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THE MULTI-CHANNEL SCATTERING WITH VELOCITY-DEPENDENT ASYMPTOTIC POTENTIALS

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1. Introduction

The earliest investigations of atomic scattering processes proposed two commonly used expansions for the wave function. The first was the closed coupling method based on an atomic states and using Jacobian coordinates (see Fig.1) for the description of two fragments movement[1]. The advantage of this method is the correct behaviour of the wave function of a truncated system in the asymptotic region. However, it leads to the Schrödinger equation with potential containing the integral term which significantly complicates the numerical integration of this problem[2]. The alternative approach was connected with the use of adiabatic molecular states for the expansion and an internuclear separation vector for the relative motion (so-called PSS method)[3]. This approach allows one to get rid of the integral term in the reduced equation but meets with other serious difficulties concerning with improper behaviour of the wave function in the asymptotic region due to the non-physical strong coupling of the channels at the infinity. That partialy explains that the major part of works using this approach treats only two level approximations taking into account only the ground states of atoms. The compromise was found in the so-called hyperspherical approach[4,5] where the hyperradius is used as a parameter for the radial equation. This parametrization continuously transforms the coordinate system of reactants into the coordinate system of products of the reaction. But this progress was achieved by the loss of some physical clarity - the asymptotic states are defined on the curved manifold of a fifth-dimensional sphere. The aim of this paper is to investigate the properties of a finite component Schrödinger equation with velocity-dependent potential in asymptotic region with special emphasis on the self-consistent formulation of asymptotic boundary conditions for the truncated scattering problem. We hope that this work will stimulate the use of PSS or related methods in application to the slow atomic collisions.

The matrix Schrödinger equation under investigation in this paper is determined by the Hamiltonian ($\hbar = 1$)

$$H = -\frac{1}{2M}\Delta_{\mathbf{R}} + 2\overline{\mathcal{Q}}(\mathbf{R})\,\nabla_{\mathbf{R}} + \mathcal{H}(\mathbf{R}), \tag{1}$$

where $\overline{\mathcal{Q}}(\mathbf{R}) = \{\mathcal{Q}_x, \mathcal{Q}_y, \mathcal{Q}_z\}$ and $\mathcal{H}(\mathbf{R})$ are real $n \times n$ matrices of effective potentials and M is the reduced mass of the system. The effective potentials are subject to the conditions providing self-adjointness of the differential operator. It means that $\overline{\mathcal{Q}}(\mathbf{R})$ is antisymmetric and $\mathcal{H}^T(\mathbf{R}) = \mathcal{H}(\mathbf{R}) - 2\nabla_{\mathbf{R}}\overline{Q}(\mathbf{R})$, where $\mathcal{H}^T$ means transposed matrix. When $\mathbf{R} \to \infty$, $\overline{Q}(\mathbf{R})$ becomes constant and $\mathcal{H}$ is symmetric. The asymptotic matrix $\mathcal{H}$ can be diagonalized by some orthogonal transformation and we assume hereafter that it was already done. We assume also that nondiagonal part of potential $\overline{Q}$ does not vanish at the infinity. Thus for the scattering processes with a fixed energy ε the asymptotic solution is not concentrated in certain component of the wave function as it normally takes place in standard potential scattering but distributes between different components. More over, as it will be shown later we cannot even hope to achieve the separation of the channels in the asymptotic region by any similarity transformation of the wave function components.

We meet this situation in the standard multichannel generalization of the PSS method (also called *multichannel adiabatic approach*)[6–8] and in its modification named *improved adiabatic approach*[9].

We need to make some remarks on the notation. We distinguish here the meenings of the i-th component of the wave function and the i-th incoming or outgoing channel understanding under the channel of the reaction the subspace of asymptotic wave functions which are simple monochromatic waves $\bar{c}e^{\pm ikR}$ corresponding to a solution with a fixed energy of the interaction.

It will be useful to illustrate all the problems encountered in this paper by a simple example. To do that we introduce the three-body closed coupling expansion using an internuclear position vector $\mathbf{R}$ (Fig.1) for the description of the external motion of fragments:

$$\Psi(\mathbf{R},\mathbf{r}) = \sum_i \varphi_{ia}(\mathbf{r}_a)\,\psi_a(\mathbf{R}) + \sum_i \varphi_{ib}(\mathbf{r}_b)\,\psi_b(\mathbf{R}), \tag{2}$$

here $\mathbf{r}$ is a position vector of a light particle with respect to the center of mass of the nuclei and $\mathbf{r}_a$, $\mathbf{r}_b$ are position vectors of the light particle with respect to the nuclei a and b. Functions φ_{ia} and φ_{ib} are atomic functions. Inserting the finite sum of this expansion into the three-body Schrödinger equation we come to a system of differential equations of variable $\mathbf{R}$ without the integral interaction term but having additional velocity-dependent potential $\overline{Q}$ that doesn't vanish at the infinity due to the correlation term $\nabla_{\mathbf{R}}\nabla_{\mathbf{r}_a}$ (or $\nabla_{\mathbf{R}}\nabla_{\mathbf{r}_b}$) in the kinetic energy operator which (for the dissociation limit $(ac)+b$) can be expressed:

