Faddeev equations in one-dimensional problems with resonant interactions

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A problem of three one-dimensional bosons with resonant multichannel interactions is considered. The problem is reduced to a single-channel Faddeev-Lovelace equation by elimination of the closed and output channels. The equation is regularized using algebraic properties of their singularities.

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Introduction

Quasi-one-dimensional (quasi-1D) quantum gases can be formed in prolonged potentials (atom waveguides) whenever the atom energies are much less then the transverse excitation energies and only the ground transverse state is substantially populated. Such gases have been recently realized in 2D optical lattices [1, 2, 3, 4, 5, 6, 7, 8], elongated atomic traps [9, 10, 11, 12, 13, 14], and atomic chips [15, 16, 17, 18, 19]. Properties of quasi-1D gases are drastically different from the 3D ones (see review [20] and the references therein) Under certain conditions quasi-1D gases can be described by the integrable Lieb-Liniger-McGuire (LLMG) model [21, 22, 23] of 1D indistinguishable Bose atoms with zero-range energy-independent interactions. This model has an exact Bethe-ansatz solution and can describe di- and multi-atomic molecules in the case of attractive interactions. However, reflection and dissociation in atom-molecule collisions and three-atomic association are forbidden within the LLMG model. Its high internal symmetry can be lifted in more realistic systems, leading to observable effects of integrability, such as atom-diatom reflection for non-identical atoms [24]. Richer physical phenomena can be provided by resonant interactions.

Resonances in interactions of quasi-1D atoms can arise both from virtual excitation of transverse modes (confinement-induced resonance, or CIR, [25, 26]) and from atomic internal structure (Feshbach resonance, see [27]). Combined effects of Feshbach resonances and CIR on two-atomic systems were analyzed in [28, 29], where parameters of 1D scattering were related to parameters of 3D scattering and harmonic waveguide. Effects of an anharmonic confinement, finite-range interactions, and other additional effects were analyzed in [31, 32, 33, 34, 35, 36].

Resonant interactions can lift integrability already in three-body systems. CIR can lead to atom-diatom reflection [37] (a similar process of atom-soliton reflection was analyzed in [38]) and to thermalization in three-atom collisions [39]. Narrow Feshbach resonances can provide richer physical phenomena, such as association in three-atom collisions, dissociation in atom-diatom collisions [40] and stabilization of Feshbach molecules [41].

An effective approach to three-body problems was developed on the base of Faddeev equations (see books [42, 43] and the references therein). Exact analytical [44, 45] and numerical [46] solutions of Faddeev equations for the LLMG model agree with the Bethe-ansatz solution. Numerical solution of Faddeev-Lovelace equations has been applied in [24] to asymmetric systems and in [47] to 1D systems with generic separable interactions. An equivalent method was used in [37]. An alternative method of numerical solution of the Schrödinger equation in hyperspherical coordinates was applied to 1D problems in [48]. Three-body bound states for resonant interactions were analyzed in [49] using a variational approach.

The present work gives a comprehensive description of the Faddeev approach to 1D problems, generalizing the approach of [40, 41] to multichannel resonant interactions. The second-quantized Hamiltonian for this case is introduced in Sec. I A. Two-body scattering and bound states are analyzed in Sec. I B. Section I C describes the three-body multichannel problem. Asymptotic states and transition amplitudes for this problem are introduced in Sec. I D. Section I E relates the multichannel transition amplitudes to solutions of the Faddeev-Lovelace equation for an effective single-channel problem. Probabilities of bound-bound and bound-free transitions are presented in Sec. I F. Section I G describes special cases of the two-channel system and deactivation problem. The solution method of Faddeev-Lovelace equations is described in Sec. I H. The present regularization procedure is applicable to generic 1D problems with separable interactions. The singularities related to the poles of two-body $T$ matrix, which are similar to the 3D case, are treated here using a generalization of the approach [24]. The present approach also regularizes the singularities of the free-atom Green function, which are different from the 3D case. They appear in the processes of dissociation and association and were not considered in [24]. Derivation of certain properties of resonant two- and three-body models is included in the Appendices.
I. ONE-DIMENSIONAL BOSONS WITH MULTICHLANEL ZERO-RANGE INTERACTIONS

A. Hamiltonian

Consider a gas of 1D Bose atoms described by the annihilation operators $\hat{\Psi}_a(z)$. The model includes several two-body channels described by the annihilation operators $\hat{\Psi}_m(z)$ of molecules with the energies $D_m$. The Hamiltonian of the system has the form (using units with Plank’s constant $\hbar = 1$),

$$\hat{H} = \int dz \left\{ \hat{\Psi}^\dagger_a(z) \left[ -\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{U_a}{2} \hat{\Psi}^\dagger_a(z) \hat{\Psi}_a(z) \right] + \sum_m \hat{\Psi}^\dagger_m(z) \left( -\frac{1}{4m} \frac{\partial^2}{\partial z^2} + D_m \right) \hat{\Psi}_m(z) + \sum_m \left[ \hat{V}_{am}(z) + \hat{V}_{am}^\dagger(z) \right] + \sum_{m \neq m'} \hat{V}_{mm'} \rho(z) \right\}, \quad (1)$$

where $m$ is the atomic mass and $U_a$ is the non-resonant interatomic interaction strength. At negative values of $U_a$ the open channel, formed by two atoms in the initial state $\hat{\Psi}_a$, has a bound state too. The interactions $\hat{V}_{am}(z) = g_m \hat{\Psi}^\dagger_m(z) \hat{\Psi}_a(z)$ couple the open channel to other (molecular) channels and

$$\hat{V}_{mm'}(z) = d_{mm'} \hat{\Psi}^\dagger_m(z) \hat{\Psi}_{m'}(z), \quad d_{m'm} = d_{mm'}^*, \quad (3)$$

couple the molecular channels [the matrix $d_{m'm}$ will be completed by diagonal elements, see Eq. (9) below]. The system with a single molecular state was analyzed in [28, 29], where the one-dimensional parameters were related to the atomic collision and waveguide parameters. Additional molecular states with large negative $D_m$ were introduced in [41].

B. Two-body system

A state vector of the two-atom system can be represented as a superposition of atomic and molecular states,

$$|\Psi_2\rangle = \int dz e^{iPz} \left[ \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} dz \varphi^{(0)}(z) \hat{\Psi}^\dagger_a \left( z - \frac{z}{2} \right) \hat{\Psi}_{a} \left( z + \frac{z}{2} \right) + \sum_m \varphi^{(m)}(z) \hat{\Psi}^{\dagger}_m \right] |\text{vac}\rangle, \quad (4)$$

where $z_c$ and $P$ are the center-of-mass position and momentum, respectively, $z$ is the interatomic distance, and $|\text{vac}\rangle$ is the physical vacuum state. Substitution of the state vector (4) into the Schrödinger equation with the Hamiltonian (1) leads to the coupled equations for the channel functions $\varphi^{(0)}(z)$ and $\varphi^{(m)}$,

$$E\varphi^{(0)}(z) = \left[ -\frac{1}{m} \frac{d^2}{dz^2} + U_a \delta (z) \right] \varphi^{(0)}(z) + \sqrt{2}\delta(z) \sum_m g_m^* \varphi^{(m)} \quad (5)$$

$$E\varphi^{(m)} = D_m \varphi^{(m)} + \sqrt{2}g_m \varphi^{(0)}(0) + \sum_{m' \neq m} d_{m'm'} \varphi^{(m')} \quad (6)$$

Here $E$ is the energy in the center-of-mass system.

