Ultracold Resonant Processes in Atomic and Molecular Traps

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Results were obtained in collaboration with

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Innsbruck experiment:

Elmar Haller

Hans-Chrisroph Nägerl

Outline

- Ultracold atoms in optical traps: why it is interesting?
- Confinement-induced resonances (CIRs)
- Feshbach resonances in quasi-1D atomic traps (bosons and fermions)
- Dipolar CIRs in quasi-1D traps
- Anisotropic quantum scattering in two dimensions
- Resonant molecule formation with energy transfer to CM excitation
- Conclusion and outlook



Lattices formed by applying orthogonal standing waves in one, two, and three directions.



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experimental aspects

Experiments with deterministically prepared quantum systems

control interparticle interaction

magnetic field [G]



Experiments with deterministically prepared quantum systems

control interparticle interaction



 control over quantum states and particle number with long lifetime



counts

Experiments with deterministically prepared quantum systems

control interparticle interaction



quantum simulation with fully controlled few-body systems

G.Zürn et. al. Phys. Rev. Lett. 108, 075303 (2012)

Quantum simulation with fully controlled few-body systems

control over: quantum states, particle number, interaction

- attractive interactions **→** BCS-like pairing in finite systems
- repulsive int.+splitting of trap → entangled pairs of atoms (quantum information processing)
- + periodic potential

 quantum many-body physics (systems with low entropy to explore such as quantum magnetism)

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Bose-Hubbard Physics



R. P. Feynman's Vision

A Quantum Simulator to study the quantum dynamics of another system.

R.P. Feyman, Int. J. Theo. Phys. (1982) R.P. Feynman, Found. Phys (1986)



theoretical aspects



theoretical aspects

3D free-space scattering theory is no longer valid and development of low-dimensional theory including influence of the trap is needed

What happens if atoms scatter in confined geometry (quasi-1D) ?



What happens in collision of two distinguishable atoms in harmonic trap, or identical atoms in anharmonic trap ?

$$H'(\rho_{\mathbf{R}}, \mathbf{r}) = -\frac{1}{2M} \left(\frac{\partial^2}{\partial \rho_R^2} + \frac{1}{4\rho_R^2}\right) - \frac{1}{2M\rho_R^2} \frac{\partial^2}{\partial \phi_R^2} + \frac{1}{2} (m_1 \omega_1^2 + m_2 \omega_2^2) \rho_R^2$$
$$\cdot \frac{1}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{L^2(\theta, \phi)}{2\mu r^2} + \frac{\mu^2}{2} \left(\frac{\omega_1^2}{m_1} + \frac{\omega_2^2}{m_2}\right) \rho^2 + \mu(\omega_1^2 - \omega_2^2) \rho \rho_R \cos(\phi - \phi_R) + V(r)$$

5D \rightarrow { $r, \theta, \phi, \rho_R, \phi_R$ }

non-separable two-body problem



non-direct 2D discrete-variable representation (2D DVR)

1D DVR: J.C.Light et al J.Chem.Phys. 1985

2D DVR: V.Melezhik Phys.Rev. A 1993 Phys.Lett. 1997 V.Melezhik & D.Baye Phys.Rev. C 1999 V.Melezhik & P.Schmelcher Phys.Rev.Lett. 2000

• multi-channel scattering problem as a boundary-value problem

V.Melezhik J.Comp.Phys. 1991 V.Melezhik & C.-Y. Hu Phys.Rev.Lett. 2003 S.Saeidian & V. Melezhik & P.Schmelcher Phys.Rev.A 2008

• splitting-up method for time-dependent 3D and 4D Schrödinger eqs.

G.I.Marchuk 1971 V.Melezhik Phys.Lett. 1997 V.Melezhik & D.Baye Phys.Rev. C 1999 J.I.Kim & V.Melezhik & P.Schmelcher Phys.Rev. A 2007 V.Melezhik & P.Schmelcher New J. Phys 2009

confinement-induced resonances (CIRs)



Tuning the interaction in 3D



3D

Tuning the interaction in 3D



single-channel pseudopotential

$$\frac{2\pi\hbar^2 a_{3\mathrm{D}}(\mathrm{B})}{\mu}\delta(\mathrm{r})$$

Tuning the interaction in 1D: B and ...







tensorial sructure of molecular state



tensorial sructure of molecular state



tensorial sructure of molecular state

Innsbruck experiment with Cs atoms:

Feshbach Resonanzen





two-channel model of Lange et. al. Phys.Rev.79,013622(2009)



3 fitting parameters:

$$\frac{1}{a-\bar{a}} = \frac{1}{a_{\rm bg}-\bar{a}} + \frac{\Gamma/2}{\bar{a}E_c}$$
$$E_c = \delta\mu(B-B_c)$$

 $V_e V_c \Omega$



TABLE I. Fitting parameters for the s-, d-, and g-wave Feshbach resonances, determining the scattering length in the magnetic-field range of interest; see Fig. 3. The background scattering length $a_{bg}=1875a_0$, the mean scattering length of cesium, $\bar{a}=95.7a_B$, and the bare s-wave state magnetic moment $\delta\mu_1=2.50\mu_B$ [28] are set constant. Poles $B_{0,i}$ and zeros B_i^* of the scattering length are derived; see text. Uncertainties in the parentheses are statistical. The systematic uncertainty of the magnetic field is 10 mG.