$$T = -\frac{1}{2M}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{\mathbf{r}_a} - \frac{1}{2M}\nabla_{\mathbf{R}}\nabla_{\mathbf{r}_a}, \tag{3}$$

where $M^{-1} = M_a^{-1} + M_b^{-1}$, $m_a^{-1} = M_a^{-1} + M_c^{-1}$ and M_a, M_b, M_c are masses of particles. So we can write out the operator $\overline{Q}$ in a form

$$\overline{Q}^{(a)}_{ij} = \langle\varphi_{ia}|\frac{1}{2M_a}\nabla_{\mathbf{r}_a}|\varphi_{ja}\rangle,$$
$$\overline{Q}^{(b)}_{ij} = \langle\varphi_{ib}|\frac{1}{2M_b}\nabla_{\mathbf{r}_b}|\varphi_{jb}\rangle,$$

and

$$\overline{Q}_{ia,jb} = \langle\varphi_{ia}|\frac{1}{2M_b}\nabla_{\mathbf{r}_b}|\varphi_{jb}\rangle = 0, \qquad \text{when } \mathbf{R}\to\infty.$$

As we have assumed above, the matrix $\mathcal{H}$ is diagonal at the infinity, its diagonal elements h_{ii} determine energy thresholds of the reaction. This definition is justified in a view that we can associate with every spectral point of $\mathcal{H}$ marked in the energy region some asymptotic wave function with $k \to 0$.

2. Conservation law for the particle flux

To define properly parameters of the scattering process (such as the S-matrix of the reaction) we should know how many particles are brought into or out of the interaction region by a wave function of a channel. It is reasonable to balance ingoing and outcomining waves comparing them with the unit flux coming through some large sphere. So we need to determine the operator of particle flux density.

Let us regard the time-dependent Schrödinger equation and its conjugate

$$i\frac{\partial\psi}{\partial t} = \left\{-\frac{1}{2M}\Delta_{\mathbf{R}} + 2\overline{Q}(\mathbf{R})\nabla_{\mathbf{R}} + \mathcal{H}(\mathbf{R})\right\}\psi(\mathbf{R}),$$
$$-i\frac{\partial\psi^*}{\partial t} = \left\{-\frac{1}{2M}\Delta_{\mathbf{R}} + 2\overline{Q}(\mathbf{R})\nabla_{\mathbf{R}} + \mathcal{H}(\mathbf{R})\right\}\psi^*(\mathbf{R}).$$

Multiplying the first equation on ψ^*, the second on ψ and extracting one from another we get the evolution equation for the density of particles

$$i\frac{\partial}{\partial t}|\psi|^2 = \psi^* H\psi - \psi H\psi^* =$$
$$= \nabla_{\mathbf{R}}\left[-\frac{1}{2M}(\psi^*\nabla_{\mathbf{R}}\psi - \psi\nabla_{\mathbf{R}}\psi^*) + (\psi^*\overline{Q}\psi - \psi\overline{Q}\psi^*)\right].$$

If we integrate equation over some volume V bounded by closed surface S we will receive the conservation law for the particle density in a bounded domain for the dynamical system described by the Hamiltonian (1):

$$\frac{\partial}{\partial t}\int_V |\psi|^2 d\mathbf{R} = -i\oint_S d\mathbf{S}\left[-\frac{1}{2M}\left(\psi^*\nabla_{\mathbf{R}}\psi - \psi\nabla_{\mathbf{R}}\psi^*\right) + \left(\psi^*\overline{\mathcal{Q}}\psi - \psi\overline{\mathcal{Q}}\psi^*\right)\right]. \quad (4)$$

The expression under the integral sign determines the operator of particle flux. It is worthful to note that this expression differs from the usual definition by the additional Q-potential term. First of all it connects with space translational properties of the Hamiltonian (1). Existence of velocity-dependent potential in the asymptotic Hamiltonian implies some modifications in definition of such dynamical parameters of the system like velocity or mass of the physical object.

We can show that in the case of expansion (2) with the full set of atomic states this definition coinsides with the generally known expression as only we transfer our coordinate system to conventional Jacobian coordinates which are orthogonal in a six-dimensional space of the three-particle relative movement. Let us regard the operator of density for the particle flux in a $(ac)+b$ subdivision of the three-particle system. In terms of expansion (2) and cooridate system $(\mathbf{R},\mathbf{r}_a)$ the operator has the following form (see Eq. (3)):

$$i\left[\frac{1}{2M}\left(\psi^*\nabla_{\mathbf{R}}\psi - \psi\nabla_{\mathbf{R}}\psi^*\right) - \frac{1}{2M_a}\left(\psi^*\nabla_{\mathbf{r}_a}\psi - \psi\nabla_{\mathbf{r}_a}\psi^*\right)\right]. \quad (5a)$$