The molecular channel functions can be expressed as

$$\varphi^{(m)} = \sqrt{2} \varphi^{(0)}(0) G_m(E), \quad (7)$$

where the vector $G_m$ is a solution of the system of linear equations

$$\sum_{m'} d_{m'm'}(E) G_m(E) = -g_m \quad (8)$$

and the diagonal elements of the matrix $d_{m'm'}(E)$ are defined as

$$d_{mm}(E) = D_m - E - i0. \quad (9)$$
If \( g_m = -\delta_{mm'} \), then \( G_m (E) \) has a physical sense of a Green function, and the infinitesimal imaginary part of \( d_{mm} (E) \) specifies its retarding behavior.

Elimination of the molecular channels leads to a single equation for the open-channel function,

\[
E \varphi^{(0)}(z) = \left[ -\frac{1}{m} \frac{d^2}{dz^2} + U_{\text{eff}} (E) \delta (z) \right] \varphi^{(0)}(z),
\]

where the effective energy-dependent interaction strength

\[
U_{\text{eff}} (E) = U_a + 2 \sum_m g_m^* G_m (E).
\]

incorporates effects of all channels. In the case of a single molecular channel it is reduced to the expression for \( U_{\text{eff}} (E) \) in [28].

Obviously, the wavefunction of a two-body scattering state can be expressed as

\[
\varphi^{(0)}(z) = (2\pi)^{-1/2} \left[ e^{ikz} - i \frac{m}{2k} T_{1D} (k) e^{ik|z|} \right]
\]

in terms of the two-body \( T \) matrix

\[
T_{1D} (k) = \left[ U_{\text{eff}}^{-1} (k^2/m) + i \frac{2mk}{m} \right]^{-1},
\]

which depends on the relative momentum \( k \) of two colliding atoms \( (E = k^2/m) \). \( T_{1D} (k) \) has poles on the positive imaginary axis, \( k = i\kappa_n \), where \( \kappa_n \) are solutions of the equation

\[
\kappa = -\frac{m}{2} U_{\text{eff}} \left( -\frac{\kappa^2}{m} \right).
\]

The poles correspond to two-body bound states (diatoms) with the energies \( E_n = -\kappa_n^2/m \). The diatom states are orthogonal (see App. [A]) and the orthonormality conditions have the form

\[
\int_{-\infty}^{\infty} dz \varphi^{(0)*}_{n'} (z) \varphi^{(0)} (z) + \sum_m \varphi^{(m)*}_{n'} \varphi^{(m)}_{n} = \delta_{nn'}.
\]

Solutions of Eq. (8) can be expressed in terms of \( \det (d) \), the determinant of the matrix \( d_{mm'} (\kappa^2/m) \), which is a polynomial of the degree \( 2M_{\text{mol}} \) in \( \kappa \), and the cofactors \( \partial \det (d) / \partial d_{mm'} \), which are polynomials of the degree \( 2 (M_{\text{mol}} - 1) \) in \( \kappa \) (where \( M_{\text{mol}} \) is the number of the molecular channels). Using Eq. (11), Eq. (14) can be represented then in the polynomial form,

\[
\left( \frac{2}{m} \kappa + U_a \right) \det (d) - \sum_{m,m'} g_{mm'} \frac{\partial \det (d)}{\partial d_{mm'}} g_m^* = 0,
\]

This equation has \( 2M_{\text{mol}} + 1 \) roots (only the real positive roots correspond to the bound states). Thus the energy-dependent interaction can lead to multiple bound states in spite of its zero range. The diatoms are superpositions of the open and molecular channels. The open-channel component can be expressed as

\[
\varphi^{(0)}_{n} (z) = \varphi^{(0)}_{n} (0) \exp (-\kappa_n |z|),
\]

where \( \varphi^{(0)}_{n} (0) \) is determined by the normalization conditions (15), and the open-channel contribution to the bound state is

\[
W_n = \int_{-\infty}^{\infty} dz |\varphi^{(0)}_{n} (z)|^2 = \left( 1 + 2 \sum_m |G_m (E_n)|^2 \kappa_n \right)^{-1}.
\]

Although the present model approximates the molecular-channel states to be infinitesimal in size, the diatoms have finite sizes \( (\sim \kappa_n^{-1}) \).
C. Three-body systems

A system of three atoms is described by the state vector

$$|\Psi_3\rangle = \left[ \frac{1}{\sqrt{6}} \int d^3z \psi^{(0)}(z_1, z_2, z_3) \hat{\Psi}_a^\dagger(z_1) \hat{\Psi}_a^\dagger(z_2) \hat{\Psi}_a^\dagger(z_3) + \sum_m \int dq dz_m \psi^{(m)}(z, z_m) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_m^\dagger(z_m) \right] |\text{vac}\rangle,$$  \tag{19}

leading to the coupled equations for the wavefunctions of the three-atom $\psi^{(0)}(z_1, z_2, z_3)$ and atom-molecule $\psi^{(m)}(z, z_m)$ channels. Their momentum representations, $\tilde{\psi}^{(0)}(q, k)$ and $\tilde{\psi}^{(m)}(q)$, are defined by

$$\psi^{(0)}(z_1, z_2, z_3) = (2\pi)^{-3/2} \int dq_j dk_j \tilde{\psi}^{(0)}(q_j, k_j) \exp \left( i q_j \left( z_j - \frac{z_j' + z_j''}{2} \right) + i k_j \left( z_j' - z_j'' \right) + i P \frac{z_j' + z_j'' + z_j'}{3} \right),$$

$$\psi^{(m)}(z, z_m) = (2\pi)^{-1} \int dq \tilde{\psi}^{(m)}(q) \exp \left( i q (z - z_m) + i P \frac{z + 2z_m}{3} \right),$$ \tag{20}

where $P$ is center-of-mass momentum and $q_j, k_j$ are momenta in any of the three sets of Jacobi coordinates ($j = 1, 2, 3$). The momentum $q_j$ is the relative momentum of the $j$ th atom and the center-of-mass of the $j'$ th and $j''$ th atoms, while $k_j$ is the relative momentum of the $j'$ th and $j''$ th atoms, where $j, j', j''$ are cyclic permutations of 1, 2, and 3. The momenta in different Jacobi coordinate sets are related as

$$q_{j', j''} = -\frac{1}{2} q_j \pm k_j, \quad k_{j', j''} = \pm \frac{3}{4} q_j + \frac{1}{2} k_j.$$ \tag{21}

These relations correspond to permutations of the atoms. In what follows the center-of-mass system ($P = 0$) is used.

The channel wavefunctions in the momentum representation satisfy the following equations

$$E \tilde{\psi}^{(0)}(q_j, k_j) = \left( \frac{3}{4m} q_j^2 + \frac{1}{m} k_j^2 \right) \tilde{\psi}^{(0)}(q_j, k_j) + \frac{U}{2\pi} \sum_{l=1}^3 \int dk'_l \tilde{\psi}^{(0)}(q_l, k'_l) + (3\pi)^{-1/2} \sum_m q_m^* \sum_{l=1}^3 \tilde{\psi}^{(m)}(q_l),$$

$$E \tilde{\psi}^{(m)}(q_j) = \left( \frac{3}{4m} q_j^2 + D_m \right) \tilde{\psi}^{(m)}(q_j) + \left( \frac{3}{\pi} \right)^{1/2} g_m \int dk_j \tilde{\psi}^{(0)}(q_j, k_j) + \sum_{m' \neq m} d_{m'm} \tilde{\psi}^{(m')}(q_j),$$ \tag{22}

where $E$ is the energy in the center-of-mass system. These equations are invariant over transformations \eqref{21} and can describe indistinguishable Bose atoms.

