Multi-Channel Computations in Low-Dimensional Few-Body Physics

Vladimir S. Melezhik

Bogoliubov Laboratory of Theoretical Physics,
Joint Institute for Nuclear Research, 141980 Dubna, Russian Federation
melezhik@theor.jinr.ru
http://theor.jinr.ru/~melezhik/

Abstract. In this lecture I give a brief review of low-dimensional few-body problems recently encountered in attempting a quantitative description of ultracold atoms and molecules confined in 2D and 1D optical lattices. Multi-channel nature of these processes has required the development of special computational methods and algorithms which I discuss here as well as the most interesting results obtained with the offered computational technique and future perspectives.

Key words: optical trap, ultracold atoms, Feshbach resonance, confinement-induced resonance, few-body problem, Schrödinger equation, scattering problem, discrete variable representation, boundary-value problem, splitting-up method

1 Introduction

Recent advances in physics of ultracold quantum gases have opened a unique opportunity to study of low-dimensional quantum systems (see, for example [1,2]). In experiments with ultracold atoms and molecules the particle motion is “frozen” along one or two variables by using the optical potential and its dynamics is limited to a plane or a line. In this case, the physical properties of the low-dimensional system can be dramatically altered under the action of the optical trap. Moreover, one can effectively manage interatomic interactions by varying the parameters of the trap. This opens up new possibilities for studying strongly correlated quantum systems [1], few-body and many-body effects in low-dimensional systems [2,3], new mechanisms of molecule formation [4], and possible elements for quantum computer [1].

The simplest example of few-body systems, a quantum two-body system, acquires in a confined geometry of a 1D trap unique properties as compare to the conventional two-body problem in a 3D free space [12]. Confining of the motion in the transversal directions leads to transverse quantization of the motion and makes the pair collisions in a 1D trap essentially multichannel ones. Possible transverse excitation energies of the particle define the channel thresholds for the scattering in the trap. Depending on the initial conditions, the parameters of the trap and the interatomic interaction, different multichannel effects may
occur at pair atomic collisions in the 1D confining trap. It is a confinement-induced resonance (CIR) defined for zero-energy limit when the ground state energy threshold of the colliding pair coincides with the resonance in the closed transverse channel [5,6], transverse excitations/deexcitations during the collision [7], center-of-mass effects [8,9,10], a new mechanism for molecule formation [11], a CIR-splitting in anisotropic traps [12], anharmonicity effects [10], and three-body effects [2].

A quantitative description of the mentioned effects has demanded to develop new computational methods that we consider in the next section. Some results obtained with the elaborated computational techniques are briefly discussed in the section 3. Concluding remarks are given in the last section 4.

2 Methods

2.1 Quantum Two-Body Problem in Confined Geometry of 1D Harmonic Trap

The collisional dynamics of two distinguishable atoms with coordinates \( r_1, r_2 \) and masses \( m_1, m_2 \) moving in the harmonic waveguide with the transverse potential \( \frac{1}{2} \sum_i m_i \omega_i^2 \rho_i^2 \) (\( \rho_i = r_i \sin \theta_i \)) is described by the 4D time-dependent Schrödinger equation (\( \hbar = 1 \))

\[
i \frac{\partial}{\partial t} \psi(\rho_R, r, t) = H(\rho_R, r) \psi(\rho_R, r, t)
\]

with the Hamiltonian

\[
H(\rho_R, r) = H_{CM}(\rho_R) + H_{rel}(r) + W(\rho_R, r) .
\]

(1)

Here

\[
H_{CM} = -\frac{1}{2M} \bigg( \frac{\partial^2}{\partial \rho_R^2} + \frac{1}{\rho_R^2} \frac{\partial^2}{\partial \phi^2} + \frac{1}{4 \rho_R^2} \bigg) + \frac{1}{2} \left( m_1 \omega_1^2 + m_2 \omega_2^2 \right) \rho_R^2
\]

(2)

and

\[
H_{rel} = -\frac{1}{2 \mu} \frac{\partial^2}{\partial r^2} + \frac{L^2(\theta, \phi)}{2 \mu r^2} + \mu^2 \left( \frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2} \right) \rho^2 + V(r)
\]

(3)

describe the center-of-mass (CM) and relative atomic motions. The potential \( V(r) \) describes the atom-atom interaction, \( \rho_R \) and \( r = r_1 - r_2 \rightarrow (r, \theta, \phi) \rightarrow (\rho, \phi, z) \) are the polar radial CM and the relative coordinates and \( M = m_1 + m_2, \mu = m_1 m_2 / M \). The term \( \frac{L^2(\theta, \phi)}{2 \mu r^2} = -\frac{1}{2 \mu r^2} \sin^2 \theta \left( \frac{\partial^2}{\partial \theta^2} \sin \theta + \frac{\partial^2}{\partial \phi^2} \right) \) represents the angular part of the kinetic energy operator of the relative atomic motion.