Translating the origin of the vector $\mathbf{R}$ from the nuclei to the center of mass of the (ac) atom we define the proper dynamics of two compound particles and the expression for the operator of flux will become:

$$i\left[\frac{1}{2\mathcal{M}_a}\left(\psi^*\nabla_{\mathbf{R}_a}\psi - \psi\nabla_{\mathbf{R}_a}\psi^*\right) - \frac{1}{2M_a}\left(\psi^*\nabla_{\mathbf{r}_a}\psi - \psi\nabla_{\mathbf{r}_a}\psi^*\right)\right], \quad (5b)$$

where

$$\mathbf{R}_a = \mathbf{R} - \tau\mathbf{r}_a, \qquad \tau = \frac{M_c}{M_a+M_c}$$

$$\nabla_{\mathbf{R}} = \nabla_{\mathbf{R}_a}, \qquad \nabla_{\mathbf{r}_a} = \nabla_{\mathbf{r}_a} - \tau\nabla_{\mathbf{R}_a}$$

and where $\mathcal{M}_a^{-1} = M_b^{-1} + (M_a+M_c)^{-1}$ defines the correct reduced mass for the atom-particle movement. The last term in (5b) appears due to the slope of the surfice $S_{R=\text{const}}$ in the six-dimensional space (see Fig.2) with respect to orthogonal coordinates $(\mathbf{R}_a,\mathbf{r}_a)$ and if the boundary surface will be adjusted to $S_{R_a=\text{const}}$ the last term will be eliminated.

The validity of these discussions can be checked by the direct insertion of the correct asymptotic wave function $\Psi(\mathbf{R}_a,\mathbf{r}_a) = \varphi_{ia}(\mathbf{r}_a)\, e^{i\mathbf{k}_i\mathbf{R}_a} = \left[\varphi_{ia}(\mathbf{r}_a)\, e^{i\tau\mathbf{k}_i\mathbf{r}_a}\right] e^{i\mathbf{k}_i\mathbf{R}}$, representing some asymptotic atomic state φ_{ia}, into expresions (5a) and (5b). It is clearly seen that the last term of Eq. (5b) is equal to zero while in the first expression the last term adds non-zero correction (connected with the so-called translational factor $e^{i\tau\mathbf{k}_i\mathbf{r}_a}$).

Formally the scattering problem can be formulated in terms of a Hamiltonian of *free* motion,

$$H_0(\bar{\mathbf{P}}) = \frac{1}{2M}\bar{\mathbf{P}}^2 + 2i\overline{\mathcal{Q}}(\infty)\bar{\mathbf{P}} + \mathcal{H}(\infty), \quad (6)$$

which provides necessary observables for the theory, such as the velocity of the "complex" particle (compare it with the flux density operator from Eq. (4)),

$$\bar{\mathbf{V}} = \partial H_0/\partial\bar{\mathbf{P}} = \frac{1}{M}\bar{\mathbf{P}} + 2i\overline{\mathcal{Q}}(\infty),$$

and the effective mass of the particle,

$$M^{eff} = P/V,$$

which varies depending on the channel number and on the velocity of the particle in the channel. One can compare the effective mass of two different channels in example (2) corresponding to two different limits of dissociation of the molecule, it coincides with the reduced mass of systems $(ac)+b$ and $(bc)+a$ respectively.

After the "free" Hamiltonian is defined we can use the standard Møller operators,

$$\Omega^{(\pm)} = \operatorname*{s-lim}_{t\to\mp\infty} e^{iHt}e^{-iH_0t},$$

and the S-matrix operator expressed in terms of Møller operators,

$$S = \left[\Omega^{(-)}\right]^*\Omega^{(+)}$$

for the formal scattering theory description[11,12].

In what follows we assume that (1) is invariant under three-dimensional rotations. (For the expansion (2) it means that a truncated basis set is rotationally invariant.) So applying the partial wave expansion to the wave function of the problem we get the system of the radial Schrödinger equations:

$$\left\{-\frac{1}{2M}\frac{d^2}{dR^2} + 2\mathcal{Q}(R)\frac{d}{dR} + \mathcal{H}(R)\right\}\psi(R) = \varepsilon\psi(R). \quad (7)$$

This system of coupled equations can connect the channels with different orbital momentum of relative motion of fragments, so it will be convenient to omit from consideration all the details concerned with orbital momentum. All the more that the phase shift corrections can be easily included afterwards. For brevity of notations we will make use of the units: $\hbar = e = 2M = 1$.

3. Description of asymptotic channels

We need to investigate the asymptotic behaviour of a common solution of the Eq. (7) when $R \to \infty$. To do that we will look for the wave functions of exponential type $\psi(R) \sim \exp(ikR)$. This leads us to the determinant equation

$$\|k^2 + 2ikQ + H - \varepsilon\| = 0, \tag{8}$$

where $Q = \mathcal{Q}(\infty)$ and $H = \mathcal{H}(\infty)$. The diagonal element h_{ii} of matrix H determines threshold above which an i-th channel will be open and the internal energy of this scattering channel can be written as $\varepsilon_i = \varepsilon - h_{ii}$.