Equations \eqref{22} can be represented in a compact vector form. Consider for the moment distinguishable atoms and introduce the vector wavefunction $\tilde{\psi} = \{ \tilde{\psi}^{(\alpha)} \}$, where $\alpha$ has values 0, m1, m2, and m3 for all $m$. The component $\tilde{\psi}^{(mj)} = \tilde{\psi}^{(m)}(q_j)$ describes the atom-molecule channel with free $j$ th atom. Equations \eqref{22} can be then written out in the form

$$E \tilde{\psi} = \left( \hat{H}_0 + \sum_{l=1}^3 \hat{U}_l \right) \tilde{\psi},$$ \tag{23}

where elements of the matrices $\hat{H}_0$ and $\hat{U}_l$ are defined, respectively, as

$$\hat{H}_0^{\alpha' \alpha} = \left[ \left( \frac{3}{4m} q_j^2 + \frac{1}{m} k_j^2 \right) \delta_{\alpha 0} + \sum_{m,j} \left( \frac{3}{4m} q_j^2 + D_m \right) \delta_{\alpha, mj} \right] \delta_{\alpha' \alpha'},$$ \tag{24}

$$\hat{U}_l^{\alpha' \alpha} \left[ \tilde{\psi}^{(\alpha)} \right] = \left[ \frac{U}{2\pi} \delta_{\alpha 0} + \left( \frac{3}{\pi} \right)^{1/2} \sum_{m,j} g_m \delta_{\alpha', mj} \delta_{lj} \right] \delta_{\alpha 0} \int dk'_l \tilde{\psi}^{(0)}(q_l, k'_l)$$

$$+ \sum_{m,j} \left( (3\pi)^{-1/2} g_m^* \delta_{\alpha' 0} + \sum_{m',j'} d_{m'm} \delta_{\alpha', mj'} \delta_{lj'} \right] \delta_{\alpha, mj} \delta_{lj} \tilde{\psi}^{(mj)}(q_j).$$ \tag{25}
The definition of $\hat{H}_0^{\alpha \beta}$ is unambiguous since the kinetic energy $\frac{1}{2m}q_j^2 + \frac{1}{m}k_j^2$ keeps the same value in the three Jacobi coordinate sets.

The atom-molecule channel wavefunctions can be expressed in terms of the three-atom one,

$$\tilde{\psi}^{(m)}(q_j) = \left(\frac{3}{\pi}\right)^{1/2} G_m \left(E - \frac{3}{4m}q_j^2\right) \int dk_j \tilde{\psi}^{(0)}(q_j, k_j),$$

(26)

where $G_m$ is defined by Eq. (5). Elimination of the atom-molecule channels leads to a single equation for the three-atom wavefunction,

$$E\tilde{\psi}^{(0)}(q_j, k_j) = \left(\frac{3}{4m}q_j^2 + \frac{1}{m}k_j^2\right) \tilde{\psi}^{(0)}(q_j, k_j) + \sum_{l=1}^3 \hat{U}_l^{\text{eff}} \tilde{\psi}^{(0)}(q_l, k_l'),$$

(27)

where the interaction operators are defined as

$$\hat{U}_l^{\text{eff}} \tilde{\psi}^{(0)}(q_l, k_l') = \frac{1}{2\pi} U_{\text{eff}} \left(E - \frac{3}{4m}q_l^2\right) \int dk_l' \tilde{\psi}^{(0)}(q_l, k_l')$$

(28)

with $U_{\text{eff}}$ given by Eq. (11). Elimination of channels and energy-dependent potentials in 3D three-body problems were considered in [50, 51, 52].

However, in three-body problems effects of the eliminated channels extend beyond the interaction strength. The additional effects are analyzed below.

D. Multichannel Faddeev approach

Equation (23) describes a vector three-body problem. Similar scalar problems were extensively studied using Faddeev equations (see books [42, 43]). In line with this approach let us introduce vector functions $\tilde{X}_{0Q}$ and $\tilde{X}_{lpn}$, describing the asymptotic channels. The wavefunction of three free atoms with the momenta $Q_1$, $Q_2$, and $Q_3$, such that $Q_1 + Q_2 + Q_3 = P = 0$, has the form

$$\tilde{X}_{0Q}^{(\alpha)}(q_j, k_j) = \delta_{\alpha 0} \delta(q_j - Q_j) \delta \left(k_j - \frac{Q_{\alpha'} - Q_{\alpha''}}{2}\right)$$

(29)

in each of the Jacobi coordinate sets. The asymptotic function containing the free $l$th atom and a diatom in the state $n$ is

$$\tilde{X}_{lpn}^{(0)}(q_l, k_l) = \delta(q_l - p) \tilde{\varphi}_n^{(0)}(k_l), \quad \tilde{X}_{lpn}^{(mj)}(q_l) = \delta_{lj} \delta(q_l - p) \varphi_n^{(m)},$$

(30)

where $p$ is the relative momentum of the atom and diatom and

$$\tilde{\varphi}_n^{(0)}(k) = \left(\frac{2n^3W_n}{\pi}\right)^{1/2} \frac{1}{k^2 + \kappa_n^2}$$

(31)

is the momentum representation of the two-body wavefunction. The asymptotic functions satisfy the following equations

$$E\tilde{X}_{0Q} = \hat{H}_0 \tilde{X}_{0Q},$$

(32)

$$E\tilde{X}_{lpn} = \left(\hat{H}_0 + \hat{U}_l\right) \tilde{X}_{lpn}$$

where $E = Q^2/(2m)$ in the first equation and $E = 3p^2/(4m) - \kappa_n^2/m$ in the second one.

The elements of the scattering matrix can be expressed as

$$S_{l'n'lpn} = \delta(p' - p) \delta_{nn'} \delta_{ll'} - 2\pi i \delta \left(3\frac{p'^2 - p^2}{4m} - \frac{\kappa_{n'}^2 - \kappa_n^2}{m}\right) X_{l'n'lpn},$$

$$S_{0Q,lpn} = -2\pi i \delta \left(\frac{Q^2}{2m} - 3\frac{p^2}{4m} + \frac{\kappa_n^2}{m}\right) X_{0Q,lpn}$$

(33)
in terms of the transition amplitudes

\[ X_{l'n'p',lnp} = \langle \chi_{l'n'p'} | \sum_{l'' \neq l'} \hat{U}_{l''} | \tilde{\psi}_{lnp} \rangle \]  \tag{34} 

\[ X_{0Q,lnp} = \langle \tilde{\chi}_{0Q} | \sum_{l''=1}^{3} \hat{U}_{l''} | \tilde{\psi}_{lnp} \rangle \]  \tag{35} 

Here the scattering-state solutions \( \tilde{\psi}_{lnp} \) of Eq. (23) have \( \chi_{lnp} \) as the incident wave.

Given energy \( E \) and internal state \( n \), the momentum \( p \) can have values \( \pm p_n \), where

\[ p_n = 2\sqrt{(mE + \kappa_n^2)/3}. \]  \tag{36} 

The bound-bound \( S \) matrix elements can be then represented as

\[ S_{l'n'p',ln \pm p_n} = \delta (p' \mp p_n) \delta_{nn'} \delta_{ll'} - \frac{4\pi im}{3p_{n'}} \left( \delta (p' - p_n) + \delta (p' + p_n) \right) X_{l'n'p',ln \pm p_n}, \]  \tag{37} 

describing transmission and reflection in atom-diatom collisions with possible rearrangement of atoms and change of the diatom internal state.