The term

\[
W(\rho_R, r) = \mu (\omega_1^2 - \omega_2^2) r \rho_R \sin \theta \cos \phi
\]

(4)

in the Hamiltonian (1) leads for two distinguishable atoms that feel different confining frequencies \( \omega_1 \neq \omega_2 \) to a coupling of the CM and relative atomic
motion, i.e. to the nonseparability of the quantum two-body problem in confined geometry of the 1D harmonic trap. The problem is to integrate the Schrödinger equation from time \( t = 0 \) to the asymptotic region \( t \to +\infty \) with the initial wave-packet

\[
\psi(\rho_R, r, t = 0) = N r \sqrt{\rho_R} \exp\left\{-\frac{\rho_R^2}{2a_1^2} - \frac{r^2}{2a_z^2} - \frac{(z - z_0)^2}{2a_z^2} + ik_0 z\right\}
\]

representing two different noninteracting atoms in the transversal ground state of the waveguide with \( a_i = (1/m_i\omega_i)^{1/2} \) and the overall normalization constant \( N \) defined by \( <\psi(0)|\psi(0)> = 1 \). We choose \( z_0 \to -\infty \) to be far from the origin \( z = 0 \) and \( a_z \to \infty \) to obtain a narrow width in momentum and energy space for the initial wave-packet. The wave-packet moves with a positive interatomic velocity \( v_0 = k_0/\mu = \sqrt{2\epsilon_0/\mu} \) (defined by the longitudinal colliding energy \( \epsilon_0 \)) to the scattering region at \( z = 0 \) and splits up after the scattering into two parts moving in opposite directions \( z \to \pm \infty \). If the initial conditions permit opening inelastic channels it can lead to the collisional excitation of the transverse vibrations [7] or formation of molecular bound states [11]. Multichannel character of the scattering is also developing at the region of the CIR where resonance in the closed channel leads to the resonant behaviour of the elastic scattering amplitude if the initial colliding energy coincides with the resonant energy of molecular state in the closed channel [6,9,7].

The modeling of the interatomic interaction \( V(r) \) was discussed in [6,9,11].

2.2 Discretization of the Angular-Subspace: 2D Nondirect Product Discrete Variable Representation

For discretization of the angular part in (1) we apply the 2D nondirect discrete variable representation [13,14,15]. For 1D quantum problems discrete variable representation (DVR) was suggested in [16] and broadly applied in the quantum chemistry computations [17]. However, it happened that the attempts to extend this approach for the case of more higher dimensions as a direct product of 1D DVRs were not so efficient [17,18]. In 1997 we have suggested a 2D nondirect product DVR (NDDVR) in application to the time-dependent 3D Schrödinger equation describing hydrogen atom in a laser field of arbitrary polarization [13,14]. The method happened to be very efficient in application to different few-dimensional quantum problems [16,19,20,21]. Mathematical aspects of the 2D NDDVR were discussed recently in [18].

In the 2D NDDVR we seek for the time-dependent solution \( \psi(\rho_R, r, t) \) of the problem (1-5) according to the expansion [13,15,9]

\[
\psi(\rho_R, r, \Omega, t) = \sum_{j=1}^{N} f_j(\Omega) \psi_j(\rho_R, r, t)
\]

with respect to the two-dimensional basis

\[
f_j(\Omega) = \sum_{\nu=1}^{N} Y_\nu(\Omega) (Y^{-1})_{\nu j}
\]
associated with a mesh $\Omega_j = (\theta_{j\theta}, \phi_{j\phi})$. For the $\theta$ variable, the $N_\theta$ mesh points $\theta_{j\theta}$ correspond to the zeros of the Legendre polynomial $P_{N_\theta}(\cos \theta_{j\theta}) = 0$. For the $\phi$ variable, the $N_\phi$ mesh points are chosen as $\phi_{j\phi} = \pi(2j\phi - 1)/N_\phi$. The total number $N = N_\theta \times N_\phi$ of grid points $\Omega_j = (\theta_{j\theta}, \phi_{j\phi})$ is equal to the number of basis functions in the expansion (6) and the number of terms in the definition (7), where the symbol $\nu$ represents the twofold index $\{l, m\}$ and the sum over $\nu$ is equivalent to the double sum

$$
\sum_{\nu=1}^{N} \sum_{m=-N_\theta}^{N_\theta-1} \sum_{l=|m|}^{N-1} \nu
$$

The $l$ and $m$ indexes show the number of zeros over $\theta$ and $\phi$ variables of the polynomials $Y_\nu(\Omega)$ which we specify in the next paragraph. Due to the definition (8) the values $N_\theta$ may be chosen only odd. $N_\phi$ can take on arbitrary values. The coefficients $(Y^{-1})_{\nu j}$ in the definition (7) are the elements of the $N \times N$ matrix $Y^{-1}$ inverse to the matrix given by the values $Y_{\nu \mu} = Y_\nu(\Omega_j)$ of the polynomials $Y_\nu(\Omega)$ at the grid points $\Omega_j$. It is clear that $f_j(\Omega_j) = \delta_{j j'}$ at such definition (i.e. the basis (7) belongs to the class of Lagrange functions [22]) and the coefficients $\psi_j(\rho_R, r, t)$ in the expansion (6) are the values of the searching solution $\psi(\rho_R, r, t)$ at the points of angular grid $\Omega_j$: $\psi_j(\rho_R, r, t) = \psi(\rho_R, r, \Omega_j, t)$.

