calculations for the process (2a), in the cross section of which the Ramsauer effect, well known from the time of Refs. 6 and 7, is observed. It can be seen that taking into account higher states of the two-center problem shifts the location of the minimum in the scattering cross section for (2a) from the collision energy $\varepsilon_0 = 0.6$ eV (at $N = 1$) to $\varepsilon_0 = 1.5$ eV (at $N = N_B$). (In Refs. 6 and 7 values $\varepsilon_0 = 0.2$ and 0.6 were found, respectively.) In addition, for $\varepsilon \to \infty$ the cross sections calculated for $N = 1$ and $N = N_B$ differ by a factor of three.

In Fig. 3 we have shown the functions $t_N(k_N)$ for reaction (2a). Up to energies $\varepsilon \approx 0.2$ eV the $t_N(k_N)$ dependence can be represented with accuracy $\sim 10^{-1}$ by the expansion ($t \equiv t_N$, $k \equiv k_N$, $a \equiv a_N$, $M \equiv M_N$)

$$kt^{-1} = -a^{-1} + 3M\pi(2a^2)^{-1}k + 3Ma^{-1}k^2 \ln\left(\frac{9Mk^2}{32}\right), \qquad (18)$$

which is well known from the theory of single-channel scattering[26] by a potential $U(R)$ with asymptotic behavior

$$U(R) \underset{R\to\infty}{=} -9M/2R^4. \qquad (19)$$

The scattering lengths a_N for various N are respectively: $a_1 = -1.1$, $a_3 = -1.4$, $a_6 = -1.5$, and $a_B = -1.6$. However, it should be noted that the region of applicability of the concept of scattering length, i.e., region of energies in which the relation $\sigma_N = 4\pi a_N^2$ is valid, is very limited ($\varepsilon \lesssim 0.05$ eV, $k \lesssim 10^{-2}$).

The validity of the expansion (18) in the case of the multichannel problem (5) and (14) indicates that in spite of the presence of terms $\sim R^{-1}$ in the matrix of the potentials

$$U_{ij}(R) = H_{ij}^{(0)} + Q_{ij}^{(0)}\frac{d}{dR} + H_{ij}^{(1)}R^{-1} + 2Q_{ij}^{(1)}R^{-1}\frac{d}{dR} + \ldots \qquad (20)$$

of the system (5) for $R \to \infty$, it is equivalent to some effective polarization potential (19) in the open channel. [We recall that the first two terms of the expansion (20) provide the correct momentum k_{1a} for $N \to \infty$ in Eq. (11b).]

For reaction (2b) the effective potentials $U_{ij}(R)$ differ from the similar potentials for reaction (2a) only by the obvious substitutions of the particle masses. In Figs. 4 and 5 we give the cross sections for reaction (2b) with $J = 0$ and $J = 1$ as a function of the collision energy ε and the dimension N of the system of equations (5).

The behavior of the s-wave cross section is determined to a significant degree by the level ($J = 0$, $v = 1$) of the mesic molecule $dt\mu$ with a relatively low energy $\varepsilon_{Jv} \approx -35$ eV. Since variation of N changes the energy of this level relatively weakly [$\varepsilon_{Jv}(N = 1) = -32.2$ MeV, $\varepsilon_{Jv}(N = N_B) = -34.9$ eV; see Ref. 18], in the region of collision energies $\varepsilon \lesssim 5$ eV we have $\sigma_1 \approx \sigma_B$.

In contrast to this, the cross section in the wave changes qualitatively as a function of N (see Fig. 5): for $N = 1$ there is

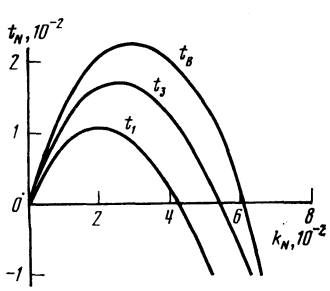

FIG. 3. The scattering parameters $\delta_N(\varepsilon)$ for the reaction $d\mu + p \to d\mu + p$ for $J = 0$ and $N = 1$, 3, and $N_B = 81$.