When $\varepsilon_i = 0$ Eq. (8) has a solution $k_i = 0$, and respective asymptotic solution of Eq. (7) is concentrated in the component "i". However, when ε_i increases the asymptotic incoming wave stretches along the components of the wave function ($k_i \geq 0$),

$$\{\psi_{in}^{(i)}\}_j(R) \simeq c_j e^{ik_iR}, \tag{9a}$$

where a vector $\bar{c} = \{c_j\}$ is a non-zero solution of equation

$$\left[k_i^2 + 2ik_iQ + (H - \varepsilon)\right]\bar{c} = 0. \tag{9b}$$

An outgoing wave has a similiar form

$$\{\psi_{out}^{(i)}\}_j(R) \simeq d_j e^{-ik_iR}, \tag{10a}$$

with d_j satisfying the transposed equation

$$\left[k_i^2 - 2ik_iQ + (H - \varepsilon)\right]\bar{d} = \left[k_i^2 + 2ik_iQ + (H - \varepsilon)\right]^T\bar{d} = 0. \tag{10b}$$

Unless matrix Q is zero, vectors $\bar{c}$ and $\bar{d}$ are not collinear and incoming and outgoing waves cannot be transformed into one component of Eq. (7) by some local similarity transformation.

In what follows we assume c_i is real and $c_i \neq 0$ for a channel "i". This restriction is reasonable in a view that we need to connect all eigenvalues of the problem (9b) with the channel numbers (asymptotic potentials derived from physical problems usually provide a dominant value for c_i and the connection is evident). For an open channel, when k_i is real, vector $\bar{d}$ can be taken as a complex-conjugate to the vector $\bar{c}$. Dividing vector $\bar{c}$ into real and imaginary parts:

$$\bar{v}^{(i)} = \frac{1}{\|\bar{c}^{(i)}\|_Q}\mathcal{R}e\{\bar{c}\}, \quad \bar{w}^{(i)} = \frac{1}{k_i\|\bar{c}^{(i)}\|_Q}\mathcal{I}m\{\bar{c}\}, \tag{11}$$

where in accordance with Eq. (4) (plus sign means transpose and conjugate)

$$\|\bar{c}\|_Q = \left|k_i\|\bar{c}\|^2 - i\bar{c}^+Q\bar{c}\right|^{\frac{1}{2}}, \tag{12}$$

we get the necessary asymptotic solutions of open channels,

$$\bar{\phi}_i^{(\pm)}(R) = \left(\bar{v}^{(i)} \pm ik\bar{w}^{(i)}\right)e^{\pm ikR}. \tag{13}$$

The wave function normalyzed by this way has a unit flux of particle transfer through a sphere bounded the interaction region.

We can describe an asymptotic solution of the channel "i" via the i-th component of the wave function

$$\psi_j^{(i)}(R) \simeq \frac{1}{v_i^{(i)}}\left\{v_j^{(i)} + w_j^{(i)}\frac{d}{dR}\right\}\psi_i^{(i)}(R), \qquad j = 1, \ldots, n. \tag{14}$$

Inserting the asymptotic solutions (14) for the wave function components into the i-th equation of (7) we get

$$\left(1 - 2\sum_j q_{ij}w_j^{(i)}\right)\psi_i'' + (\varepsilon - u_{ii})\psi_i = 0,$$

where the first derivative term disappeared due to the self-adjointness of the operator (one can check it directly using equation (9b)).

When expansion (2) has a full basis set, an outgoing wave $\Psi(R, \mathbf{r}_a) = \varphi_i(\mathbf{r}_a)e^{ik_iR_a} = \left[\varphi_i(\mathbf{r}_a)e^{i\tau(\mathbf{k}_i\mathbf{r}_a)}\right]e^{ik_iR}$, where $\tau = M_c/(M_c + M_a)$ and $k_i^2 = 2\varepsilon_i\mathcal{M}_a$, satisfies the stationary equation

$$-\frac{1}{2M}\frac{d^2}{dR^2}\Psi - \frac{1}{2M_a}\left(\frac{\mathbf{R}}{R}\nabla_{\mathbf{r}_a}\right)\frac{d}{dR}\Psi + (H - \varepsilon)\Psi =$$
$$= -\frac{1}{2\mathcal{M}}\frac{d^2}{dR^2}\Psi + (H - \varepsilon)\Psi = 0.$$

The wave number k_i and the wave function $\phi_i = \varphi_i(\mathbf{r}_a)\, e^{i\tau(\mathbf{k}_i\mathbf{r}_a)}$ compose a nonzero solution of the respective determinant equation

$$\left[k_i^2 + 2ik_i\left(\frac{\mathbf{R}}{2M_aR}\nabla_{\mathbf{r}_a}\right) + (H-\varepsilon)\right]\phi_i = 0.$$

If a finit basis set contains the wave function ϕ_i or the function can be linearly expressed by this set, then truncated scattering equation should have a solution with correct asymptotic behaviour. It is easyly seen that this function depends on the colliding energy thus it is rather possible to introduce such a set of basis functions that includes all necessary functions. Anyhow we can hope that it can be done approximately (for example with the use of pseudostates). So when the number n of basis functions increases the quantities of $k_i^{(n)}$ and $M_i^{(n)} = k_i^{(n)}/\dot{v}_i^{(n)}$ $(v_i^{(n)} = \|\bar{c}^{(i,n)}\|_Q^2)$ converge respectively to correct values of k_i and $\mathcal{M}_a$.