The polynomials $Y_\nu(\Omega)$ in Eq.(7) are chosen as

$$
Y_\nu(\Omega) = Y_{\ell m}(\Omega) = e^{im\phi} \sum_{\nu} C_l^{\mu} \times P_l^{\nu}(\theta),
$$

where $C_l^{\mu} = \delta_{l \nu}$ holds in general, and thus $Y_\nu(\Omega)$ coincides with the usual spherical harmonic with a few possible exceptions for large values of $\nu$ such that we receive the orthogonality relation

$$
\int Y_\nu^*(\Omega)Y_{\nu'}(\Omega)d\Omega \approx \sum_j \lambda_j Y_{\nu j}^* Y_{\nu' j} = \delta_{\nu \nu'}
$$

for all $\nu$ and $\nu' \leq N$. Here the $N$ weights $\lambda_j$ are the standard Gauss-Legendre weights multiplied by $2\pi/N_\phi$. For most $\nu$ and $\nu'$ the above relation is automatically satisfied because the basis functions $Y_\nu(\Omega)$ are orthogonal and the Gaussian quadrature is exact. For these $\nu$ we have $C_l^{\mu} = \delta_{l \nu}$ in Eq.(9). However, in a few cases involving the highest $l$ values, some polynomials $P_l^{\nu}(\theta)$ have to be orthogonalized in the sense of the Gaussian quadrature ($C_l^{\mu} \neq \delta_{l \nu}$ for these specific values of $l$). With this choice, the matrix $S_{\nu \mu} = \lambda_j^{1/2} Y_{\nu j}$ is orthogonal.

The basis in the form (7) was initially introduced in [23] for the one-dimensional angular space $\Omega = \theta$. The fact, that values of the searching wave function $\psi(\rho_R, r, t)$ at the grid points of the 2D angular space $\psi(\rho_R, r, \Omega_j, t) = \psi_j(\rho_R, r, t)$ are utilized in the 2D NDDVR, drastically simplifies the calculations as compared to the usual partial-wave analysis.
2.3 Splitting-up Method for 4D Time-Dependent Schrödinger Equation

It is an attractive feature of the 2D NDDVR (6-10) that for the grid representation \( f_j(\Omega) \) the only nondiagonal part of the Hamiltonian (1) is the angular part of the kinetic energy operator (see Eqs. (2,3))

\[
\frac{1}{2\mu r^2} L^2(\theta, \phi) - \frac{1}{2M \rho^2_R} \frac{\partial^2}{\partial \rho^2} \sum_{\nu} \left( \frac{1}{2} \right) \sum_{\nu} \frac{N}{Y_{\nu} (\Omega)} (Y_\nu^{-1})_{\nu'} \mid_{\nu=\nu_j} = \\
\sum_{\nu} Y_{\nu}^\dagger \left( \frac{l(l+1)}{2\mu r^2} + \frac{m^2}{2M \rho^2_R} \right) (Y_\nu^{-1})_{\nu'}
\]

which can be diagonalized by the simple unitary transformation \( S_{j\nu} = \lambda_j^{1/2} Y_{\nu} \). This property has been exploited for developing an efficient algorithm with a computational time scaling proportional to the number \( N = N_\theta \times N_\phi \) of unknowns in the system of equations [14].

For the propagation \( \psi_j(\rho_R, r, t_n) \rightarrow \psi_j(\rho_R, r, t_{n+1}) \) in time \( t_n \rightarrow t_{n+1} = t_n + \Delta t \) we have developed a computational scheme [9] based on the component-by-component split-operator method suggested by G.I. Marchuk in 1971 [24]. The Hamiltonian in (11) permits the splitting into the following three parts

\[
H_{jj'}(\rho_R, r) = h_{jj'}^{(0)}(\rho_R) + h_{jj'}^{(1)}(r) + U_j(\rho_R, \rho) \delta_{jj'}
\]

where

\[
h_{jj'}^{(0)}(\rho_R) = -\frac{\delta_{jj'} \rho^2}{2M \rho^2_R} + \frac{1}{4\rho^2_R} + \frac{1}{2M \rho^2_R \sqrt{\lambda_j \lambda_{j'}}} \sum_{\nu} (Y_{\nu}^{-1})_{\nu'} m^2 (Y_\nu^{-1})_{\nu'} ,
\]

\[
h_{jj'}^{(1)}(r) = -\frac{\delta_{jj'} \rho^2}{2\mu \rho_R} + \delta_{jj'} V(r) - \frac{1}{2\mu r^2} \frac{\partial}{\partial r} \sqrt{\lambda_j \lambda_{j'}} \sum_{\nu} (Y_{\nu}^{-1})_{\nu'} l(l+1)(Y_\nu^{-1})_{\nu'} ,
\]

\[
U_j(\rho_R, \rho) = \frac{1}{2} (m_1 \omega_1^2 + m_2 \omega_2^2) \rho^2_R + \frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2} \rho^2 + \mu(\omega_1^2 - \omega_2^2) \rho_R \cos \phi_j .
\]

