Resonances in ultracold collisions confined by atomic traps

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Abstract. We have developed a method for treating ultracold pair collisions in confined geometry of tight atomic waveguides. With this approach we have predicted and analyzed a few novel resonant and multichannel effects induced by confining traps in ultracold atomic collisions. In this report we discuss our model yielding the shifts and widths of magnetic Feshbach resonances in tight atomic waveguides. We also briefly discuss a resonant mechanism of molecule formation in atomic traps with transferring the energy release to the center-of-mass excitation while forming molecule and dipolar confinement-induced resonances in waveguides. These results could potentially be used experimentally.

1. Introduction

Impressive progress of the physics of ultracold quantum gases have opened new pathways for the study of low-dimensional few-body systems (see, for example [1]) as well as strongly correlated many-body systems [2]. It has stimulated the necessity of detailed and comprehensive investigations of collisional processes in the confined geometry of atomic traps. It soon became clear that here the free-space scattering theory is no longer valid and the development of the low-dimensional theory including the influence of the confinement is needed [3]. In our works [4, 5, 6, 7] we have developed a computational method for pair collisions in tight atomic waveguides and have found several novel effects in its application: the confinement-induced resonances (CIRs) in multimode regimes including effects of transverse excitations and deexcitations [5], the so-called dual CIR yielding a complete suppression of quantum scattering [4, 8], and resonant molecule formation with a transferred energy to center-of-mass (CM) excitation while forming molecules [9]. Our calculations have also been used for planning and interpretation of the Innsbruck experiment on investigation of CIRs in ultracold Cs gas [10]. Our computational schemes are based on the works [11, 12], where a method for solving stationary few-dimensional scattering problem as a boundary value problem was suggested, and [13] devoted to a component-by-component splitting up method for three-dimensional time-dependent Schrödinger equation. A key element of the developed economic computational schemes is the non-direct product 2D discrete-variable representation we suggested for approximation angular variables [14].

In this report, we discuss the most important results obtained recently in our study of resonances in ultracold collisions confined by atomic waveguides. It is the development of a theoretical model for describing Feshbach resonance shift and width induced by an atomic waveguide [15]. It is a resonant mechanism of molecule formation in an atomic waveguide with transferring the energy release to the CM excitation while forming molecule we suggested in [9]. We briefly discuss this model, which becomes actual in connection with recent experiments in Heidelberg on the resonant formation of Li molecules in atomic traps [16]. We also briefly discuss our nonperturbative model to treat pair collisions with long-range anisotropic interactions in quasi-one-dimensional geometries [17]. This model avoids the limitations of pseudopotential theory [18, 19] and gives exact prediction of the positions of dipolar CIRs in waveguides, which may pave the way for the experimental realization of special phases in one-dimensional dipolar gases (see, for example [20]).

2. Shifts and widths of Feshbach resonances in atomic waveguides

Already at the initial stage of the investigation of ultracold pair collisions in atomic traps, it was shown that the confining geometry can drastically change the scattering properties of ultracold atoms and induce resonances in the collisions (confinement-induced resonances (CIRs)) [3]. Further research in this field has shown that a necessary ingredient for the experimental realization of the CIR in a confining trap is the existence of magnetic Feshbach resonances in free-space [1, 2, 10, 21]. However, until recently, single-channel potential models with zero-energy bound states were used for simulating the magnetic Feshbach resonances in the 3D free-space (see, for example, the papers [3, 4, 5, 7, 9, 16, 17, 18, 19, 22, 23]). The simplified models were used despite that the single-channel interatomic interaction approach permits to explore only the main attribute of the Feshbach resonances in the 3D free-space, namely the appearance of a singularity in the s-wave scattering length $a \to \pm\infty$ when the molecular bound state with energy E_c crosses the atom-atom scattering threshold at energy $E = 0$ in the entrance channel. Other important parameters of the Feshbach resonance, such as the rotational and spin structure of the molecular bound state in the closed channel, background scattering length a_{bg} as well as the width Δ of the resonance characterizing the coupling Γ of the molecular state with the entrance channel [1], were ignored.

The main goal of our work [15] was to exit from the frame of the single-channel theoretical approaches developed earlier for the CIRs and take into account the effects of different rotational structure of the Feschach resonance, the resonance width and the background scattering. We have developed and a theoretical model [15] which yields the shifts and widths of Feshbach resonances (having different tensorial structure) in an atomic waveguide. It is based on our multichannel approach for CIRs and atomic transitions in the waveguides in the multimode regime [5]. We replace in this scheme the single-channel scalar interatomic interaction by the four-channel tensorial potential $\hat{V}(r)$ modeling resonances of broad, narrow and overlapping character according to the two-channel parametrization of A.D.Lange et. al. [24].