Indistinguishable Bose atoms are described by the wavefunctions \( \psi^{(0)}(z_1, z_2, z_3) \) which are independent over permutations of each pair of the atomic coordinates \( z_1, z_2, \) and \( z_3 \). Then the momentum-representation wavefunctions \( \tilde{\psi}^{(0)}(q_j, k_j), \tilde{\psi}^{(m)}(q_j) \) are invariant over transformations (21), and the components \( \tilde{\psi}^{(mj)} \) are independent of \( j \). A symmetric scattering-state solution \( \tilde{\psi}_{lnp} = 3^{-1/2} \sum \tilde{\psi}_{lnp} \) is obtained with a symmetrized incident wave \( 3^{-1/2} \sum \chi_{lnp} \) since Eqs. (22) and (23) are invariant over transformations (21). Then a symmetric atom-diatom collision wavefunction in the coordinate representation [see Eq. (20)] has the asymptotic

\[ \psi_{lnp} \sim 3^{-1/2} \sum_{l=1}^{3} \chi_{lnp} - \frac{4\pi im}{3} \sum_{n',j} \frac{1}{p_{n'}} \left( X_{jn,p_n',lnp} X_{jn',p_n,ln} + X_{jn',p_n',lnp} X_{jn,p_n,,ln} \right) \]

\[ -2\pi i \int d^3Q \delta (Q_1 + Q_2 + Q_3) \delta \left( \frac{Q^2}{2m} - E \right) X_{0Q,lnp} \chi_{0Q}, \]  \tag{38} 

where the three terms in the square brackets correspond to the incident wave, transmission-reflection, and dissociation of the diatom, respectively, and \( \chi \) are the coordinate representations of the functions \( \tilde{\chi} \).

E. Effective single-channel problem

Taking into account Eqs. (25) and (30), and expressing \( \tilde{\psi}^{(mj)} \) in terms of \( \tilde{\psi}^{(0)} \) using Eq. (20), one can represent the transition amplitudes in the form of

\[ X_{l'n'p',lnp} = \langle \chi_{l'n'p',lnp} | \sum_{l'' \neq l'} \hat{U}_{l''}^{\text{eff}} | \tilde{\psi}_{lnp}^{(0)} \rangle \]  \tag{39} 

\[ X_{0Q,lnp} = \langle \tilde{\chi}_{0Q} | \sum_{l''=1}^{3} \hat{U}_{l''}^{\text{eff}} | \tilde{\psi}_{lnp}^{(0)} \rangle \]  \tag{40} 

involving only the three-atom components of the wavefunctions. These components are proportional to solutions of the effective single-channel three-body problem with interaction \( \hat{U}_{l}^{\text{eff}} \). Indeed, consider the solution of the scalar equation

\[ E \tilde{\chi}_{lnp}(q_l, k_l) = \hat{R}^{00}_{l} \tilde{\chi}_{lnp}(q_l, k_l) + \hat{U}_{l}^{\text{eff}} \tilde{\chi}_{lnp}, \]  \tag{41} 

of the form

\[ \tilde{\chi}_{lnp}(q_l, k_l) = \left( \frac{2\kappa_n^3}{\pi} \right)^{1/2} \frac{\delta (q_l - p)}{\sqrt{3}q_l^2 + k_l^2 - mE}. \]  \tag{42}
where only the normalization factor depends on $n$ for fixed $p$. The solutions are normalized as $\langle \tilde{\chi}_{n'p} | \tilde{\chi}_{n'p} \rangle = A \delta (p' - p)$, where $A = 1$ for $p = p_n$. Taking into account Eqs. (30), (31), and (36), the wavefunctions in Eq. (39) can be related to the single-channel solutions for an arbitrary diatom state $n = 0$, chosen as the reference state,

$$
\tilde{\chi}^{(0)}_{n'p_n} (q_l, k_l) = \left( \frac{W_n}{\kappa_0} \right)^{1/2} \tilde{\chi}_{n'p_n} (q_l, k_l)
$$

(43)

$$
\tilde{\psi}^{(0)}_{n'p_n} (q_j, k_j) = \left( \frac{W_n}{\kappa_0} \right)^{1/2} \tilde{\psi}_{n'p_n} (q_j, k_j).
$$

Here $\tilde{\psi}_{n'p_n}$ is the scattering-state solution of Eq. (27) with the incident wave $\tilde{\chi}_{n'p_n} (q_l, k_l)$ which is off-shell $|3p_n^2/(4m) + \kappa_0^2/m \neq E|$ for $n \neq 0$. Therefore, all transition amplitudes in Eq. (38) can be related to off-shell amplitudes for the effective single-channel interaction $\hat{U}^{\text{eff}}$ and a single diatom state $n = 0$ as,

$$
X_{n'n'\pm p_n', lnp} = \sqrt{W_n W_n} \frac{(\kappa_0 \kappa_0)}{\kappa_0} \sum_{l' \neq l'} \langle \tilde{\chi}^{(0)}_{n'p_n'} | \hat{U}^{\text{eff}} | \tilde{\psi}^{(0)}_{n'p_n} \rangle
$$

(44)

$$
X_{0Q, lnp} = \left( \frac{W_n}{\kappa_0} \right)^{1/2} \langle \tilde{\chi}^{(0)}_{0Q} | \hat{U}^{\text{eff}} | \tilde{\psi}^{(0)}_{n'p_n} \rangle
$$

(45)

where $\tilde{\chi}^{(0)}_{0Q}$ is the three-atom component only, see Eq. (29). Thus, solutions of the effective single-channel problem (27) provide all necessary information on multichannel scattering.

Equation (27) describes a three-body problem with separable two-body interactions. Following Lovelace (see also books [42, 43] and an adaptation of this approach to 1D problems in [47]), the problem can be reduced to an integral equation

$$
X (q', q_0) = 2Z (q', q_0) + \frac{m^2}{2\kappa_0} \int dq Z (q', q) T_{1D} (k (q)) X (q, q_0)
$$

(46)

for the symmetric transition amplitude

$$
X (q', q) = \sum_{i=1}^{3} \langle \tilde{\chi}^{(0)}_{i'0q'} | \hat{U}^{\text{eff}} | \tilde{\psi}^{(0)}_{i0q} \rangle
$$

(47)

(it is independent of $l'$, see [42, 43, 53]). Here

$$
Z (q', q) = \frac{2\kappa_0^3}{\pi m m E + i0 - q - q' - q'^2}
$$

(48)

is the Green function for three free atoms, expressed in terms of the momenta $q$ in two Jacobi coordinate sets, the two-body $T$ matrix $T_{1D} (k)$ is given by Eq. (19), and the relative momentum of two atoms is expressed in terms of $q$ as

$$
k (q) = \sqrt{mE + i0 - 3q^2/4},
$$

F. Transition probabilities

Identifying the transmission and reflection amplitudes in Eq. (38) and using Eqs. (44) and (46) one can express the reflection and transmission probabilities in terms of the symmetric transition amplitude

$$
p_{\text{ref}}^{n'n} = \frac{16\pi^2 m^2 W_n W_n \kappa_0^3 \kappa_n^3}{9 \kappa_0^3 p_n p_n} |X (-p_n', p_n)|^2
$$

(49)

$$
p_{\text{tran}}^{n'n} = \frac{16\pi^2 m^2 W_n W_n \kappa_0^3 \kappa_n^3}{9 p_n p_n} |X (p_n', p_n)|^2
t\neq n
$$

(50)

$$
p_{\text{tran}}^{nn} = \left| 1 - i \frac{4\pi m}{3p_n} W_n \left( \frac{\kappa_n}{\kappa_0} \right)^3 X (p_n, p_n) \right|^2
$$
Atom-diatom collisions can also result in dissociation of the diatom. This process is described by the last term in Eq. \([38]\). However, the total dissociation probability is related to probabilities of other processes as

\[
P_{n}^{\text{diss}} = 1 - \sum_{n'} \left( P_{n'n}^{\text{tran}} + P_{n'n}^{\text{ref}} \right). \tag{50}
\]