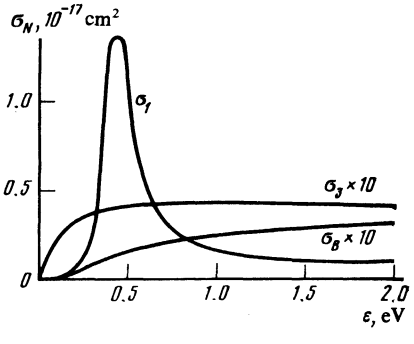

FIG. 5. Elastic scattering cross sections for $t\mu + d \to t\mu + d$ for $J = 1$ as a function of the number of pairs $N = 1,3$, and $N_B = 129$ of equations to be solved in the system (5).

TABLE I

Keys	σ, 10^{-21} cm^2
Cross section for elastic scattering $p\mu(\uparrow\downarrow)+p$	1.2
Source	8.2
cm^2	167 ± 30
Zel'dovich and Gershteĭn (1960)	7.6 ± 0.7
Cohen *et al.* (1960)	2.5
Dzhelepov *et al.* (1965)	0.2
Matveenko and Ponomarev (1970)	35
Matveenko *et al.* (1975)	14 ± 2
Ponomarev *et al.* (1978)	19
Present work*	

*The result was obtained at energy $\varepsilon = 0.04$ eV and $N = N_B$; for $N = 1, 3$, and 6 the calculated cross sections are respectively $\sigma_1 = 0.1$, $\sigma_3 = 8.4$, $\sigma_6 = 12$ (see Fig. 6).

a resonance in the cross section at energy $\varepsilon = 0.46$ eV which disappears on enlargement of the system (5) up to $N = 3$, and with further increase of N the cross section changes only quantitatively. (The fictitious nature of the resonance at $N = 1$ has already been pointed in Ref. 27.) For $N \geqslant 3$ the cross section $\sigma_N(J = 1)$ is determined by the energy ε_{J_v} of the weakly bound state ($J = v = 1$) of the $dt\mu$ mesic molecule, which for values $N = 3$ and $N = N_B = 128$ is respectively $\varepsilon_{11} = -0.11$ and -0.64 eV. The total cross section for reaction (2b) $\sigma = \sigma(J = 0) + \sigma(J = 1)$ for $N = N_B$ is given in Fig. 4.

The results of many years of experimental and theoretical studies of reaction (2c) are given in Table I. Note the large spread of the data.

The system of equations for description of this reaction is given in Ref. 5. For reaction (2c) the effective potentials $\overline{U}_{ij}(R)$ in the system of equations (5) are obtained from $U_{ij}(R)$ by the transformation[5,7]

$$\overline{U} = BUB^{-1}, \quad B_{ij} = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \delta_{ij}, \quad (21)$$

and the value of γ_N^2 in equations (9)–(11) is given by the formula

$$\gamma_N^2 = -2M_N(\varepsilon - \Delta E),$$

where $\Delta E = 0.182$ eV. In constructing the effective potentials (21) for reaction (2c), we have used from among the relativistic corrections to the potentials only the contact term. Numerical checks showed that the relative contribution to the cross section from the discarded terms due to interaction of the muon and nucleus spins does not exceed $\sim 10^{-3}$.

It can be seen from Fig. 6 that in the transition from $N = 1$ to $N = 3$ the calculated cross section for reaction (2c) changes by about 100 times, and with further increase up to $N = N_B$ it rises another factor of two. It follows from this that the two-level approximation used in all previous calculations is utterly inapplicable in the present case. We note, however, that the cross sections calculated in the so-called simple approach of Ref. 28, which differs from the usual two-level approximation only in the substitution $M \to \mathcal{M}_a$, differs by less than a factor of two from the values of the present work for $N = N_B$ (see Table I and also Fig. 5).

In Figs. 7 and 8 we show the quantities t_N and $a_N = -t_N/k_N$ for reaction (2c). The curves $a_N(k_N)$ reveal a characteristic maximum which corresponds to the point of inflection of the functions t_N in Fig. 7. From comparison of Figs. 3 and 7 the reason for the rapid dependence of the results of the calculations on the number of equations N in the case of reaction (2c) becomes clear. It can be seen that in this case we have a situation which for $N = 1$ simulates the Ramsauer effect, but this is just as fictitious as the resonance in the p wave of reaction (2b) at $N = 1$ and disappears in exactly the same way on enlargement of the system of equations (5).