Subsequently we can approximate the time-step \( \psi_j(\rho_R, r, t_n) \rightarrow \psi_j(\rho_R, r, t_{n+1}) \) where \( t_n \rightarrow t_{n+1} = t_n + \Delta t \) according to

\[
\psi(t_n + \Delta t) = \exp(-i \Delta t \hat{U}) \exp(-i \Delta t \hat{h}^{(1)}) \exp(-i \Delta t \hat{h}^{(0)}) \times \exp(-i \Delta t \hat{U}) \psi(t_n) + O(\Delta t^3) .
\]
The time evolution proceeds as follows. For the first and the last steps according to the relation (13) we write the function $\psi$ and the operators $\exp(-i\Delta t\hat{U}/2)$ in our 2D NDDVR (7) on the 2D grid $\Omega_j = \{\theta_j, \phi_j\}$. Since the potential $U_j(\rho_R, \rho)$ is diagonal in this representation the first and last steps represent simple multiplications of the diagonal matrices $\exp(-i\Delta tU_j(\rho_R, \rho))$. Two intermediate steps in (13) depending on $\hat{h}^{(0)}$ and $\hat{h}^{(1)}$ are treated in the basis $Y_{\nu}^{(9)}$ where the matrix operators $\hat{h}^{(0)}(\rho_R)$ and $\hat{h}^{(1)}(\rho)$ are diagonal with respect to the indices $m$ and $l$. For that we approximate the exponential operators according to

$$\exp(-i\Delta t\hat{A}) \approx (1 + \frac{i}{2}\Delta t\hat{A})^{-1}(1 - \frac{i}{2}\Delta t\hat{A}) + O(\Delta t^2), \quad (14)$$

which ensures the desired accuracy of the numerical algorithm (13). Thus, after the discretization of $r$ (or $\rho_R$) with the help of finite-differences the matrix $\hat{A}$ possesses a band structure and we arrive at the following boundary-value problems

$$(1 + \frac{i}{2}\Delta t\hat{A})\psi(t_n + \frac{\Delta t}{4}) = (1 - \frac{i}{2}\Delta t\hat{A})\psi(t_n),$$

which can be solved rapidly due to the band structure of the matrix $\hat{A}$. This computational scheme is unconditionally stable \[24\], preserves unitarity and is very efficient, i.e. the computational time is proportional to the total number $N$ of grid points over the radial and angular variables \[14\]. The efficiency of the computational procedure is based on the fast transformation with help of the unitary matrix $S_j \nu = \lambda_j^{1/2} Y_{\nu}$ between the two relevant representations: the 2D NDDVR (7) and the $Y_{\nu}$-representation (9).

### 2.4 2D Multichannel Scattering Problem as Boundary-Value Problem

In the case of the pair collisions of two identical atoms in harmonic trap the problem reduces to scattering of a single effective particle with the reduced mass $\mu$, off a scatterer $V(r)$ at the origin, under transverse harmonic confinement with frequency $\omega (\hbar = 1)$ \[7\]

$$\left[-\frac{1}{2\mu} \nabla^2 + \frac{1}{2} \mu \omega^2 \rho^2 + V(r)\right] \psi(r) = \epsilon \psi(r). \quad (15)$$

Here the energy of the relative two-body motion $\epsilon = \epsilon^{(n,m)}_{\perp} + \epsilon_{||}$ is a sum of the transverse $\epsilon^{(n,m)}_{\perp}$ and longitudinal collision $\epsilon_{||}$ energies. Due to our definition of the confining potential, the transverse excitation energies $\epsilon^{(n,m)}_{\perp}$ can take the possible values $\epsilon^{(n,m)}_{\perp} = \epsilon - \epsilon_{||} = \omega(2n + |m| + 1) > 0$ of the discrete spectrum of the 2D oscillator $\frac{1}{4} \mu \omega^2 \rho^2$.

The problem was in integration of the 3D stationary Schrödinger equation (15) with the scattering asymptotic conditions

$$\psi_{n,m}(r) = e^{ik_n z} \phi_{n,m}(\rho, \varphi) + \sum_{n'=0}^{n_o} f_{n'n} e^{ik_{n'} z} \phi_{n', m}(\rho, \varphi) \quad (16)$$
at $|z| \to +\infty$ and finding the unknown matrix elements $f_{nn'}$ of the scattering amplitude, which describe transitions between the initial $n$ and final $n'$ channels of scattering. The quantum numbers $n$ of the two-dimensional harmonic oscillator denote the transversal excitations/deexcitations $n \leftrightarrow n'$ of colliding atoms. In addition to the quantum number $n$ the asymptotic scattering state is defined also by the momentum $k_n$ of the channel

$$k_n = \sqrt{2\mu \epsilon \parallel}.$$  

The energy $\epsilon$ defines the number $n_o$ of open channels in (16), where the longitudinal collision energy must be positive $\epsilon \parallel = \epsilon - \epsilon^{(n,m)}_{\perp} > 0$.