Diatoms can be formed in three-atom collisions. The probability of association per unit time can be found, like in the 3D case \([34]\), from the equation

\[
u_{n}^{\text{assoc}} (Q) = 2\pi \int \frac{Ld\rho}{2\pi} |\langle Q | \sum_{l=1}^{3} \hat{U}_l | n, p \rangle|^2 \delta \left( \frac{3p^2}{4m} - \frac{k_n^2}{m} - E \right). \tag{51}
\]

Here

\[
|Q\rangle = \frac{2\pi}{L} 6^{-1/2} \sum_{\Pi} \hat{\chi}_{\Pi} (Q)
\]

is the wavefunction of three free atoms with momenta \(Q_1, Q_2,\) and \(Q_3, (Q_1 + Q_2 + Q_3 = 0)\), and the energy is \(E = Q^2 / (2m)\). The wavefunction \(\psi_{n}(Q)\) is normalized per unit in the box of the length \(L\) and symmetrized over all 6 possible permutations \(\Pi (Q)\) of the momenta \(Q_i\). The wavefunction of the interacting atom and diatom in the state \(n\),

\[
|n, p\rangle = \left( \frac{2\pi}{3L} \right)^{1/2} \sum_{l=1}^{3} \psi_{lnp},
\]

has the box normalization too and is symmetrized over the atom permutations.

In the system of \(N_{\text{at}}\) atoms with momenta \(Q_i\) the rate of formation of molecules in the state \(n\) can be evaluated by summation over all trios

\[
\frac{dN_n}{dt} = \sum_{1 \leq i_1 < i_2 < i_3 \leq N_{\text{at}}} \nu_{n}^{\text{assoc}} \left( Q_{i_1} - \frac{Q_{i_1} + Q_{i_2} + Q_{i_3}}{3}, Q_{i_2} - \frac{Q_{i_1} + Q_{i_2} + Q_{i_3}}{3}, Q_{i_3} - \frac{Q_{i_1} + Q_{i_2} + Q_{i_3}}{3} \right) . \tag{54}
\]

Replacing the summation by integration with the atomic momentum distribution \(f_{\text{at}} (Q)\), one obtains the rate equation for the molecular density \(\rho_n = n_n / L\),

\[
\frac{d\rho_n}{dt} = \rho_{\text{at}}^3 \int d^3Q K_{3n} \left( Q_1 - \frac{Q_1 + Q_2 + Q_3}{3}, Q_2 - \frac{Q_1 + Q_2 + Q_3}{3}, Q_3 - \frac{Q_1 + Q_2 + Q_3}{3} \right) f_{\text{at}} (Q_1) f_{\text{at}} (Q_2) f_{\text{at}} (Q_3) , \tag{55}
\]

where \(\rho_{\text{at}} = N_{\text{at}} / L\) is the atomic density and

\[
K_{3n} (Q_1, Q_2, Q_3) = \frac{L^2}{3!} \nu_{n}^{\text{assoc}} (Q_1, Q_2, Q_3)
\]

\[
= \frac{2\pi^2 m^3 \kappa^3}{9\kappa_0^6 \rho_n} W_n \left[ \sum_{j=1}^{3} T_{1D} (k (Q_j)) X (Q_j, p_n) |^2 + \sum_{j=1}^{3} T_{1D} (k (Q_j)) X (Q_j, -p_n) |^2 \right] \tag{56}
\]

is the association rate coefficient. [Here \(p_n\) is given by Eq. \([36]\) and \(Q_1 + Q_2 + Q_3 = 0\) again.] This expression is derived using Eqs. \([51], [52], [53], [55], [44]\), and the general relation between bound-free and bound-bound transition amplitudes (see \([42, 43]\)).

\[
\langle \chi_{0Q} | \sum_{l''=1}^{3} \hat{U}_{l''r}^{\text{eff}} | \tilde{\psi}_{l''p_n} \rangle = - \frac{m}{2} (2\pi \kappa_{0}^2)^{-1/2} \sum_{j=1}^{3} T_{1D} (k (Q_j)) \langle \chi_{0Q} | \sum_{l'' \neq j}^{3} \hat{U}_{l''r}^{\text{eff}} | \tilde{\psi}_{l''p_n} \rangle \tag{57}
\]

The rate coefficient \([56]\) is defined according to conventional chemical notation and is three times larger then the \(K_3\) used in \([20, 40]\).
G. Special cases

1. Two-channel case

In this case \[10\], when only one molecular channel \((m = c)\) is present, the vector \(G_m (E)\) contains only one element,

\[
G_c (E) = \frac{g_c}{E + i0 - D_c}.
\]

Therefore, the effective interaction strength is

\[
U_{\text{eff}} (E) = U_a + \frac{2|g_c|^2}{E + i0 - D_c}
\]

and Eq. (10) for the poles of \(T_{1D}\) is reduced to the cubic equation \[28, 49\]

\[
\kappa^3 + \frac{m}{2} U_a \kappa^2 + m D_c \kappa + \frac{1}{2} m^2 D_c U_a - m^2 |g_c|^2 = 0.
\]

It has two positive roots \(\kappa_{0,1}\) whenever \(U_a < 0\) and \(D_c < 2|g_c|^2 / U_a\), and one positive root \(\kappa_0\) otherwise. The open-channel contributions to the corresponding bound states are \[29\],

\[
W_n = \frac{\kappa_n^2 + m D_c}{3 \kappa_n^2 + m U_a \kappa_n + m D_c}.
\]

2. Deactivation case

The general problem with multiple molecular channels can be substantially simplified in the case when one of the molecular channels, the closed channel \((m = c)\), is coupled to all other channels, while other molecular channels, the deactivation products \((m \in \{d\})\), are not mutually coupled \((d_{dd'} = 0, d \neq d')\). In this case the effective interaction strength can be expressed as

\[
U_{\text{eff}} (E) = U_a + 2 \sum_d \frac{|g_d|^2}{E + i0 - D_d} + 2 \left(|g_c|^2 + g_c^* \sum_d \frac{d_{cd} g_d}{E + i0 - D_d} \right) \left(E + i0 - D_c - \sum_d \frac{|d_{cd}|^2}{E + i0 - D_d} \right)^{-1}.
\]

If the deactivation product states lie far below the open channel threshold, i.e. \(D_d < 0\) and

\[
|D_d| > \max(|d_{cd}^2 / D_c|, |g_d d_{cd} / g_c|, |g_d^2 / U_a|, |E|, |D_c|, m U_a^2),
\]

the effective interaction strength is approximately the same as in the two-channel case \[59\], and Eq. (14) has roots which are approximately determined by the same cubic equation \[60\].