In Fig. 9 we show the energy dependence of the elastic scattering cross section for reaction (2d). Note the steep de-

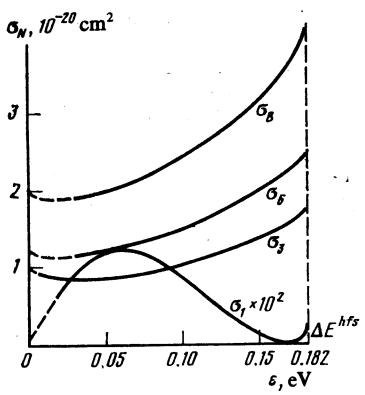

FIG. 6. The cross section $\sigma_N(\varepsilon)$ for the reaction $p\mu(\uparrow\downarrow) + p \to p\mu(\uparrow\downarrow) + p$ for $N = 1,3,6$, $N_B = 81$ ($J = 0$). The dashed portions are extrapolations of $\sigma_N(\varepsilon)$ to $\varepsilon = 0$.

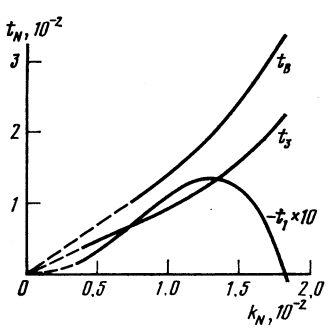

FIG. 7. Elastic-scattering parameters $\delta_N(\varepsilon)$ for the reaction $p\mu(\uparrow\downarrow) + p \to p\mu(\uparrow\downarrow) + p$ with $N = 1,3$, and $N_B = 81$ ($J = 0$). The dashes are extrapolations of $\delta_N(\varepsilon)$ to $\varepsilon = 0$.

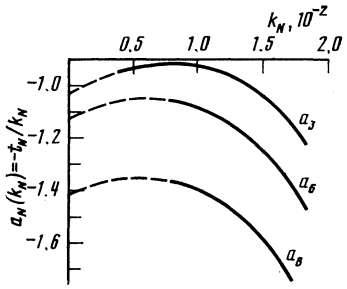

FIG. 8. The functions $a_N(k_N) = -t_N(k_N/k_N$ calculated for the reaction $p\mu(\uparrow\uparrow) + p \to p\mu(\uparrow\downarrow) + p$ with $N = 3,6$, and $N_B = 81$ $(J = 0)$. The scattering lengths $a_N = \lim_{\varepsilon\to 0} a_N(\varepsilon)$ were obtained by extrapolation to $\varepsilon = 0$.

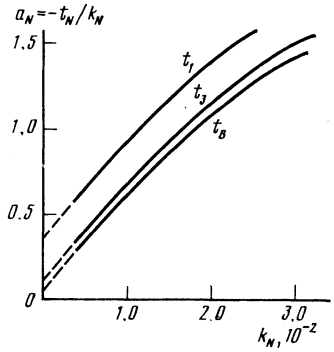

FIG. 10. The functions $a_N(k_N) = -t_N(k_N)/k_N$ calculated for the reaction.

pendence of the cross section on the collision energy and also its anomalously small value for $\varepsilon \to 0$. From Fig. 10, where we have shown the functions $a_N = -t_N/k_N$, we can see that in this case the region of applicability of the scattering-length concept ($\varepsilon \lesssim 2\cdot 10^{-4}$ eV, $k \lesssim 10^{-3}$) is already narrower than in the case of the reactions (2a)–(2c).

We note also the threshold dependence[29] in the cross section for reaction (2d), which was noted in Ref. 7. On enlargement of the system of equations this feature is preserved.

In Figs. 2–10 we can trace the dependences of σ_N and t_N on the number of pairs N of equations (5) used in their calculation. It is easy to see that in all cases considered in the transition from the two-level approximation ($N = 1$) to the multilevel case ($N = 3$, 10, N_B) the behavior of the cross sections as functions of the collision energy ϵ changes qualitatively.[3)] The greatest qualitative changes are observed in the transition form $N = 1$ to $N = 3$ (or to $N = 4$ for $J = 1$) and with further increase of N only quantitative changes of the scattering parameters occur. In all reactions considered, the contribution of continuum states ($N > 10$) to the elastic scattering cross section amounts to about 40% of the contribution of all states in the range $2 \leqslant N \leqslant 10$, i.e., it is of the same order as the contribution of the continuum to the binding energy of the mesic molecule.[18]

In Table II we have given the cross sections and scattering lengths for the processes (2) found from the system of