It is clear that the scattering amplitude depends also on the index $m$, however, remains unchanged during the collision due to the axial symmetry of the problem. Hereafter we consider only the case $m = 0$ and the index is omitted in the following. Due to the axial symmetry of the interactions in (15) we separate the $\phi$-variable and reduce the problem to 2D one in the variables $(r, \theta)$ (or $(z, \rho)$).

First, we discretize the 2D Schrödinger equation (15) on a 2D grid of angular $\{\theta_j\}_{j=1}^{N_\theta}$ and radial $\{r_j\}_{j=1}^{N_r}$ variables. The angular grid points $\theta_j$ are defined as the zeroes of the Legendre polynomial $P_{N_\theta}(\cos \theta)$ of the order $N_\theta$. Using the completeness property of the normalized Legendre polynomials which remains valid also on the chosen angular grid

$$\sum_{l=0}^{N_\theta-1} P_l(\cos \theta_j) P_l(\cos \theta_{j'}) \sqrt{\lambda_j \lambda_{j'}} = \delta_{jj'},$$

(17)

where $\lambda_j$ are the weights of the Gauss quadrature, we expand the solution of equation (15) in the basis $f_j(\theta) = \sum_{l=0}^{N_\theta-1} P_l(\cos \theta)(P^{-1})_{lj}$ according to

$$\psi(r, \theta) = \frac{1}{r} \sum_{j=1}^{N_\theta} f_j(\theta) u_j(r).$$

(18)

Here $P^{-1}$ is the inverse of the $N_\theta \times N_\theta$ matrix $P$ with the matrix elements defined as $P_{lj} = \sqrt{\lambda_j} P_l(\cos \theta_j)$. Due to this definition one can use the completeness relation (17) in order to determine the matrix elements $(P^{-1})_{lj}$ as $(P^{-1})_{lj} = \sqrt{\lambda_j} P_l(\cos \theta_j)$. It is clear from (18) that the unknown coefficients $u_j(r)$ in the expansion are the values $\psi(r, \theta_j)$ of the two-dimensional wave function $\psi(r, \theta)$ at the grid points $\theta_j$ multiplied by $\sqrt{\lambda_j} r$. Near the origin $r \to 0$ we have $u_j(r) \approx r \to 0$ due to the definition (18) and the demand for the probability distribution $|\psi(r, \theta_j)|^2$ to be bounded. Substituting (18) into (15) results a system of $N_\theta$ Schrödinger-like coupled equations with respect to the $N_\theta$-dimensional unknown vector $u(r) = \{\lambda_j^{1/2} u_j(r)\}_{j=1}^{N_\theta}$

$$[H^{(0)}(r) + 2(\epsilon I - V(r))]u(r) = 0,$$

(19)
where

\[ H^{(0)}_{j'j}(r) = \frac{d^2}{dr^2} \delta_{j'j} - \frac{1}{r^2} \sum_{l=0}^{N_\theta-1} P_{jl}(l+1)(P^{-1})_{lj'} , \] (20)

\[ V_{j'j}(r) = V(r, \theta_j) \delta_{j'j} = \{V(r) + \frac{1}{2} \omega^2 \rho_j^2 \} \delta_{j'j}, \quad \rho_j = r \sin \theta_j , \] (21)

and \( I \) is the unit matrix. We solve the system of equations (19) on the quasi-uniform radial grid (13)

\[ r_j = R \frac{e^{\gamma x_j}}{e^\gamma - 1}, \quad j = 1, 2, ..., N \] (22)

of \( N \) grid points \( \{r_j\} \) defined by mapping \( r_j \in [0, R \rightarrow +\infty] \) onto the uniform grid \( x_j \in [0, 1] \) with the equidistant distribution \( x_j - x_{j-1} = 1/N \). By varying \( N \) and the parameter \( \gamma > 0 \) one can choose more adequate distributions of the grid points for specific interatomic and confining potentials.

By mapping the initial variable \( r \) in Eq. (19) onto \( x \) we obtain

\[ [H^{(0)}(x) + 2(eI - V(r(x)))] u(r(x)) = 0 , \] (23)

with

\[ H^{(0)}_{j'j}(x) = f^2(x) \delta_{j'j} \left( \frac{d^2}{dx^2} - \gamma \frac{d}{dx} \right) - \frac{1}{r^2(x)} \sum_{l=0}^{N_\theta-1} P_{jl}(l+1)(P^{-1})_{lj'} , \] (24)

where

\[ f(x) = \frac{e^\gamma - 1}{Re^{\gamma x}} . \] (25)