Equation (14) also has roots

\[
\kappa_d \approx \sqrt{m |D_d|},
\]

one per each deactivation product state. The open-channel contributions to the corresponding bound states are

\[
W_d \approx \frac{1}{2} \sqrt{m |g_d|^2 |D_d|}^{-3/2}.
\]

The rate coefficient for deactivation of the diatom state \(n\) onto all states \(\{d\}\) can be expressed, using Eqs. (49), (65) and \[C3\], as

\[
K_{2n} = \frac{3 \gamma_n}{2m} \sum_d \left(P_{d \rightarrow n}^{\text{ref}} + P_{d \rightarrow n}^{\text{tran}}\right) \sum_{\{d\}} |\gamma_{ad} \psi_n(0) (0,0,0) + \gamma_{cd} \psi_n(0) (0,0,0)|^2,
\]

where the coefficients \(\gamma_{ad}\) and \(\gamma_{cd}\) are expressed as

\[
\gamma_{ad} = \left(\frac{3^4 5^4 m}{|D_d|^5}\right)^{1/4} |g_d| U_a, \quad \gamma_{cd} = 2 \left(\frac{3^3 m}{|D_d|^5}\right)^{1/4} |g_d| g_c^*
\]

(67)
and the symmetric wavefunctions
\[
\psi^{(0)}_{npn}(0,0,0) = \frac{\sqrt{3}W_n\kappa_n}{2\pi} \left[ 1 + \frac{im^2\kappa_n}{4\kappa_0^2} \int dq \frac{T_{1D}(k(q))X(q, pn)}{k(q)} \right]
\]
(68)
\[
\psi^{(c)}_{npn}(0,0,0) = - \frac{mg_e}{\pi} \frac{W_n\kappa_n}{2} \left[ \frac{1}{\kappa_n^2 + mD_e} + \frac{m\kappa_n}{2\kappa_0^3} \int dq \frac{T_{1D}(k(q))X(q, pn)}{U_e(k^2(q) - mD_e) + 2mg_e^2} \right]
\]
are calculated with the symmetric transition amplitudes \( X(q, pn) \) and the two-body \( T \) matrix \( T_{1D}(k) \) for the two-channel case (see App. [3]).

II. REGULARIZATION OF ONE-DIMENSIONAL FADEEV-LOVELACE EQUATIONS

The previous section demonstrates that a solution of Eq. (45) provides all necessary information for evaluation of transition probabilities. This equation is a particular case of the general Lovelace equation (see [42, 43, 47, 53]) for separable potentials \( Vv^*(z)\tilde{v}(z') \), where the energy lies above the lowest bound state, \( E > m\kappa_0^2 + 2 \) [see Eq. (39)]. The free Green function \( Z(q', q) \) has singularities at \( q = q_n \pm (q_n') \) and \( k(q_n) = -q_n/2 \pm k(q_n') \), where the function \( k(q) \) is given by Eq. (48). Since \( q' \) and \( k(q) \) are the momenta and \( k \) in one of the Jacobi coordinate systems, Eq. (21) allows to recognize \( q_{n\pm}(q') \) as the momenta \( q_n \) in other systems, where the atoms are permuted. Therefore the poles correspond to non-diffractive collisions where the momenta keep their values and are only exchanged by the atoms. Then the transformations \( q_{n\pm}(q_n'(q')) \) can lead only to one of the two solutions \( q_0^+ \), \( q_0^-(q') \), and \( q_0^- \). This property will be used below (see Tab. [1]). Since they lie outside of the real axis for \( q' = \pm p_n \), the singularities of \( Z(q', q) \) play a role only in the case when \( q' \) corresponds to three free atoms. In the source term \( Z(q', q_0) \) of Eq. (45) the singularities can appear only when both \( q' \) and \( q_0 \) correspond to three free atoms. However, the present work does not deal with this case of free-free transitions. Unlike the 3D case, where a partial wave expansion leads to logarithmic singularities of \( Z(q', q) \), in the present 1D case they are simple poles.

For further derivation let us introduce dimensionless variables. Convenient energy and momentum scales are based on \( g \), a characteristic value of the channel coupling strengths \( g_m \). The dimensionless momentum and energy are expressed as
\[
\zeta = \frac{\sqrt{3}}{2} (mg)^{-2/3} q, \quad \epsilon = m^{-1/3} g^{-4/3} E.
\]
(70)
An introduction of new functions in place of the transition amplitude, the free Green function, and the two-body \( T \) matrix,
\[
F(\zeta, \zeta_0) = -\frac{\pi}{\sqrt{3}} m^{7/3}g^{4/3} \kappa_0^{-3} \sqrt{\epsilon + i0 - \zeta^2} X(q, q_0)
\]
(71)
\[
S(\zeta', \zeta) = -\frac{2\pi}{\sqrt{3}} m^{7/3}g^{1/3} \kappa_0^{-3} \sqrt{\epsilon + i0 - \zeta'^2} Z(q', q) = \frac{1}{\zeta - \zeta + (\zeta') - \zeta - \zeta - (\zeta')}
\]
(72)
\[
r(\zeta) = -\frac{m^{1/3}}{2\pi g^{2/3}} (\epsilon + i0 - \zeta^2)^{-1/2} T_{1D}(k(q)) = -\frac{1}{2\pi} \left( \tilde{U}^{-1}_{\text{eff}} \sqrt{\epsilon + i0 - \zeta^2 + \frac{i}{2}} \right)
\]
(73)
allows to exclude the square-root singularity from \( X(q, q_0) \). Here
\[
\zeta_{\pm} (\zeta) = -\frac{1}{2} \zeta \pm \frac{\sqrt{3}}{2} \sqrt{\epsilon + i0 - \zeta^2}, \quad \tilde{U}_{\text{eff}} = m^{1/3} g^{-2/3} U_{\text{eff}}.
\]
(74)
Equation (45) is transformed then to the form

$$F (\zeta', \zeta_0) = S (\zeta', \zeta_0) + \int_{-\infty}^{\infty} d\zeta S (\zeta', \zeta) r (\zeta) F (\zeta, \zeta_0).$$  

(75)

### A. Singularities of the free Green function

According to Eq. (72), $S (\zeta', \zeta)$ has simple poles on the real axis whenever $\zeta'^2 \leq \epsilon$. The pole contributions can be separated using the symbolic expression

$$\frac{1}{\zeta - \zeta_0 - i0} = \text{v.p.} \frac{1}{\zeta - \zeta_0} + i\pi \delta (\zeta - \zeta_0),$$

leading to the integral equation

$$F (\zeta', \zeta_0) - i\pi r (\zeta) F (\zeta', \zeta_0) - i\pi r (\zeta') F (\zeta', \zeta_0) = \frac{1}{\zeta_0 - \zeta_+} - \frac{1}{\zeta_0 - \zeta_-} + \int_{-\infty}^{\infty} d\zeta \text{v.p.} \left( \frac{1}{\zeta - \zeta_+} - \frac{1}{\zeta - \zeta_-} \right) r (\zeta) F (\zeta, \zeta_0).$$

(77)

Here $\zeta_{\pm} = \zeta_{\pm} (\zeta')$, symbol v.p. means Cauchy principal value integral in the vicinity of $\zeta_{\pm}$, and the source term is non-singular for the problems considered here, as it was mentioned above. The following derivation is based on the algebraic properties of the transformation $\zeta_{\pm} (\zeta)$. A direct calculation of products of these transformations (see Tab. II) demonstrates that $\zeta_{\pm} (\zeta_{\pm})$ leads again to one of the three values $\zeta', \zeta_+, \text{ or } \zeta_-$. Therefore, replacement $\zeta'$ by $\zeta_+$ or by $\zeta_-$ in Eq. (77) leads to two additional linear equations in $F (\zeta', \zeta_0)$, $F (\zeta_+, \zeta_0)$, and $F (\zeta_-, \zeta_0)$. Then they form a system of linear equations with the matrix

$$A = \begin{pmatrix}
\frac{1}{\zeta_0 - \zeta_+} & -i\pi r (\zeta_+) & -i\pi r (\zeta_-) \\
-i\pi r (\zeta') & \frac{1}{\zeta_0 - \zeta_-} & -i\pi r (\zeta_-) \\
-i\pi r (\zeta') & -i\pi r (\zeta_+) & 1
\end{pmatrix}.$$  

(78)

Solution of this system leads to the integral equation in $F (\zeta', \zeta_0)$

$$F (\zeta', \zeta_0) = S (\zeta', \zeta_0) + \int_{-\infty}^{\infty} d\zeta \text{v.p.} S (\zeta', \zeta) r (\zeta) F (\zeta, \zeta_0).$$

(79)

Here

$$S (\zeta', \zeta) = \left\{ \begin{array}{ll}
\frac{s_+}{\zeta - \zeta_+} + \frac{s_-}{\zeta - \zeta_-} & \zeta' \leq \sqrt{\epsilon} \\
\frac{s_0}{\zeta - \zeta_0} & \zeta' > \sqrt{\epsilon}
\end{array} \right.$$  

(80)

and the parameters $s$, $s_+$, and $s_-$ are expressed as

$$s = (A^{-1})_{12} \text{sign} (\zeta' + \sqrt{\epsilon}/2) + (A^{-1})_{13} \text{sign} (\zeta' - \sqrt{\epsilon}/2)$$  

$$s_+ = (A^{-1})_{11} - (A^{-1})_{13} \text{sign} (\zeta' - \sqrt{\epsilon}/2)$$  

$$s_- = - (A^{-1})_{11} - (A^{-1})_{12} \text{sign} (\zeta' + \sqrt{\epsilon}/2)$$  

(81)

in terms of the inverted matrix $A^{-1}$. 