In this approach the scattering amplitude $f(k, B)$ describing a pair collision in free-space ($\omega_\perp = 0$) is calculated for different magnetic field strengths B and varying parameters of the potential $\hat{V}$ by solving the Schrödinger equation

$$\left([-\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_\perp^2\rho^2]\hat{I} + \hat{B} + \hat{V}(r) \right) |\psi\rangle = E|\psi\rangle \tag{1}$$

with the scattering boundary conditions

$$\psi_e(\mathbf{r}) \to \exp\{ikz\} + f(k,B)/r \exp\{ikr\}\,, \;\; \psi_{c,i}(\mathbf{r}) \to 0$$

at $kr \to \infty$ for the fixed $E \to 0$ ($k = \sqrt{2\mu E}/\hbar \to 0$) [12]. The diagonal matrix $\hat{B}$ in (1) is defined as $B_{ii} = \delta\mu_i(B - B_i)$ (here $\delta\mu_i$ is the relative magnetic moment of the channel i, $i = 1, 2, 3$)

and $B_{ee} = 0$. After separation of the angular part in (1) we come to the system of four coupled radial equations

$$[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l_\alpha(l_\alpha+1)}{2\mu r^2} + B_{\alpha\alpha}]\phi_\alpha(r) + \sum_\beta V_{\alpha\beta}(r)\phi_\beta(r) = E\phi_\alpha(r) \quad (2)$$

for the radial part $\phi_\alpha(r)$ of the desired wave function $|\psi\rangle = \sum_\alpha \psi_\alpha(\mathbf{r})|\alpha\rangle = \sum_\alpha \phi_\alpha(r)Y_{l_\alpha 0}(\hat{r})|\alpha\rangle$, where $\alpha = \{e, i = 1,2,3\}$, $(l_e = 0, l_1 = 0, l_2 = 2, l_3 = 4)$ and the matrix elements $V_{\alpha\beta}(r)$ are defined by four diagonal parameters $V_{c,i}$, V_e and three non-diagonal ones Ω_i [15]. The centrifugal barrier $\frac{\hbar^2 l_\alpha(l_\alpha+1)}{2\mu r^2}$ in (2) models at $r \to 0$ the correct asymptotic behavior $\phi_i(r) \sim r^{l_i+1}$ of the molecular bound states $|c,i\rangle$ in the closed channels which couple to the entrance s-wave ($l_e = 0$) channel $|e\rangle$ by the nondiagonal terms $V_{\alpha\beta}(r)(\alpha \neq \beta)$.

By varying the $V_{c,i}$, V_e and Ω_i we have obtained an excellent agreement of the calculated s-wave scattering length $a(B) = -f(k \to 0, B)$ with the analytical results from [24] for Cs atoms in the hyperfine state $|F = 3, m_F = 3\rangle$ for the considered magnetic field regime $-40G < B < 60G$, corresponding to the conditions of Innsbruck experiments [10]. In this regime, we observe three resonances B_i in $a(B)$, which correspond to the coupling to the s-, d-, and g-wave molecular states in the closed channels $|c,i\rangle$.

Then, after finding the parameters of interparticle interaction $\hat{V}(r)$, we have analyzed the scattering properties of the s-, d- and g-wave magnetic Feshbach resonances in harmonic waveguides by integrating the Schrödinger equation (1) for $\omega_\perp \neq 0$ with the scattering boundary conditions

$$\psi_e(\mathbf{r}) = \left(\cos(k_{||}z) + f_e(B)\exp\{ik_{||} \mid z \mid\}\right)\Phi_0(\rho)\ ,\ \ \psi_{c,i}(\mathbf{r}) \to 0 \quad (3)$$