Let us fix the incident channel i of the reaction. A respective solution of the multichannel stationary Schrödinger equation (7) with m open channels has an asymptotic form

$$\psi^{(i)}(R) \simeq \vec{\phi}_i^{(-)} - \sum_{j=1}^{m} S_{ij}\vec{\phi}_j^{(+)}, \tag{15}$$

and elements S_{ij} define the S-matrix of the scattering problem. Or course, it is necessary to show that this new definition of S-matrix coincides with the one given in the previous section. But we lay aside a rigorous consideration of this problem.

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:

$$\vec{\phi}_i^{(1)} = \frac{1}{2i}\left(\vec{\phi}_i^{(+)} - \vec{\phi}_i^{(-)}\right) = \bar{\mathbf{v}}^{(i)}\sin k_iR + k_i\bar{\mathbf{w}}^{(i)}\cos k_iR,$$

$$\vec{\phi}_i^{(2)} = \frac{1}{2}\left(\vec{\phi}_i^{(+)} + \vec{\phi}_i^{(-)}\right) = \bar{\mathbf{v}}^{(i)}\cos k_iR - k_i\bar{\mathbf{w}}^{(i)}\sin k_iR.$$

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

$$\hat{\psi}^{(i)} \simeq \vec{\phi}_i^{(1)} - \sum_{j=1}^{m} K_{ij}\vec{\phi}_j^{(2)}, \tag{16}$$

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[11,12].

4. Boundary conditions

Let us consider the n component system of radial equations with m open channels. The asymptotic solutions (15) define boundary conditions in the infinity. For practical use it will be better to impose boundary conditions somewhere at a finite point R_p. For this purpose we will assume that potentials $\mathcal{Q}$ and $\mathcal{H}$ can be represented by asymptotic expansions

$$\mathcal{K}(R) = \frac{1}{2}\left(\mathcal{H}(R) + \mathcal{H}^T(R)\right) = \mathcal{E} + \sum_{l=1}^{M} A^{(l)}R^{-l},$$

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

where $\mathcal{E}$is a diagonal matrix whose elements are the threshold energies of the different channels. Matrices $A^{(l)}$ are symmetric and $B^{(l)}$ are antisymmetric.

We can continue the solution (13) from the infinity to a finite point R_p using the asymptotic expansion

$$\vec{\phi}_i^{(\pm)}(R) = e^{\pm ik_iR}R^{i\beta_i}\left[\bar{c}_0^{(i)} + \sum_{n=1}^{N}\bar{c}_nR^{-n}\right]. \tag{17}$$

Inserting (17) into equation (7) yields us a sequence of equations providing solutions for unknown quantities in (17)

$$\left[k_i^2 + 2ik_iB_0 + \mathcal{E} - \varepsilon\right]\bar{c}_0 = 0; \tag{18a}$$

$$\left[k_i^2 + 2ik_iB_0 + \mathcal{E} - \varepsilon\right]\bar{c}_1 + \left[2k_i\beta_i + 2i\beta_iB_0 + 2ik_iB_1 + A_1\right]\bar{c}_1 = 0; \tag{18b}$$

$$\dots$$

and

$$\beta_i = -\frac{(\bar{c}_0, [2ik_iB_1 + A_1]\,\bar{c}_0)}{(\bar{c}_0, [2k_i + iB_0]\,\bar{c}_0)}. \tag{19}$$

So for a given accuracy ϵ we can find a value R_p of R such that expansion (17) differs in absolute value from the exact solution by an amount smaller than ϵ for all $R \geq R_p$.

Now let us suppose that all the necessary solutions (and their derivatives) are obtained at a given point R_p. We denote by $\Phi^{(+)}(R)$ the $n\times m$ matrix composed of open channel solutions which we assume to have a maximal rank m.

We look for the boundary conditions of the form

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

which selects from the common asymptotic solution functions having an asymptotic behaviour as in (15). 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 left pseudoinverse $\left[\Phi^{(+)}\right]^{-1}$ of the matrix $\Phi^{(+)}(R)$, satisfying the condition: $\left[\Phi^{(+)}\right]^{-1}\Phi^{(+)} = I$, where I is the identity matrix. 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. (7) 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.

5. The number of asymptoticaly bounded solutions

The complexity of the problem can be illustrated by the two component equation. So let asymptotic potentials be determined by the following matrices:

$$Q = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix}, \qquad H = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix};$$

the determinant equation (8) can be expanded:

$$\left(k^2 - \varepsilon\right)\left(k^2 - \varepsilon + 1\right) - 4q^2k^2 = 0.$$

The solutions of it describing a wave number k as a function of energy ε, for different values of q are shown on Figures 3–5 (solid line is the real part of the function $k(\varepsilon)$ or $k^2(\varepsilon)$ and the dashed line is the imaginary part of it). The asymptotic wave function is determined by the wave number k as $\psi(R) = e^{ikR}$, so when k has an imaginary part, the solution decays or increases exponentially and it corresponds to a closed channel.