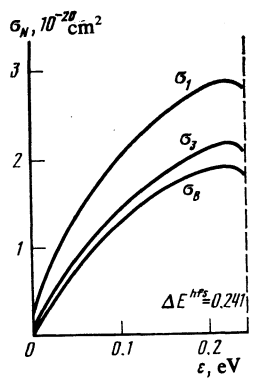

FIG. 9. Cross section $\sigma_N(\varepsilon)$ for the reaction $t\mu(\uparrow\downarrow) + t \to t\mu(\uparrow\downarrow) + t$ with $N = 1$, 3, and $N_B = 81$ $(J = 0)$. The value $\sigma_B(0) = 2\cdot 10^{-23}$ cm^2 was obtained by extrapolation to $\varepsilon = 0$.

equations (5) with $N = N_B$. The scattering lengths given were used for calculation of the cross sections $\sigma = 4\pi a^2$ at $\varepsilon = 0$.

The error in calculation of the elastic scattering cross sections for the reactions (2) in our opinion amounts to about 10% and is determined both by the error in approximation of the initial infinite system of equations by the finite system (5), and by the accuracy of the computational scheme used to find the states $\varepsilon_N^{(a)}$.

The algorithms used[14] permit calculation of $\varepsilon_N^{(a)}$ and the scattering phase shifts with an absolute accuracy $\sim 10^{-4}$. Algorithms of higher order of accuracy have been described in Ref. 30. The results of calculations carried out in this approach with $N = 1$ agree with similar calculations carried out by the method of phase functions[25] (the variable-phase method) with a relative accuracy 10^{-2}–10^{-3}. For calculation of the contribution of higher states of the two-center problem to the reaction (2) scattering cross sections it is possible to use also the method proposed in Ref. 31 for the extrapolation $N \to \infty$ in calculation of the energy levels of μ-mesic molecules.

5. CONCLUSION

In the present work we have developed a method of solution of the multichannel problem of scattering with one open channel and many closed channels. The method permits generalization to the case of several open channels, which will permit calculation of cross sections for inelastic processes. The effectiveness of the method has been demonstrated with calculation of elastic-scattering cross sections in a system of three charged particles as an example. However, the method itself does not depend on the specific properties of the adiabatic basis used for solution of the initial scattering problem. One of the advantages of the method developed is that it permits solution of the Cauchy problem for a system of equations even in the presence of strong coupling of channels in the asymptotic region, which for most methods presents substantial difficulties.[23,32–35] The basic idea of the problem—reduction of the Cauchy problem to the Sturm-Liouville problem for a system of equations of large size—is carried out here for the first time.

TABLE II

ε, eV	Process					
	$p^{\mu}(\uparrow\downarrow)+p$	$t^{\mu}(\uparrow\downarrow)+t$	$d^{\mu}+p$	$t^{\mu}_{J=0}+d$	$t^{\mu}_{J=1}+d$	$t^{\mu}+d$
0	2.0	0,002	2.4	12	0	12
0.04	1.9	0.62	1.6	16	0	16
0.10	2.4	1.2	1.2	17	2	19
0.15	3.1	1.6	1.0	18	4	22
0.3	—	—	0.65	21	9	30
0.5	—	—	0.38	22	14	36
1	—	—	0.07	24	26	50
3	—	—	0.18	25	34	59
5	—	—	4.00	24	34	58
10	—	—	11.9	19	32	51
Scattering length, mesic atom units	−1.6	0.05	−1.7	3.8	—	—
m_{μ}/m_a	1.113	1.038	1.056	1.038	—	—

*The cross sections are given units of 10^{-20} cm^2, and the scattering length in mesic atom units $\mu = \hbar^2/m_{\mu}e^2 = 2.559\cdot10^{-11}$ cm.

The proposed method possesses sufficient generality and can be used for solution of diverse problems of atomic and nuclear physics, in wave-propagation theory, solid-state physics, and so forth. The natural region of application of the method is in scattering at low energies when only a few partial waves contribute to the cross sections, i.e., just the energy region in which approximate methods of solution of the scattering problem turn out to be ineffective.

The examples considered by us from the field of mesic-atom physics demonstrate the substantial diversity of the possibilities of the method: it permits description in a unified manner of various physical phenomena—the Ramsauer effect, threshold behavior and resonances in a cross section, and also effects due to the influence of closed channels (such as Feshbach resonances[26]).

In conclusion the authors express their gratitude to S. I. Vinitskiĭ, I. V. Puzynin, and L. N. Somov for helpful discussions at various stages of the work.

