Mathematical Modeling of Resonant Processes in Confined Geometry of Atomic and Atom-Ion Traps

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MMCP2017, Dubna, 5 July 2017

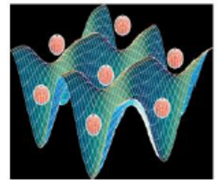
Outline

- Why it is interesting
- Confined ultracold atom-atom and atom-ion collisions
- npDVR: scattering problem as boundary-value problem
  splitting-up method for 4D Schrödinger eq.
- Atom-atom CIRs
- Atom-ion CIRs
- Impact of ion micromotion-induced heating
- Outlook

Why it is interesting

- ultracol atoms

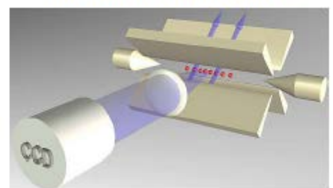
Atoms in an optical lattice:
Artificial solids



optical traps

Trapped ions:
Arrays of interacting spins

- cold ions



RF Paul traps

- last few years: hybrid systems ``atom+ion''

new quantum systems with different energy and length scales

with respect to ultracold atoms and molecules

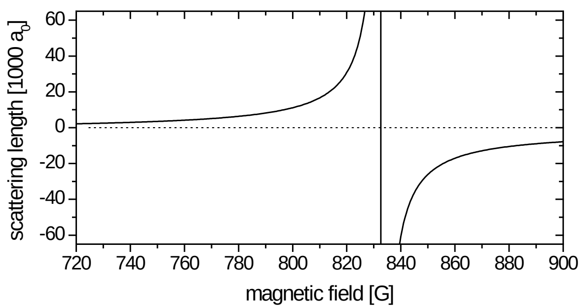
motivation in brief

experimental aspects

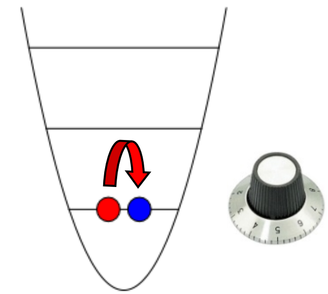
Experiments with deterministically prepared quantum systems

- control interparticle interaction

2 interacting particles in a 1D potential



magnetic Feshbach resonance



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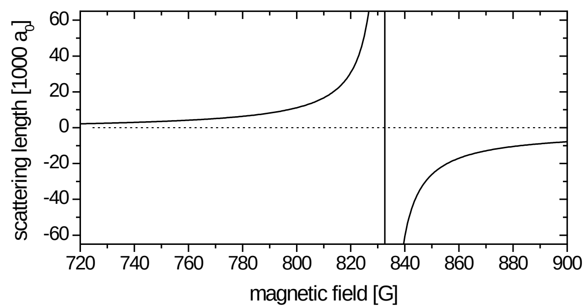

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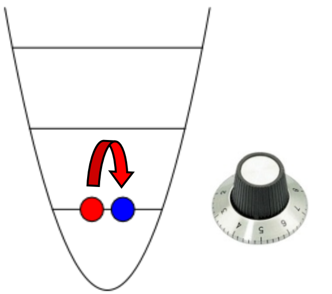
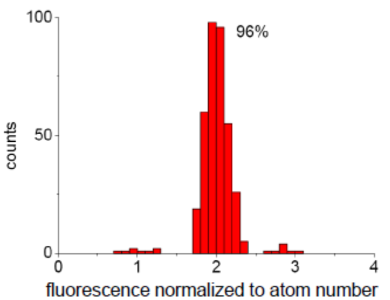