at $\mid z \mid = \mid r\cos\theta \mid \to \infty$ adopted for a confining trap [5]. $f_e(B,E)$ is the scattering amplitude, corresponding to symmetric states with respect to the exchange $z \to -z$ (we consider collisions of identical bosonic Cs atoms), $\Phi_0(\rho)$ is the wave function of the ground-state of the two-dimensional harmonic oscillator and $k_{||} = \sqrt{2\mu(E - \hbar\omega_\perp)}/\hbar = \sqrt{2\mu E_{||}}/\hbar$. In the presence of of the harmonic trap ($\omega_\perp \neq 0$) the problem (1),(3) becomes non-separable in the plane $\{\rho, z\}$, i.e. the azimuthal angular part is separated in the wave function $|\psi\rangle$ and Eq.(1) is reduced to the coupled system of four 2D Schrödinger-type equations. To integrate this coupled channel 2D scattering problem in the plane $\{r,\theta\}$ we have applied the extended version of the computational scheme [5]. The computations have been performed in a range of variation of $\omega_\perp$ close to the experimental values of the trap frequencies $\omega_\perp \sim 2\pi \times 14.5$kHz [10]. We have integrated Eq.(1) for varying B and fixed longitudinal colliding energy $E_{||} = E - \hbar\omega_\perp \to 0$.

As an input the experimentally known parameters of Feshbach resonances in the absence of the waveguide [24], namely the resonant energies $E_{c,i}$ (or the corresponding values of the field strengths B_i of the external magnetic field), the widths of the resonances $\Delta_i(\Gamma_i)$, spin characteristics and the background scattering length a_{bg}, were used. The output of the model is the calculated scattering amplitude $f_e(B)$ in the confining trap $\omega_\perp$ and the transmission $\mathrm{T}(B) = \mid 1 + f_e(B) \mid^2$.

We have calculated the shifts and widths of s-, d- and g-wave magnetic Feshbach resonances of Cs atoms emerging in harmonic waveguides as CIRs (the minimums in the transmission $\mathrm{T}(B)$) and resonant enhancement of transmission T(B) at zeros $a(B) = 0$ of the free-space scattering length. The results are illustrated by the curves T(B) calculated near the d-wave resonance for different $\omega_\perp$ (Fig.1) corresponding to the transverse frequencies of the optical trap being used in the experiment [10]. It is shown that the position of B_{min} of the transmission coefficient T(B) minimum is dependent on the transverse trap width $a_\perp = \sqrt{\hbar/(\mu\omega_\perp)}$ according to simplified Olshanii model [3]. Actually, the corresponding scattering length $a(B_{min})$ at the point B_{min} is accurately described by the formulas $a(B_{min}) = a_\perp/C$ obtained in [3] for the position of the CIR in s-wave case. Our analysis has shown that this law is fulfilled with high accuracy for Feshbach resonances of different tensorial structure which holds in spite of the fact that the formulas defining the position of CIR was originally obtained in the framework of the s-wave single-channel pseudopotential approach (see Fig.2). This property was experimentally confirmed for d-wave Feshbach resonances in a gas of Cs atoms [10].

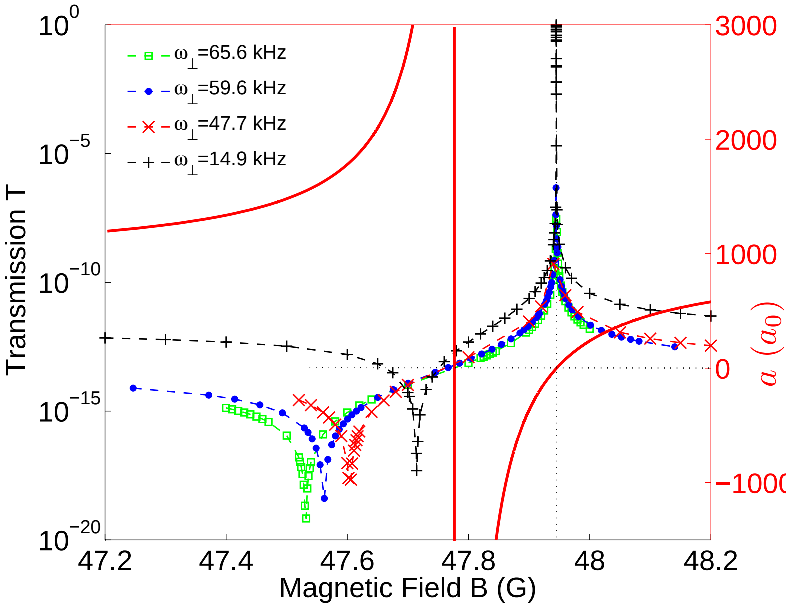

Figure 1. The transmission T(B) as a function of the strength of the magnetic field for several trap frequencies $\omega_\perp$. Here the s-wave free-space scattering length $a(B)$ as a function of B is also given in atomic units a_0 (solid curve).