---

**TABLE I: Algebraic properties of transformations $\zeta_{\pm}$**

| $\zeta' < -\sqrt{\epsilon}/2$ | $\zeta' > \sqrt{\epsilon}/2$ | $\zeta_+ (\zeta')$ | $\zeta_- (\zeta')$ | $\zeta_+ (\zeta')$ | $\zeta_- (\zeta')$ |
|-----------------------------|-----------------------------|------------------|------------------|------------------|------------------|
| $\zeta' < -\sqrt{\epsilon}/2$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ |
| $-\sqrt{\epsilon}/2 < \zeta' < \sqrt{\epsilon}/2$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ |
| $\zeta' > \sqrt{\epsilon}/2$ | $\zeta_+ (\zeta')$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ | $\zeta_+ (\zeta')$ | $\zeta'$ |

---
B. Singularities of two-body $T$ matrix

Following derivation is a generalization of the approach \cite{24} to the case of multiple bound states. Since $r (ζ)$ is an even function of $ζ$ [see Eq. (73)] and $S (−ζ', ζ) = S (ζ', −ζ)$ (this property can be directly proven), the equations for the odd and even components,

$$F_\pm (ζ, ζ_0) = F (ζ, ζ_0) \pm F (−ζ, ζ_0),$$  \hspace{1cm} (82)

can be separated as

$$F_\pm (ζ', ζ_0) = \bar{S}_\pm (ζ', ζ_0) + \int_0^\infty dζ \text{ v.p.} \bar{S}_\pm (ζ', ζ) r (ζ) F_\pm (ζ, ζ_0),$$  \hspace{1cm} (83)

where

$$\bar{S}_\pm (ζ', ζ) = \bar{S} (ζ', ζ) \pm \bar{S} (−ζ', ζ).$$  \hspace{1cm} (84)

The odd and even component in 1D scattering are analogs of 3D partial waves \cite{55}.

Equations (83) still contain singularities related to poles of $r (ζ)$ at $ζ = ζ_n + i0$, where $ζ_n = \frac{\sqrt{3} \pi}{2} (mg)^{2/3} p_n$. In the pole vicinity the function $r (ζ)$ has the limiting behavior

$$r (ζ) \sim \frac{-ir_n}{ζ - ζ_n - i0^+}, r_n = i \text{ Res } (r (ζ), ζ = ζ_n) = \frac{1}{π} \frac{\kappa_n^2}{m^{1/3} g^{2/3}} \frac{W_n}{ζ_n}$$  \hspace{1cm} (85)
[see Eqs. (12) and (73)]. The contributions of the singularities can be separated using Eq. (76) leading to the regularized equations

$$F_\pm (ζ', ζ_0) = \bar{S}_\pm (ζ', ζ_0) + \pi \sum_n r_n \bar{S}_\pm (ζ', ζ_n) F_\pm (ζ_n, ζ_0) + \text{ v.p.} \int_0^\infty dζ \bar{S}_\pm (ζ', ζ) r (ζ) F_\pm (ζ, ζ_0),$$  \hspace{1cm} (86)

where the Cauchy principal value integral is taken for all singularities in $\bar{S}_\pm (ζ', ζ)$ and $r (ζ)$.

Source terms in these equations have forms of linear combinations of the functions $\bar{S}_\pm (ζ', ζ_n)$ (for the problems under consideration $ζ_0$ is equal to one of $ζ_n$). Thus the solution can be expressed as a linear combination

$$F_\pm (ζ', ζ_0) = \bar{F}_\pm (ζ', ζ_0) + \pi \sum_n r_n F_\pm (ζ_n, ζ_0) \bar{F}_\pm (ζ', ζ_n)$$  \hspace{1cm} (87)

of solutions $\bar{F}_\pm (ζ', ζ_0)$ of integral equations

$$\bar{F}_\pm (ζ', ζ_n) = \bar{S}_\pm (ζ', ζ_n) + \text{ v.p.} \int_0^\infty dζ \bar{S}_\pm (ζ', ζ) r (ζ) \bar{F}_\pm (ζ, ζ_n),$$  \hspace{1cm} (88)

where the source terms do not contain unknown functions. Solving of these equations also allows the evaluation of the values of $F_\pm$ at specific points, $F_\pm (ζ_n, ζ_0)$, involved into Eq. (87). They are determined by the system of linear algebraic equations

$$F_\pm (ζ_n, ζ_0) = -\pi \sum_n r_n \bar{F}_\pm (ζ_n, ζ_n') F_\pm (ζ_n', ζ_0) = \bar{F}_\pm (ζ_n, ζ_0)$$  \hspace{1cm} (89)

which are obtained by setting $ζ' = ζ_n$ in Eqs. (87).

Conclusions

Multichannel resonant interactions can be described by a model involving one atomic and several molecular states. Even in the case of zero-range interactions this model predicts several two-body bound states (diatoms), which are superpositions of two-atomic and molecular components. Orthogonality of the diatom wavefunctions is proven.
In three-body problems the multichannel behavior leads both to an effective energy-dependent interactions and multichannel asymptotic wavefunctions. The last effect leads to rescaling of the probabilities of elastic and inelastic atom-diatom collisions and of three-atom association. All the probabilities can be expressed in terms of the symmetric transition amplitude for an effective single-channel problem. This amplitude can be evaluated as a solution of the Faddeev-Lovelace equation. Singularities in this equation can be regularized using their algebraic properties.

The algorithm of solution of a resonant 1D three-body problem consists then of the following steps:

1. functions $F_\pm (\zeta, \zeta_n)$ are determined as solutions of the regularized integral equations (63) for each bound state $n$;
2. the system of linear equations (69) is solved for $F_\pm (\zeta_n, \zeta_0)$;
3. $F_\pm (\zeta, \zeta_0)$ is calculated by using of Eq. (87);
4. $X (q, q_0)$ is determined using Eqs. (71) and (82);
5. transition probabilities are evaluated using Eqs. (49), (56), (66) and (68).