- control over quantum states and particle number with long lifetime



Experiments with deterministically prepared quantum systems

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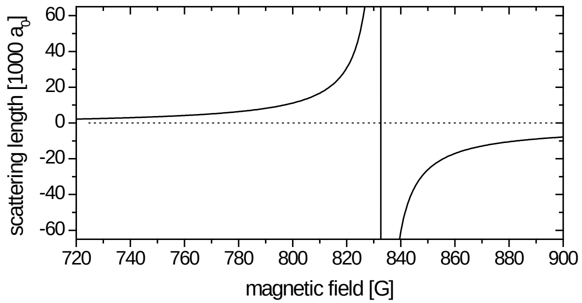
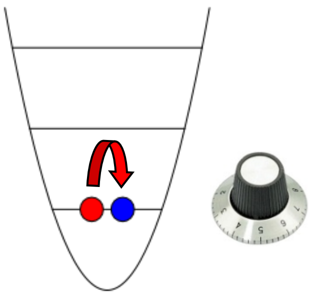
2 interacting particles in a 1D potential



magnetic Feshbach resonance



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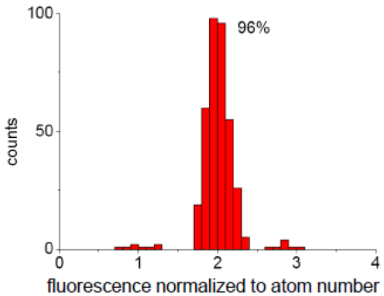

quantum simulation with fully controlled few-body systems

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)
- ...

Quantum simulation with fully controlled few-body systems

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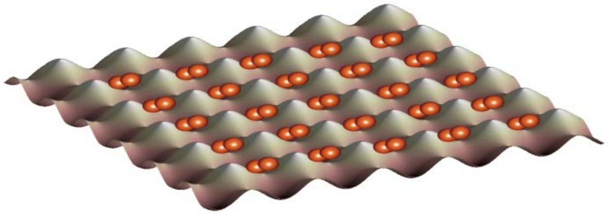
- ...

Bose-Hubbard Physics



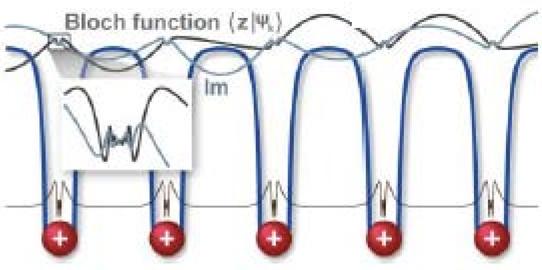
R. P. Feynman's Vision

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)

Why it is interesting

quantum simulation with cold atoms and ions



Ion crystal + atoms: Fröhlich model

U. Bissbort *et al.*, PRL 111, 080501 (2013)

other proposals: formation of molecular ions, polarons,
density bubbles, collective excitations,
quantum information processing (two-qubit gate),
mesoscopic entanglement …

all proposals assume:
atom-ion and atom-phonon interactions can be tuned

atomic confinement-induced resonances (CIRs) $\Rightarrow$ atom-ion CIR ?

motivation in brief

theoretical aspects

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

Methods:

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

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

  2D DVR: V.Melezhik Phys.Lett. 1997
  V.Melezhik AIP Conf Proc 1479, 2012
  V.Melezhik EPJ Web of Conf (MMCP15) 2016

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

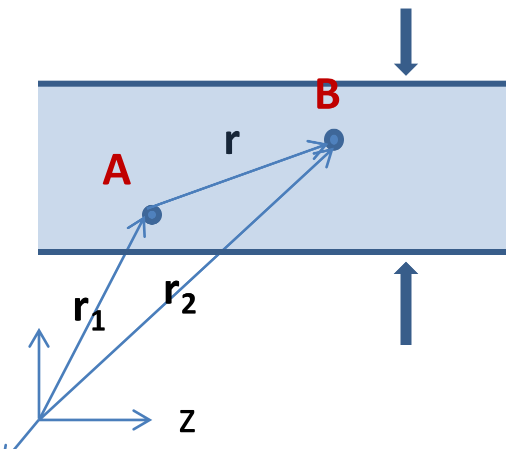
  V.Melezhik & C.-Y. Hu Phys.Rev.Lett. 2003
  S.Saeidian & V. Melezhik & P.Schmelcher Phys.Rev.A 2008
  V. Melezhik EPJ Web of Conf (MMCP15) 2016