We have also found the linear dependence of the width of the resonance in the transmission T(B^*) at the point $a(B^*) = 0$ on the longitudinal atomic momentum $k_{||} = \sqrt{2\mu(E - \hbar\omega_\perp)}/\hbar = \sqrt{2\mu E_{||}}/\hbar$ and quadratic dependence on the trap width $a_\perp$: $\Gamma_i^* = \Delta_i k_{||} a_\perp^2/a_{bg}$ (here $\Delta_i = B^* - B_i$ is the width of the Feshbach resonance at B_i and a_{bg} is the background scattering length in free-space). This formula was confirmed by numerical results at $k_{||} \to 0$. The found effect could potentially be used experimentally. Actually, one can control the width $\Gamma_i^* = \Delta_i k_{||} a_\perp^2/a_{bg}$ of the resonance by varying the trap width $a_\perp$, an increase of $\omega_\perp$ leads to a narrowing of the resonance. From the other side, by measuring the width Γ_i^* one can extract from the obtained formulae [15] important information about the longitudinal colliding energy $E_{||} = E - \hbar\omega_\perp$ and estimate the temperature of the atomic cloud in the trap.

Finally, we have calculated the populations of the molecular states in closed channels at pair atomic collisions in a trap. It was found that the molecule formation rates in a waveguide show an enhancement for the case of a corresponding zero of the s-wave scattering length $a(B^*) = 0$. The effect is illustrated by Fig.3. We have also shown that the positions of these resonances are stable w.r.t. the variation of the confining frequency $\omega_\perp$ of the waveguide.

3. Resonance mechanism of molecule formation in 1D trap with CM excitation

In our paper [9] a resonant mechanism for molecule formation in heteronuclear atomic collisions in waveguides with transferring the energy release to the CM excitation was suggested. The key point of this mechanism is the confinement-induced mixing of the relative and CM motions in the atomic collision process due to the coupling term

$$W(\rho_{CM}, \mathbf{r}) = \mu(\omega_1^2 - \omega_2^2) r \rho_{CM} \sin\theta\cos\phi \tag{4}$$

in the Hamiltonian of the atomic pair in the confining potential of the trap. Here ρ_{CM} is the radial variable of the CM, $\mathbf{r}$ are the relative variables and ω_i is the frequency of the confining trap

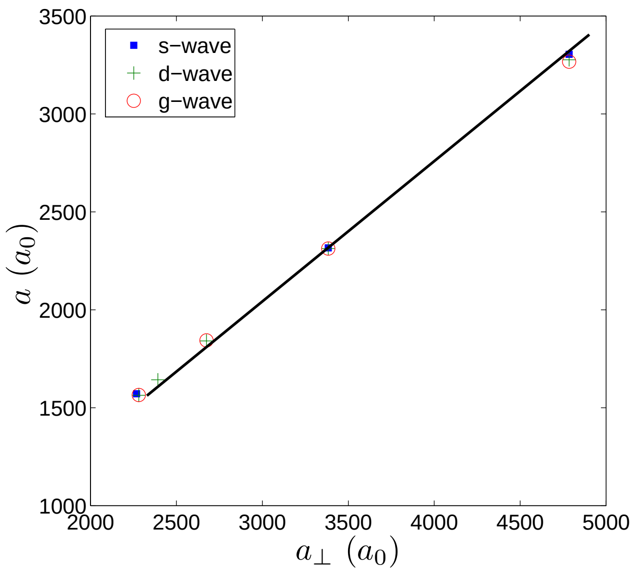

Figure 2. The dependence of the s-wave scattering length $a(B)$ on the trap width $a_\perp$ at the points B_{min} of the minimum of the transmission $\mathrm{T}(a(B), a_\perp)$ (see Fig.1). The dots, pluses and cycles correspond to the calculated points near the s-,d- and g-wave magnetic Feshbach resonances, respectively. The solid line corresponds to the formula $a = a_\perp/C$ (where C=1.4603) from [3]. The values $a(B)$ and $a_\perp$ are given in atomic units a_0.