The uniform grid with respect to \( x \) gives 6-order accuracy for applying a 7-point finite-difference approximation of the derivatives in the equation (23). Thus, after the finite-difference approximation the initial 2D Schrödinger equation (15) is reduced to the system of \( N \) algebraic matrix equations

\[ \sum_{p=1}^{3} \delta_{j-p}^l u_{j-p} + [\delta_{j}^l + 2(eI - V_j)] u_j + \sum_{p=1}^{3} \delta_{j+p}^l u_{j+p} = 0 , \quad j = 1, 2, ..., N - 3 \]

\[ u_j + \alpha_j^{(1)} u_{j-1} + \alpha_j^{(2)} u_{j-2} + \alpha_j^{(3)} u_{j-3} + \alpha_j^{(4)} u_{j-4} = g_j \quad j = N-2, N-1, N \] (26)

where each coefficient \( \delta_{j}^l \) is a \( N_0 \times N_0 \) matrix, each \( \alpha_j^l \) is a diagonal \( N_0 \times N_0 \) matrix and each \( g_j \) is a \( N_0 \)-dimensional vector. Here the functions \( u_{-3}, u_{-2}, u_{-1} \) and \( u_0 \) in the first three equations of the system (for \( j = 1, 2 \) and 3) are eliminated by using the “left-side” boundary conditions: \( u_0 = 0 \) and \( u_{-j} = u_j \) (\( j = 1, 2, 3 \)). The last three equations in this system for \( j = N, N-1 \) and \( N-2 \) are the “right-side” boundary conditions approximating at the edge points \( r_{N-2}, r_{N-1} \) and \( r_N = R \) of the radial grid, the scattering asymptotics (16) for the desired wave function \( u(r_j) \). In order to construct the “right-side” boundary conditions (20) at \( j = N-2, N-1 \) and \( N \) we used an idea of ref. (23) i.e.
the asymptotic behaviour \(16\) at the edge points \(r_{N-2}, r_{N-1}\) and \(r_N = R\) are considered as a system of vector equations with respect to the unknown vector \(f_{nn'}\) of the scattering amplitude for a fixed \(n\). By eliminating the unknowns \(f_{nn'}\) from this system we implement the “right-side” boundary conditions defined by Eqs.\(26\) at \(j = N - 2, N - 1\) and \(N\).

The reduction of the 2D multi-channel scattering problem to the finite-difference boundary value problem \(26\) permits one to apply efficient computational methods. Here we use the LU-decomposition \(26\) or sweep method \(27\), which is a fast implicit matrix algorithm. The block-diagonal structure of the matrix of the coefficients in the system of equations \(26\) with the width of the diagonal band equal to \(7 \times N_\theta\) makes this computational scheme an efficient one.

Solving the problem \(26\) for the defined initial vector \(k_n\) and a fixed \(n\) from the possible set \(0 \leq n \leq n_e\) we first calculate the vector function \(\psi(k_n, r, \theta_j)\). Then, by matching the calculated vector \(\psi(k_n, R, \theta_j)\) with the asymptotic behaviour \(16\) at \(r = R\), we calculate the \(n\)-th row of the scattering amplitude matrix \(f_{nn'}\) describing all possible transitions \(n \rightarrow n' = 0, 1, ..., n_e\). This procedure is repeated for the next \(n\) from \(0 \leq n \leq n_o\) and over upon calculating all the elements \(f_{nn'}\) of the scattering amplitude.

3 Some Results

In this section we briefly discuss some of the most interesting results obtained with the developed computational methods.

3.1 Resonant molecule formation in harmonic waveguides

In our work \([11]\) it was shown that the quantum dynamics of the coupled center-of-mass and relative motion for two different colliding atoms in a harmonic trap exhibits a resonant formation process of ultracold molecules. With the developed splitting-up method (section 2.3), permitting to treat quantitatively the collision in the 4D configuration space \((\rho_R, r, \theta, \phi)\), we have analyzed in detail the quantum dynamics of the process and demonstrated the existence of a novel mechanism for the resonant formation of polar molecules. The origin of this effect is the confinement-induced mixing \(4\) of the relative and center-of-mass motions in the atomic collision process leading to a coupling of the diatomic continuum to center-of-mass excited molecular states in closed transverse channels. The process is illustrated by Fig.1 where the probability density distribution averaged over the angular variables \(W(\rho_R, r, t) = \int |\psi(\rho_R, r, \theta, \phi, t)|^2 (\rho_R^{-1}) \sin \theta d\theta d\phi\) is given as a function of time. For \(\omega_1 \neq \omega_2\) (different atoms “feel” different frequencies \(\omega_1\) and \(\omega_2\) in the trap) we observe that a considerable part of the scattered wave-packet (see the probability density distribution \(W(\rho_R, r, t)\) at \(t = 8t_0\)) is located near origin \(r = 0\) after the collision and corresponds to a molecular bound state with excitation of the molecular center-of-mass. It is first excited state with respect to the center-of-mass motion what is indicated by the node
Fig. 1. Time evolution of the probability density distribution averaged over the angular variables \( W(\rho_R, r, t) = \int |\psi(\rho_R, r, \theta, \phi, t)|^2 (r^2 \rho_R)^{-1} \sin \theta d\theta d\phi \). (a) For the waveguide with \( \omega_1/2 = \omega_2 = 0.02 \) (b) for \( \omega_1 = \omega_2 = 0.02 \). For \( t = 8t_0 \) corresponding to a time after the collision the insets show a more detailed view of \( W \) on the scales \( 0 \leq W \leq 8 \times 10^{-7} \) corresponding to the continuum part of the wave-packet. \( \epsilon = 0.004 \), time is given in units of \( t_0 = \pi/\omega_2 \).
of the density distribution $W$ at the point about $\rho_R \simeq 3$. Note, that during collision at $t \sim 3t_0$ the main part of the wave-packet is temporarily in the ground state, decays thereafter rapidly into the continuum but part of it goes into the excited molecular state. In contrast to this the case $\omega_1 = \omega_2$ in Fig.1b (the case of the center-of-mass separation) shows an almost complete decay the molecular ground state into the continuum: The remaining minor part of the probability density distribution near $r = 0$ representing the molecular part is much smaller compared to the case $\omega_1 \neq \omega_2$.