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

  V.Melezhik Phys.Lett. 1997
  V.Melezhik & D.Baye Phys.Rev. C 1999
  V.Melezhik & P.Schmelcher New J. Phys 2009
  V.Melezhik EPJ Web of Conf (MMCP15) 2016

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

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



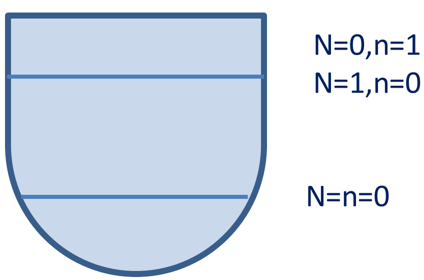
$$V(r) + \tfrac{1}{2}m_1\omega_1^2\rho_1 + \tfrac{1}{2}m_2\omega_2^2\rho_2$$

$$i\frac{\partial}{\partial t}\psi(\rho_R,\mathbf{r},t) = H(\rho_R,\mathbf{r})\psi(\rho_R,\mathbf{r},t)$$

$$H(\rho_R,\mathbf{r}) = H_{CM}(\rho_R) + H_{\text{rel}}(\mathbf{r}) + W(\rho_R,\mathbf{r})$$

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

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



$$\frac{L^2(\theta,\phi)}{2\mu r^2} = -\frac{1}{2\mu r^2\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$\boxed{W(\rho_R,\mathbf{r}) = \mu(\omega_1^2 - \omega_2^2)r\rho_R\sin\theta\cos\phi}$$ → 4D TDSE: ρ_R, r, θ, ϕ

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

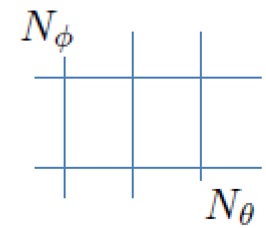
5D TDSE

- Discretization of the angular subspace:
  2D nondirect product discrete variable representation (npDVR)

$$\psi(\rho_R, r, \Omega, t) = \sum_{j=1}^{N} f_j(\Omega)\psi_j(\rho_R, r, t) \qquad \sum_{\nu=1}^{N} = \sum_{m=-(N_\phi-1)/2}^{(N_\phi-1)/2} \; \sum_{l=|m|}^{|m|+N_\theta-1}$$

$$f_j(\Omega) = \sum_{\nu=1}^{N} Y_\nu(\Omega)(Y^{-1})_{\nu j} \qquad \Omega_j = (\theta_{j_\theta}, \phi_{j_\phi})$$

$$Y_\nu(\Omega) = Y_{lm}(\Omega) = e^{im\phi}\sum_{l'} C_l^{l'} \times P_{l'}^{m}(\theta) \qquad Y_{j\nu} = Y_\nu(\Omega_j)$$



V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik, AIP Conf.Proc.1479(2012)1200

5D TDSE

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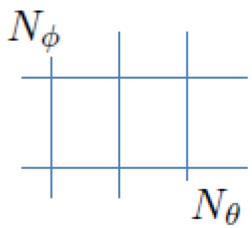


V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik, AIP Conf.Proc.1479(2012)1200