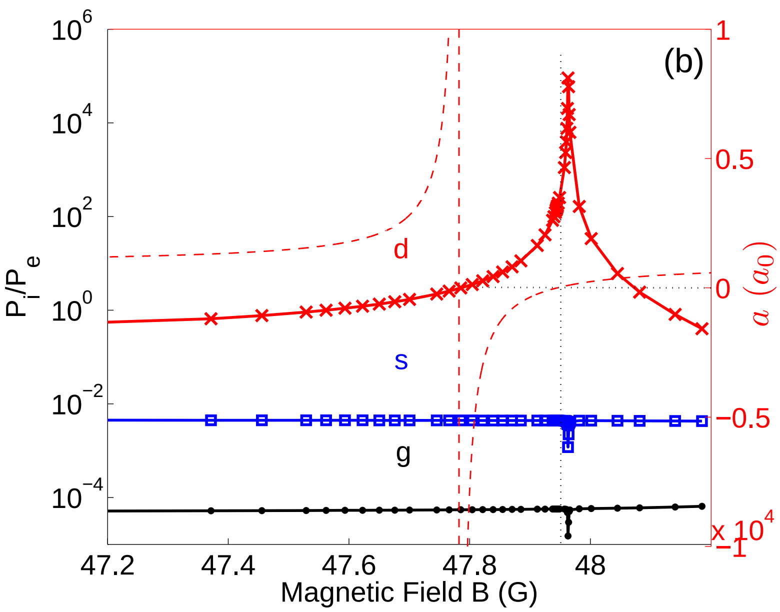

Figure 3. The relative population P_i/P_e of the molecular states i = s, d and g calculated as a function of magnetic field B near the d-wave Feshbach resonance in Cs for pair atomic collisions in the harmonic waveguide $\omega_\perp$ =59.6 kHz. The free-space scattering length $a(B)$ is given in atomic units.

corresponding to the atom i. This term leads to a coupling of the diatomic continuum to the CM excited molecular states in closed transverse channels. By using our wave-packet propagation method we have modeled the collisional dynamics of two atoms in the ground transverse state $n_1 = n_2 = 0$ $(n = N = 0)$ of the harmonic waveguide near the CIRs (n_i is the quantum number of the harmonic spectrum of the atom i, the quantum numbers n and N numerates the harmonic spectrums of the relative and the CM transverse eigenstates). The possibilities of the resonance molecule formation in a harmonic wavegaide under the scheme

$$A_{n_1=0} + B_{n_2=0} \to (AB)_{n=0,N=1}$$

with the CM excitation $n = N = 0 \to n = 0, N = 1$ was investigated in details in [9] and the crucial role of the coupling term was demonstrated. It was shown that the molecular formation probabilities can be tuned by changing the trap frequencies ω_i, that characterize the transverse modes of the atomic species, and by varying the longitudinal colliding energy $E_{\|}$.

It is known that for identical atoms (when $\omega_1 = \omega_2$) the coupling term (4) is absent but the mixing of the relative and CM variables is, nevertheless, present in the two-body Hamiltonian in anharmonic traps (see, for example, [25, 26]). In the work [26] the mechanism of molecule formation with transferring the energy release to CM excitation of forming molecule was considered for an anharmonic lattice.

Experimental confirmation of the resonate molecule formation in an atomic waveguide with transferring the energy release to CM excitation was recently obtained [16], what opens iteresting possibilities for investigations in this field.

4. Dipolar CIRs of ultracold gases in waveguides

By using our method [5, 6, 12] we develop a nonperturbative theoretical framework to treat collisions with generic anisotropic interactions in quasi-one-dimensional geometries [17]. The developed scheme avoids the limitations of pseudopotential theory [8, 19] and allows us to include accurately long-range anisotropic interactions. For ultracold dipolar collisions in a harmonic waveguide we predict dipolar confinement-induced resonances (DCIRs) which are attributed to different angular momentum states. The analytically derived resonance condition reveals in detail the interplay of the confinement with the anisotropic nature of the dipole-dipole interactions. The results are in excellent agreement with ab initio numerical calculations confirming the robustness of the presented approach. The exact knowledge of the positions of DCIRs may pave the way for the experimental realization of different exotic phases in effective one-dimensional dipolar gases [20].

5. Conclusion

In this report we have presented three novel resonant effects induced by confining waveguides in ultracold atomic collisions which we have analyzed recently with the developed computational method. These results could potentially be used experimentally. The high efficiency and flexibility of the method we observed in theses studies make it very promising in application to other resonant processes in atomic traps of different geometry.

Possible actual problems can be the fermionic atom collisions in waveguides, ultacold pair processes in pancake-like traps, triple ultracold collisions.

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