APPENDIX A: ORTHOGONALITY OF THE DIATOM STATES

Integration of Eqs. (5) and (10) over an infinitesimal interval including $z = 0$ allows to represent them in the forms

\[
\frac{1}{m} \hat{p} \varphi^{(0)} = U_n \varphi^{(0)} (0) + \sqrt{2} \sum_m g_m \varphi^{(m)} \tag{A1}
\]

\[
\frac{1}{m} \hat{p}_n \varphi^{(0)} = U_{\text{eff}} (E_n) \varphi^{(0)} (0), \tag{A2}
\]

where the wavefunction derivative discontinuity operator $\hat{\varphi}$ acts as

\[
\hat{\varphi} = \frac{\partial \varphi}{\partial z} \big|_{z=0+0} - \frac{\partial \varphi}{\partial z} \big|_{z=0-0}. \tag{A3}
\]

Equations (A1) and (A2) allow to prove the identity relation involving wavefunctions of two diatom states, $n$ and $n'$,

\[
\varphi_n^{(0)*} (0) \frac{1}{m} \hat{p}_n \varphi_n^{(0)} + E_n \sum_m \varphi_{n'}^{(m)*} \varphi_n^{(m)} = \varphi_n^{(0)*} (0) \frac{1}{m} \hat{p}_{n'} \varphi_n^{(0)} + E_{n'} \sum_m \varphi_{n'}^{(m)*} \varphi_n^{(m)}. \tag{A4}
\]

Multiplication of Eq. (10) for $\varphi_n^{(0)}$ by $\varphi_n^{(0)*}$ with following subtraction of the complex conjugate of the similar product with exchanged $n$ and $n'$ leads to the following expression

\[
(E_n - E_{n'}) \varphi_n^{(0)*} (z) \varphi_n^{(0)} (z) = - \frac{1}{m} \frac{\partial}{\partial z} \left[ \varphi_n^{(0)*} (z) \frac{\partial}{\partial z} \varphi_n^{(0)} (z) - \varphi_n^{(0)} (z) \frac{\partial}{\partial z} \varphi_n^{(0)*} (z) \right] + \delta (z) [U_{\text{eff}} (E_n) - U_{\text{eff}} (E_{n'})] \varphi_{n'}^{(0)*} (0) \varphi_n^{(0)} (0) \tag{A5}
\]

Integrating this expression from $-\infty$ to $\infty$ and using Eqs. (A4) and (A2) one gets the equation

\[
(E_n - E_{n'}) \int_{-\infty}^{\infty} dz \varphi_n^{(0)*} (z) \varphi_n^{(0)} (z) + \sum_m \varphi_{n'}^{(m)*} \varphi_n^{(m)} = 0. \tag{A6}
\]

It leads to the orthogonality conditions (13) for non-degenerate states, while the degenerate states can be always orthogonalized by a simple linear transformation.

APPENDIX B: RESIDUES OF THE TWO-BODY T MATRIX

For scattering on a generic potential $\hat{U}$, the two-body $T$ matrix, as a function of the collision energy $E$, has poles at the bound state energies $E_n$ with the residues

\[
\text{Res} (T_{1D}, E = E_n) = \hat{U} |\varphi_n\rangle \langle \varphi_n| \hat{U}. \tag{B1}
\]

In the present case $\hat{U} = U_{\text{eff}} (E) \delta (z)$ and the bound state wavefunction is given by Eq. (17). Taking into account Eqs. (13) and (18) one obtains

\[
\text{Res} (T_{1D} (k), k = ik_n) = -2i \frac{k_n^2}{m} W_n. \tag{B2}
\]
APPENDIX C: RELATIONS BETWEEN TRANSITION AMPLITUDES IN THE TWO-CHANNEL AND DEACTIVATION CASES

The three-body asymptotic functions $\tilde{\chi}_{ldp_d}(q_i, k_i)$, corresponding to the deactivation product channels, are obtained by substitution of Eqs. (63) and (50) into Eq. (42). For large $|D_d|$ they are approximately independent of the momentum $k_i$,

$$\tilde{\chi}_{ldp_d}(q_i, k_i) \approx \left(\frac{2}{\pi \kappa_d}\right)^{1/2} \delta(q_i - p_d)$$

(C1)

(this means that sizes of the deactivation-product bound states are negligibly small compared to other relevant scales). The transition amplitude (34) can be then transformed, using Eqs. (25) and (43), to the form

$$X_{ldp_d, lnp_n} \approx \frac{1}{2\pi} \left(\frac{2W_d}{\pi \kappa_d}\right)^{1/2} \int dk_{\nu} \sum_{l' \neq l''} U_a \int dk_{l''} \tilde{\psi}_m^{(0)}(q_{l''}, k_{l''}) + 2 \left(\frac{\pi}{3}\right)^{1/2} g_c^* \tilde{\psi}_m^{(c)}(q_{l''})$$

(C2)

where $n = 0, 1$ and $\tilde{\psi}^{(0,c)}_{lnp_n}$ are solutions of the two-channel problem, which does not involve deactivation product states. Changing the integration variable $k_{l''}$ by $q_{l''}$ allows us to recognize in the integrals the coordinate-representations of the open and closed channel wavefunctions [see Eq. (20)] in the origin. Finally, the symmetric transition amplitude (40) involving the deactivation product states can be expressed using Eq. (41) as

$$X(\pm p_d, p_n) = 3 \left(\frac{3}{W_n \kappa_n}\right)^{1/2} \left[ U_a \psi^{(0)}_{lnp_n}(0, 0, 0) + \frac{2}{3} g_c^* \psi^{(c)}_{lnp_n}(0, 0) \right]$$

(C3)

in terms of the values at the origin of the symmetric wavefunctions in the two-channel case

$$\psi^{(0)}_{lnp_n}(0, 0, 0) = 3^{-1/2} \sum_{l=1}^{3} \psi_{lnp_n}(0, 0, 0) = \left(\frac{W_n}{3}\right)^{1/2} (2\pi)^{-3/2} \sum_{l=1}^{3} \int dq_j dk_j \tilde{\psi}_{lnp_n}(q_j, k_j)$$

(C4)

$$\psi^{(c)}_{lnp_n}(0, 0, 0) = 3^{-1/2} \sum_{l=1}^{3} \psi_{lnp_n}(0, 0, 0) = \left(\frac{W_n}{\pi}\right)^{1/2} g_c \sum_{l=1}^{3} \int dq_j \frac{dk_j}{E + i0 - q_j^2 + i(4m)} \tilde{\psi}_{lnp_n}(q_j, k_j)$$

[see Eqs. (20), (28), and (58)].

These values can be also expressed in terms of the symmetric transition amplitude for the two-channel case in the following way. Let us write out the Lippmann-Schwinger equation for the effective single-channel problem

$$\tilde{\psi}_n^{(c)}(q_j, k_j) = \tilde{\chi}_{n}(q_j, k_j) \delta_{j0} + \left(E + i0 - \hat{H}_0^{00} - \hat{U}_j^{eff}\right)^{-1} \sum_{l' \neq j} \hat{U}_{n}^{eff} \tilde{\psi}_{l'}^{(c)}$$

(C5)

Here the Green function for the free $j$th atom and diatom is the integral operator

$$\left(E + i0 - \hat{H}_0^{00} - \hat{U}_j^{eff}\right)^{-1} \tilde{\psi} = \psi_0(q_j, k_j) \int dk'_j \left[ \delta(k'_j - k_j) + \frac{1}{2\pi} T_{1D}(k (q_j)) \right] \psi_0(q_j, k'_j)$$

(C6)

expressed in terms of the two-body $T$ matrix (13) and the Green function for three free atoms,

$$g_0(q, k) = \left[E + i0 - \frac{3}{4m} q^2 - \frac{1}{m} k^2\right]^{-1}$$

(C7)

The incident wave $\tilde{\chi}_{lnp}(q, k)$ [see Eq. (42)] is proportional to $g_0(q, k)$ (it is a general property of separable potentials, see (12) (43)). Substitution of $\psi$ given by Eq. (C5) into Eq. (C4) allows to express the integrals in Eq. (C4) in terms of the transition amplitudes for the effective single-channel problem. Some algebra leads to the values of symmetric wavefunctions (58).

[1] M. Greiner, I. Bloch, O. Mandel, T. W. Hänsch, and T. Esslinger, Phys. Rev. Lett. 87, 160405 (2001).