It was also shown that the molecular formation probabilities can be tuned by changing the trap frequencies $\omega_1$ and $\omega_2$ characterizing the transverse modes of the atomic species in the trap.

## 3.2 Multichannel Scattering and Confinement-Induced Resonances

![Fig. 2. The total transmission coefficients $T$ for bosonic collisions as a function of the dimensionless energy $\varepsilon = (\epsilon - \omega)/\omega$ for the two cases of the system being initially in (a) the ground transverse state $n = 0$ and (b) the first excited transverse state $n = 1$, for several ratios of $a_s/a_\perp$ and $\omega = 0.002$. The black solid curve corresponds to $a_s/a_\perp = 0.68$ for which the zero-energy CIR in the single-mode regime is encountered [5].](image)

The grid method for integration of the 2D multichannel scattering problem as a boundary-value problem (section 2.4) was applied to extensively analyze the transverse excitations and deexcitations as well as resonant scattering processes at pair atomic collisions in harmonic waveguides [7]. Collisions of identical bosonic and fermionic as well as distinguishable atoms in harmonic traps with a single frequency $\omega$ permitting the center-of-mass separation were explored in depth. In the zero-energy limit and single mode regime the well-known CIRs
Fig. 3. The probability density $|\psi(x, z)|^2$ for bosonic collisions as a function of $x$ and $z$ at $a_x/a_\perp = +4.39$ for two cases of the single-mode regime (left subfigures with $\varepsilon < 1$) and two-mode regime (right subfigures with $1 < \varepsilon < 2$). The corresponding transmission values $T$ are also indicated. All subfigures are for $\omega = 0.002$ and $n = 0$. The inset shows a more detailed view of $|\psi(x, z)|^2$ near the origin $z = x = 0$. 
for bosonic [5,6], fermionic [28] and heteronuclear [8,29] collisions were reproduced. In case of the multi-mode regime up to four open transverse channels were considered. Important scattering observable in the quasi-1D scattering is the transmission coefficient $T_\epsilon(\epsilon) = \sum_{n'} |\delta_{nn'} + f_{nn'}|^2$.

Fig. 2 illustrates the behaviour of the transmission $T$ with varying energy $\epsilon$ (permitting opening of the four lowest channels during the collision) and scattering length $a_s/a_\perp$ (here $a_s$ is the scattering length in the 3D free space and $a_\perp = \sqrt{1/(\mu \omega)}$ is the width of the trap). In Fig. 3 the probability density distribution $|\psi(x,z)|^2$ calculated as a function of the the transverse ($x$) and longitudinal ($z$) variables is given. Here the case $T = 0$ illustrates the appearing of the CIR in the scattering. The dual CIR [8,29] leading to a complete quantum suppression of atomic scattering was also analyzed in multi-channel regimes and possible applications were discussed.

4 Conclusion

In this lecture the computational methods have been considered which were elaborated for a quantitative analysis of multichannel effects in low-dimensional few-body systems. The efficiency of the methods was demonstrated in applications for different quantum dynamics of two-body atomic collisions in harmonic 1D traps. It is very promising further development of these approaches in applications to hot problems of the few-body physics in confined geometry of optical traps. Thus, the description of the effects of anisotropy and anharmonicity of the traps as well as strong anisotropy in the interparticle interactions (scattering of polar molecules) requires an extension to the increasing number of spatial variables. Progress in this direction also opens up new possibilities for a quantitative analysis of more complex low-dimensional few-body systems.