Res.	Γ_i/h (MHz)	$\delta \mu_i / \mu_B$	$B_{c,i}$ (G)	$B_{0,i}$ (G)	B_i^* (G)
S-WV.	11.6(3)	2.50	19.7(2)	-11.1(6)	18.1(6)
d-wv.	0.065(3)	1.15(2)	47.962(5)	47.78(1)	47.944(5)
g-wv.	0.0042(6)	1.5(1)	53.458(3)	53.449(3)	53.457(3)

extension of two-channel model of Lange et. al. to 1D geometry

Sh.Saeidian, V.S. Melezhik ,and P.Schmelcher, Phys.Rev. A86, 062713 (2012)

A four-channel square-well potential

$$\hat{V} = \begin{pmatrix} -V_{c,3} & 0 & 0 & \hbar\Omega_3 \\ 0 & -V_{c,2} & 0 & \hbar\Omega_2 \\ 0 & 0 & -V_{c,1} & \hbar\Omega_1 \\ \hbar\Omega_3 & \hbar\Omega_2 & \hbar\Omega_1 & -V_e \end{pmatrix} \qquad |\psi\rangle = \sum_{\alpha} \psi_{\alpha}(\mathbf{r})|\alpha\rangle = \sum_{\alpha} \phi_{\alpha}(r)Y_{l_{\alpha}0}(\hat{r})|\alpha\rangle$$

$$\omega_{\perp} = 0$$

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

$$\psi_{e}(\mathbf{r}) \to \exp\{ikz\} + f(k,\theta)/r \exp\{ikr\}, \qquad \psi_{c,i}(\mathbf{r}) \to 0$$

4-coupled radial equations

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$$\omega_{\perp} = 0$$

 $\omega \neq 0$

$$\begin{bmatrix} -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l_{\alpha}(l_{\alpha}+1)}{2\mu r^2} + B_{\alpha\alpha} \end{bmatrix} \phi_{\alpha}(r) + \sum_{\beta} V_{\alpha\beta}(r)\phi_{\beta}(r) = E\phi_{\alpha}(r) \qquad \text{4-coupled radial equations}$$

$$\psi_{e}(\mathbf{r}) \to \exp\{ikz\} + f(k,\theta)/r \exp\{ikr\}, \qquad \psi_{c,i}(\mathbf{r}) \to 0$$

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

4-coupled 2D equations in the plane $\{r, heta\}$

 $\psi_{e}(\mathbf{r}) = [\cos(k_0 z) + f_{e} \exp\{ik_0|z|\}] \Phi_0(\rho), \quad \psi_{c,i}(\mathbf{r}) \to 0$

 $T(B) = |1 + f_e(B)|^2$















S.Saeidian, V.S.Melezhik and P.Schmelcher, J. Phys B (2015) (in press)

p-wave magnetic Feshbach resonances of 40 K atoms emerging in harmonic waveguides as p-wave CIRs.

bosons: only s-wave in entrance channel
$$\frac{a}{a_{\perp}} = 0.68$$

fermions: only p-wave in entrance channel $\frac{V_p}{V_\perp} = ?$

$$V_{\perp} = a_{\perp}^3$$

$$k^3 \cot \delta_1(k, B) = -\frac{1}{V_p(B)}$$



S.Saeidian, V.S.Melezhik and P.Schmelcher, J. Phys B (2015) (in press)

My,

p-wave magnetic Feshbach resonances of ⁴⁰K atoms emerging in harmonic waveguides as p-wave CIRs.





 $\frac{V_p}{V_\perp} \neq const$

 $k^3 \cot \delta_1(k, B) = -\frac{1}{V_p(B)}$

S.Saeidian, V.S.Melezhik and P.Schmelcher, J. Phys B (2015) (in press)



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state $|F = 9/2, m_F = -7/2\rangle$ of Potassium atoms as a function of the the rescaled energy ϵ

B.E. Granger and D. Blume, Phys. Rev. Lett. **92**, 133202 (2004).

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B.E. Granger and D. Blume, Phys. Rev. Lett. **92**, 133202 (2004).

J.I. Kim, V.S. Melezhik, and P. Schmelcher, Progr. Theor. Phys. Supp. 166, 159 (2007).