For small values of q ($q = 0.2$ on Fig.3) we have seen quite ordinary picture — two closed channels in the lower part of the spectrum which becomes open when the energy ε increases and comes across the respective thresholds $h_1 = 0$ and $h_2 = 1$. The only remarkable peculiarity is appearing here for closed channels just below the energies of approximately $\varepsilon = -1.5$. The asymptotic solution besides an exponentially changing amplitude has also an oscillation due to the nonzero real part of the wave number k. But it does not spoil the qualitative picture of the scattering system behaviour. On Fig.4 the spectral picture for the critical value of parameter $q = 0.5$ is shown. At this point the determinant equation becomes degenerated: $k^4 = 0$, when ε reaches the first threshold ($\varepsilon = 0$). And at last, Fig.5 shows the qualitative behaviour of the system for $q > 0.5$. Here we can see two open channels right below the first threshold! They appear at some energy (in the case of $q = 1$ shown on the Figure it is about $\varepsilon = -0.6$) with a nonzero oscilation and then one of them gradually decreases to the zero and disappears at the threshold energy $\varepsilon = 0$ transforming into the closed channel, while the other developes formally as a usual open channel.

One can ask if a small nonzero Q-potential perturbs the exponential behaviour $e^{\pm|k|R}$ ($k = i|k|$) of the solution for closed channels adding some oscillatory part, why we cannot expect the similar effect for pure oscillatory solutions of open channels $e^{\pm i|k|R}$. The existence of an imaginary part in the wave number leads to exponential changes in amplitude of the wave function and thus this channel should be regarded as closed. Fortunately, the perturbation of the standard multicannel asymptotic potential H by the velocity-dependent potential Qd/dR does not reduce the number of open channels.

To prove this assert we can regard the determinant equation (8) as an equation of two real variables k and ε. If we will solve it regarding ε as an unknown for every fixed k, it will be the standard eigenvalue problem for the Hermitian matrix $k^2 + 2ikQ + H$. The solutions of it are some curves on a real (k, ε)-plane (Fig.6) symmetric with respect to the

k-axis. The number of open channels for a fix value of ε is determined as the number of crossings of these curves while k varies from zero to $+\infty$ (or $-\infty$). It is easyly seen that for large values of k these curves behaves as $\varepsilon_i \sim k^2 + h_{ii}$ so the number of crossings is not less then the number of negative eigenvalues of the matrix $H - \varepsilon$. That proves that the number of asymptotically bounded solutions — open channels — is not less than the number of thresholds below the energy ε. However, the previous two-component example shows that this number of open channels can be greater, if the Q potential is sufficiently large.

To complete the investigation we prove some results on necessary conditions providing the coincidence of the number of thresholds below the fixed energy ε and the number of open channels. Till the end of this section we assume for simplicity that the wave number $k \geq 0$. The proper behaviour of the solutions of the determinant equation obey the rule: $\varepsilon(k_1) > \varepsilon(k_2)$, if $k_1 > k_2$, for any positive k_1 and k_2. So the branches of determinant curves should monotonically increase when k goes from zero to infinity. Otherwise there exist some value of ε for which vertical line of $k > 0$ crosses some curve two or more times. We shall apply this speculations to the point of threshold where $k = 0$.

The curves are the solutions of parametrical eigenvalue equation with Hermitian matrix A:

$$\begin{cases} [A(k) - \varepsilon(k)]\, y(k) = 0, \\ (y, y) = 1, \end{cases}$$

where $A(k) = k^2 + 2ikQ + H$. Differentiating it twice we get

$$\varepsilon'(k) = \frac{(y, A'(k)\, y)}{(y, y)},$$

$$\varepsilon''(k) = \frac{(y, A''y) - 2\left(y\, [A' - \varepsilon']\, [A - \varepsilon]^{-1}\, [A' - \varepsilon']\, y\right)}{(y, y)},$$

or for $k = 0$:

$$\begin{cases} \varepsilon_i = 0, \\ \varepsilon_i' = 0, \\ \varepsilon_i'' = 2\left(1 - 4\sum_{j \neq i} \dfrac{q_{ij}^2}{h_{jj} - \varepsilon}\right). \end{cases}$$

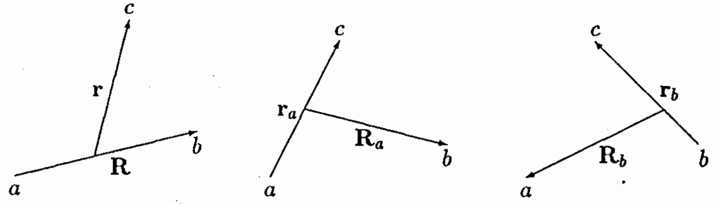

Fig.1 Three sets of Jacobian coordinates of a three-body system.