References

1. Pitaevskii, L.P.: Bose-Einstein Condensates in a Laser Radiation Field. Phys. Uspekhi 49, 333–351 (2006)
2. Chin, C., Grimm, R., Julienne, P., Tiesinga, E.: Feshbach Resonances in Ultracold Gases. Rev. Mod. Phys. 82, 1225–1286 (2010)
3. Bloch, I., Dalibard, J., Zwerger, W.: Many-Body Physics with Ultracold Gases. Rev. Mod. Phys. 80, 885–964 (2008)
4. Kohler, I., Goral, K., Julienne, P.S: Production of Cold Molecules via Magnetically Tunable Feshbach Resonances. Rev. Mod. Phys. 78, 1311–1361 (2006)
5. Olshanii, M.: Atomic Scattering in the Presence of an External Confinement and a Gas of Impenetrable Bosons. Phys Rev. Lett. 81, 938–941 (1998)
6. Bergeman, T., Moore, M.G., Olshanii, M.: Atom-Atom Scattering under Cylindrical Harmonic Confinement: Numerical and Analytic Studies of the Confinement Induced Resonance. Phys Rev. Lett. 91, 163201-1–4 (2003)
7. Saedidian, S., Melezhik, V.S., Schemelcher, P.: Multichannel Atomic Scattering and Confinement-Induced Resonances in Waveguides. Phys. Rev. A77, 042721-1–15 (2008)
8. Kim, J.I., Melezhik, V.S., Schmelcher, P.: Suppression of Quantum Scattering in Strongly Confined Systems. Phys. Rev. Lett. 97, 193203-1–4 (2006)
9. Melezhik, V.S., Kim, J.I., Schmelcher, P.: Wave-Packet Dynamical Analysis of Ultracold Scattering in Cylindrical Waveguides. Phys. Rev. A76, 053611-1–15 (2007)
10. Kestner, J.P., Duan, L.M.: Anharmonicity-induced resonances for ultracold atoms and their detection. New J. Phys. 12, 053016-1–6 (2010)
11. Melezhik, V.S., Schmelcher, P.: Quantum Dynamics of Resonant Molecule Formation in Waveguides. New J. Phys. 11, 073031-1–10 (2009)
12. Haller, E., Mark, M.J., Hart, R., Danzl, J.G., Reichsollner, L., Melezhik, V., Schmelcher, P., Nägerl, H.-C.: Confinement-Induced Resonances in Low-Dimensional Quantum Systems. Phys Rev. Lett. 104, 153203-1–4 (2010)
13. Melezhik, V.S.: Polarization of Harmonics Generated from a Hydrogen Atom in a Strong Laser Field. Phys. Lett. A 230, 203–208 (1997)
14. Melezhik, V.S.: A Computational Method for Quantum Dynamics of a Three-Dimensional Atom in Strong Fields. In: Schmelcher, P., Schweizer, W. (eds.) Atoms and Molecules in Strong External Fields, pp. 89–94, Plenum, New York (1998)
15. Melezhik, V.S., Baye D.: Nonperturbative Time-Dependent Approach to Breakup of Halo Nuclei. Phys. Rev. C 59, 3232–3239 (1999)
16. Lill, J.V., Parker, G.A., Light, J.C.: Discrete Variable Representations and Sudden Models in Quantum Scattering Theory. Chem. Phys. Lett. 89, 483–489 (1982)
17. Light, J.C., Carrington, T.: Discrete-Variable Representations and their Utilizations. In: Adv. Chem. Phys., vol.114, Prigogine, I., Rice, S.A., (eds.) John Wiley and Sons, Inc., Hoboken, NJ, USA (2007)
18. Wang, X-C., Carrington, T.: Using a Nondirect Product Discrete Variable Representation for Angular Coordinates to Compute Vibrational Levels of Polyatomic Molecules. J. Chem. Phys. 19, 194109-1–8 (2008)
19. Melezhik, V.S., Schmelcher, P.: Quantum Energy Flow in Atomic Ions Moving in Magnetic Fields. Phys. Rev. Lett. 84, 1870–1873 (2000)
20. Capel, P., Melezhik, V.S., Baye D.: Time-Dependent Analysis of the Breakup of Halo Nuclei. Phys. Rev. C 68, 014612-1–15 (2003)
21. Melezhik, V.S., Cohen, J.S., Hu, C.Y.: Stripping and Excitation in Collisions between p and He\(^+\) (n ≤ 3) Calculated by a Quantum Time-Dependent Approach with Semiclassical Trajectories. Phys. Rev. A69, 032709-1–15 (2004)
22. Baye, D.: Lagrange-Mesh Method for Quantum-Mechanical Problems. Phys. Stat. Sol. (b) 243, 1095–1109 (2006)
23. Melezhik, V.S.: New Method for Solving Multidimensional Scattering Problem. J. Comp. Phys. 92, 67-81 (1991)
24. Marchuk, G.I.: Methods of Numerical Mathematics. Sec.4.3.3, Springer-Verlag, New York (1975)
25. Melezhik, V.S., Hu, C.Y.: Ultracold Atom-Atom Collisions in Nonresonant Laser Field. Phys. Rev. Lett. 90, 083202-1–4 (2003)
26. Press, W.H., Teukolsky, S.A., Vetterling, W.T., Flannery B.P.: Numerical Recipes. Cambridge Univ. Press, Cambridge (1992)
27. Gelland, I.M., Fonin S.V.: Calculus of Variations. Dover Publ., New York (2000)
28. Granger B.E., Blume, D.: Tuning the Interactions of Spin-Polarized Fermions Using Quasi-One-Dimensional Confinement. Phys. Rev. Lett. 92, 133202-1–4 (2004)
29. Kim, J.I., Melezhik, V.S., Schmelcher, P.: Quantum Confined Scattering Beyond the s-Wave Approximation. In: Proc. Int. Conf. on Quantum Mechanics and Chaos, Nakamura K., Harayama T., Takatsuka K. (eds.) Osaka Univ. Sept. 19-20, 2006. Progr. Theor. Phys. Suppl., vol. 166, pp. 159–169 (2007)