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P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)

 $\stackrel{d}{\longrightarrow} \stackrel{d}{\longrightarrow}$

$$H = -\frac{\hbar^2}{2\mu} \nabla^2 + \underbrace{\frac{C_{12}}{r^{12}} - \frac{C_6}{r^6}}_{V_{sr}} + \underbrace{\frac{d^2}{r^3} [1 - 3(\hat{z} \cdot \hat{r})]}_{V_{sr}} \underbrace{V_{dd}}_{V_{sr}} \\ \underbrace{K^{3D}}_{K_{ds}} = \begin{pmatrix} K_{ss} & K_{sd} & 0 \\ K_{ds} & K_{dd} & K_{dg} \\ 0 & K_{gd} & K_{gg} \end{pmatrix} \\ a_{ll'} = -\frac{K_{ll'}}{k} \\ l_d = \frac{\mu d^2}{\hbar^2} \end{aligned}$$

P.Giannakeas, V. Melezhik & P.Schmelcher, PRL,111(2013)

$$H = -\frac{\hbar^{2}}{2\mu}\nabla^{2} + \frac{\mu}{2}\omega_{\perp}^{2}\rho^{2} + \frac{C_{12}}{r^{12}} - \frac{C_{6}}{r^{6}} + \frac{d^{2}}{r^{3}}[1 - 3(\hat{z} \cdot \hat{r})]$$

$$d = -\frac{d}{d} - \frac{d}{d} - \frac{d}{d}$$

reduces to \bar{a}_s = $-1/\sigma_0$ = 0.68

 $a_s = 0.68 a_{\perp}$

For $l_d = 0$, the resonance condition $\bar{a}_{ss} = \mathcal{F}_{BA}$







FIG. 8. (Color online) The total cross sections σ in the units of σ_{SC} as a function of the dipole tilt angle $\alpha = \gamma$ and the rotational angle β calculated for potential (23) at D = 1, Dq = 10.



 σ_{sc} as a function of the dipole tilt angles α and γ calculated for

potential (23) at D = 1, Dq = 10. The rotational angle β is equal to

 $\pi/2.$

FIG. 8. (Color online) The total cross sections σ in the units of σ_{SC} as a function of the dipole tilt angle $\alpha = \gamma$ and the rotational angle β calculated for potential (23) at D = 1, Dq = 10.



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Mechanism of molecule formation with transferring the energy release to CM excitation of forming molecule was considered in:

E.Bolda et.al. Phys.Rev. A71,033404 (2004) (in anharmonic lattices)

V.Melezhik & P.Schmelcher, New J.Phys.11,073031 (2009) (distinguishable atoms in harmonic waveguides)

non-separability of two-body problem in trap (distinguishable atoms in harmonic trap or identical atoms in anharmonic trap)



 $A_{n1=0} + B_{n2=0} \rightarrow (AB)_{n=0,N=1}$

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$$W(\rho_{\rm R}, r, t) = \int |\psi(\rho_{\rm R}, r, \theta, \phi, t)|^2 (r^2 \rho_{\rm R})^{-1} \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$$

CM coupling with interatomic motion:



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CM coupling with interatomic motion:

CM decouples from interatomic motion:



Resonant Formation of Ultracold Molecules in Waveguides

V. Melezhik & P. Schmelcher, New J. of Phys. 11, 073031 (2009)

coupling of the deatomic continuum with the CM of excited molecule at (N=1) in closed transverse channels:

if the atoms in the colliding pair are identical, then coupling term goes to zero and the effect disappears.

 $A_{n1=0} + B_{n2=0} \rightarrow (AB)_{n=0,N=1}$

Time evolution of the molecular states (N=0 and 1) population $P_{M}(t)$ during a pair collision:



in Heidelberg experiment, S.Sala et. al. Phys.Rev.Lett.110,203202 (2013), the mechanism of molecule formation with transferring energy release to CM molecule excitation was observed in anharmonic waveguide



signature of resonant molecule formation

- confinement-induced resonances in low-dimensional quantum systems
- s- and p-wave CIRs in quasi-1D traps
- resonant positions for dipolar CIRs in quasi-1D traps
- resonant mechanism for molecule formation in traps with energy transfer to CM excitation

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extension to quasi-2D geometry

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 $\omega_1 \neq \omega_2$



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extension to quasi-2D geometry

• resonant positions for dipolar CIRs in quasi-1D traps

 $\omega_1 \gg \omega_2$

 resonant mechanism for molecule formation in traps with energy transfer to CM excitation





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three-body collisional problem (Efimov resonances) in tight traps

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extension to quasi-2D geometry

three-body collisional problem (Efimov resonances) in tight traps

non-linear time-dependent Schrödinger equation with CM coupling

Quantum simulation with fully controlled few-body systems

control over: quantum states, particle number, interaction

Fermions in Lattices (Hubbard Model, Superconductivity)

Bose-Fermi mixtures

Disordered Systems

Quantum Magnets (in spin mixtures, Ising, XY model, Heisenberg model)

Nonequilibrium Dynamics

Spin-Liquid Systems & Topological Quantum Phases



Towards (One Way) Quantum Computing

Large Scale Entanglement, Nonclassical Field States

Decoherence

Single Site Addressing

Spin Squeezing

Quantum Metrology

High precision spectroscopy, Search for EDM Controlled Molecule Formation in arbitrary quantum states Formation of heteronuclear molecules with dipole moments Control interaction properties (mag. & opt. Feshbach resonances)