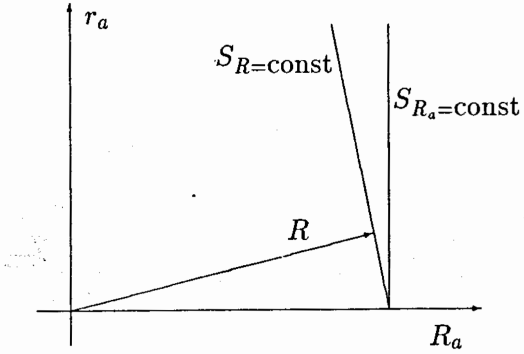

Fig.2 Surfices $S_{R=\text{const}}$ and $S_{R_a=\text{const}}$ in the six-dimensional space with respect to orthogonal coordinates $(\mathbf{R}_a, \mathbf{r}_a)$.

The second derivative of ε should be non-negative. So we get the necessary condition:

$$1 - 4\sum_{j \neq i} \frac{q_{ij}^2}{h_{jj} - \varepsilon} \geq 0,$$

if only the number of thresholds below the interaction energy ε coincides with the number of open channels of the scattering system. It gives a very hard restriction on multiple thresholds (in a case of asymptotic level degeneracy): all q_{ij} connecting different components of multiple level should be equal to zero.

If we substitute for $A'(k)$ its value $2(k + iQ)$, then insert it into the expression for ε':

$$\varepsilon'(k) = \frac{(y, 2\, [k + iQ]\, y)}{(y, y)},$$

and compare it with Eq. (4), we obtain very important relation: the energy of the system as the function of k increases within some interval of values as soon as the respective channel wave function $\bar{\mathbf{c}} \exp ikR$ has a positive balance of particle transfer through some surfice bounded the interaction region right in accordance with Eq. (4). It can be shown

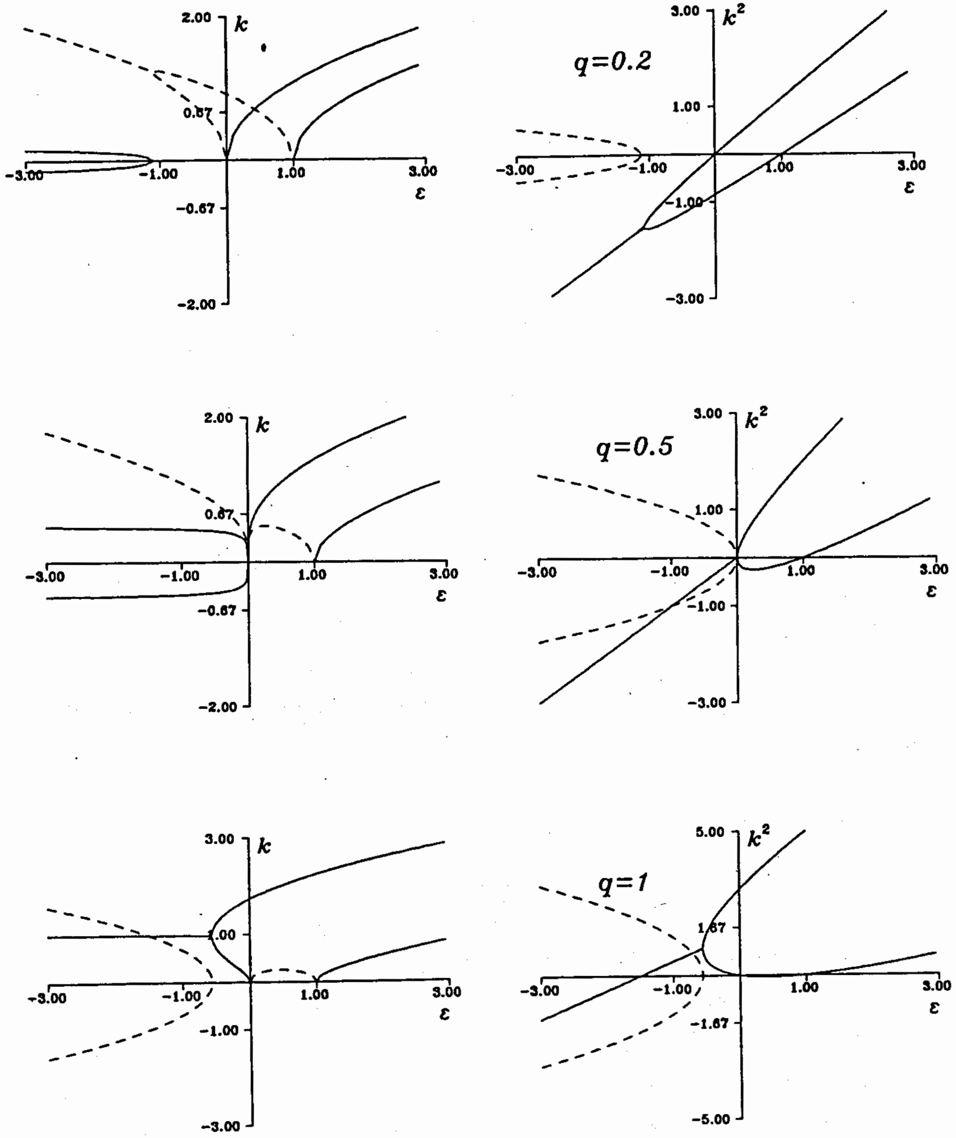

Fig.3-5 Solutions of the determinant equation in a case of two-component radial Schrödinger equation with non-zero asymptotic potential Q for three different values of parameter $q = 0.2, 0.5, 1$. Dashed curve is the imaginary part of a wave number k (left) and its square k^2 (right) respectively.