APPENDIX

For $R\to\infty$ the nondiagonal matrix elements[20] are

$$Q_{ia,\,jb}=Q_{ib,\,ja}=H_{ia,\,jb}=H_{ib,\,ja}=0$$

and the system of equations (5) breaks up into two subsystems. We shall consider the subsystem which in the asymptotic region describes the relative motion of $(a\mu)+b$. for this subsystem the system of equations (5) for $J=0$ has the form

$$\left(\frac{d^2}{dR^2}+\tilde{k}^2-2Q^{(0)}\frac{d}{dR}-H^{(1)}\frac{1}{R}\right)\chi=0, \tag{A1}$$

where

$$\tilde{k}^2=\begin{pmatrix}\tilde{k}_1^2 & 0 & 0 & \dots & 0\\ 0 & \tilde{k}_2^2 & 0 & \dots & 0\\ 0 & 0 & \tilde{k}_3^2 & \dots & 0\\ \dots & \dots & \dots & \dots & \dots\\ 0 & 0 & 0 & \dots & \tilde{k}_N^2\end{pmatrix},\quad \chi=\begin{pmatrix}\chi_1\\ \chi_2\\ \dots\\ \chi_N\end{pmatrix},$$

$$Q^{(0)}=(1+\varkappa)\begin{pmatrix}0 & q_{12} & q_{13}\dots & q_{1N}\\ -q_{12} & 0 & 0\dots & 0\\ -q_{13} & 0 & 0\dots & 0\\ \dots & \dots & \dots & \dots\\ -q_{1N} & 0 & 0\dots & 0\end{pmatrix}, \tag{A2}$$

$$H^{(1)}=2(1+\varkappa)\begin{pmatrix}0 & q_{12} & q_{13}\dots & q_{1N}\\ q_{12} & 0 & 0\dots & 0\\ q_{13} & 0 & 0\dots & 0\\ \dots & \dots & \dots & \dots\\ q_{1N} & 0 & 0\dots & 0\end{pmatrix}.$$

Here we have used the property $H^{(i)}_{ij}=2Q^{(0)}_{ij}$, $i<j$[4] Using the results of Ref. 22, we find with accuracy to terms of order $(2M)^{-2}$

$$\chi_i=\frac{2(1+\varkappa)q_{i1}}{\tilde{k}_i^2-\tilde{k}_1^2}\left(\frac{d}{dR}-\frac{1}{R}\right)\chi_1. \tag{A3}$$

Substituting (A3) into the first equation of the system (A1), we obtain

$$\left[\frac{d^2}{dR^2}+\tilde{k}_1^2-4(1+\varkappa)^2\sum_{i\neq1}^{N}\frac{q_{1i}q_{i1}}{\tilde{k}_i^2-\tilde{k}_1^2}\left(\frac{d}{dR}+\frac{1}{R}\right)\left(\frac{d}{dR}-\frac{1}{R}\right)\right]$$

$$\times\chi_1=0. \tag{A4}$$

Using the operator equality

$$\left(\frac{d}{dR}+\frac{1}{R}\right)\left(\frac{d}{dR}-\frac{1}{R}\right)=\frac{d^2}{dR^2}, \tag{A5}$$

we arrive at the equation

$$\left[\left(1-4(1+\varkappa)^2\sum_{i\neq1}^{N}\frac{q_{1i}q_{i1}}{\tilde{k}_i^2-\tilde{k}_1^2}\right)\frac{d^2}{dR^2}+\tilde{k}_1^2\right]\chi_1=0. \tag{A6}$$

In the limit $N\to\infty$ we have according to Eq. (11b)

$$\left[1-4(1+\varkappa)^2\sum_{i\neq1}^{N}\frac{q_{1i}q_{i1}}{\tilde{k}_i^2-\tilde{k}_1^2}\right]\to\frac{M}{\mathcal{M}_a}.$$

From this it follows that

$$\left[\frac{d^2}{dR^2}+k_{1a}^2\right]\chi_1=0,\quad k_{1a}^2=\frac{\mathcal{M}_a}{M}\tilde{k}_1^2.$$

This result agrees with the conclusion of Ref. 21.

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[2)]This procedure was used previously in the solution of the one-channel scattering problem (see for example Refs. 12 and 24).

[3)]We recall[18,27] that in calculation of the energy of weakly bound states of mesic molecules it is just the inclusion of terms of order $(2M)^{-2}$ in the potentials $U_{ij}(R)$ which leads to appearance of a new level $(J = v = 1)$ in the $dt\mu$ mesic molecule.

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Translated by Clark S. Robinson