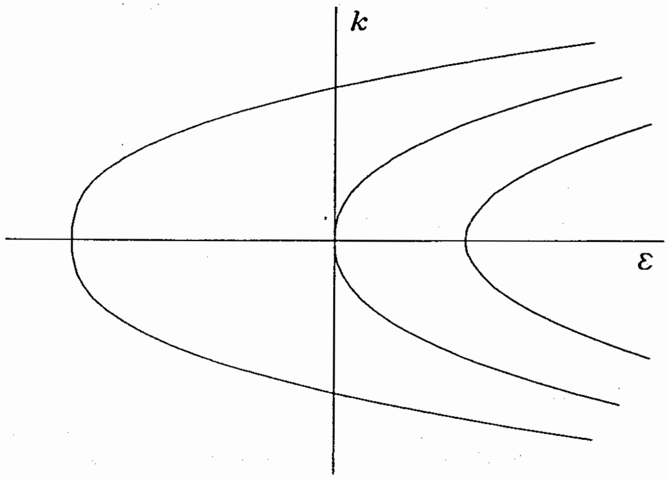

Fig.6 Solutions of the determinant equation (8) as curves on a real (k, ε)-plane.

that for the case of $q = 1$ (Fig.5), one of the open channels corresponding to the positive value of k and placed just below the first threshold (the lower one) has a convergent to the origin flux of particles.

6. Conclusions

Results considered in this paper show that the scattering system with velocity-dependent asymptotic potential has some peculiarities in behaviour comparing to the standard multichannel model. That allows us to hope that they can attract theorists attention to more deep investigation of that kind of systems. In particular, it will be very interesting to find some other physical models beyond the example (2) of this paper which represents in some sense artificial situation due to the truncation of the infinite set of radial Schrödinger equations for the three-body scattering problem.

From the other hand the expansion (2) can be used as the base for the numerical investigation for the three-body low energy scattering processes (including exchange processes). This approach allows to get rid of integral terms in reduced equations. The existence of correlation of basic channels does not complicate the problem very much and can be overcomed numerically very easy. And what is especially attractive that it closely relates to the most elaborated standard closed coupling method[1,2] and achievements of which with slight changes can be applied to the considered approach.

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Многоканальное рассеяние с асимптотическим потенциалом, зависящим от скорости

Исследуются решения системы радиальных уравнений Шредингера

$$\left[-\frac{1}{2M}\frac{d^2}{dR^2} + 2Q(R)\frac{d}{dR} + \mathcal{H}(R)\right]\psi(R) = \epsilon\psi(R)$$

с зависящими от скорости потенциалами. Теория подобных систем удивительно отличается от стандартной теории с локальными потенциалами. Так, если член с первой производной Qd/dR потенциала не исчезает на бесконечности, тогда множество характеристических чисел общего асимптотического решения может содержать комплексные числа с ненулевыми вещественной и мнимой частью одновременно. Более того, число открытых каналов (мы связываем два ограниченных решения, соответствующих вещественному положительному волновому числу k: $\psi_j^{(\pm)}(R) \approx \exp(\pm ik_j R)$ с одним открытым каналом) может превосходить число порогов, лежащих ниже энергии рассеяния. Под порогом мы подразумеваем соответствующее собственное значение h_{jj} $\mathcal{H}$-терма асимптотического потенциала. И наоборот, показано, что число открытых каналов не может быть меньше чем число порогов, удовлетворяющих условию $h_{jj} < \epsilon$. Выписываются граничные условия для многоканального радиального уравнения Шредингера на бесконечности и в некоторой конечной точке R_p.

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The Multi-Channel Scattering with Velocity-Dependent Asymptotic Potentials

Asymptotic solutions for the system of radial Schrödinger equations

$$\left[-\frac{1}{2M}\frac{d^2}{dR^2} + 2Q(R)\frac{d}{dR} + \mathcal{H}(R)\right]\psi(R) = \epsilon\psi(R),$$

with velocity-dependent potentials are investigated. The theory of that kind of systems surprisingly differs from the standard local potential theory. So, if the first derivative term Qd/dR of the potential doesn't vanish at the infinity, the set of characteristic numbers of the common asymptotic solution could contain complex numbers with nonzero real and imaginary parts simultaneously. More over, the number of open channels (we relate two bounded asymptotic solutions corresponding to a real positive wave number k: $\psi_j^{(\pm)}(R) \approx \exp(\pm ik_j R)$, with one open channel) can exceed the number of thresholds lying below the scattering energy. Under threshold we imply the respective eigenvalue h_{jj} of the $\mathcal{H}$ term of the asymptotic potential. Vice versa, it is shown that the number of open channels could not be less than the number of thresholds satisfying the condition: $h_{jj} < \epsilon$. Boundary conditions for the multichannel radial Schrödinger equation at the infinity and some finite point R_p are proposed.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1992