- Computational scheme: component-by-component split operator method

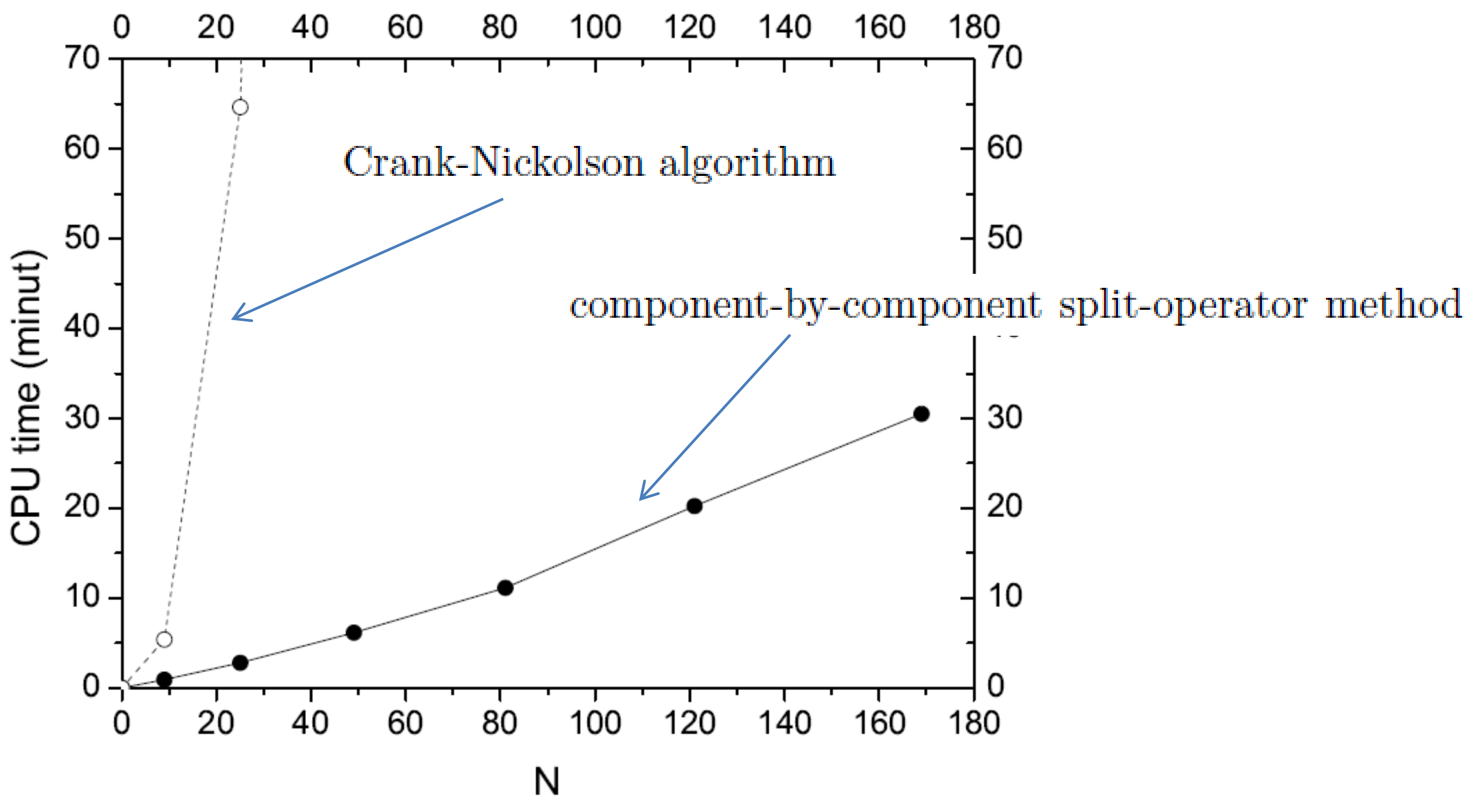
$$i\frac{\partial}{\partial t}\psi_j(\rho_R, r, t) = \sum_{j'}^{N} H_{jj'}(\rho_R, r)\psi_{j'}(\rho_R, r, t) \qquad t_n \to t_{n+1} = t_n + \Delta t$$

interaction is diagonal in ndDVR $f_j(\Omega)$
kinetic energy operator is diagonal $Y_\nu(\Omega) = Y_{lm}(\Omega)$

$$S_{j\nu} = \lambda_j^{1/2} Y_{j\nu}$$

V.Melezhik, Phys.Lett.A230(1997)203
V.Melezhik, EPJ Web of Conf 108(2007)01008

economic computational scheme



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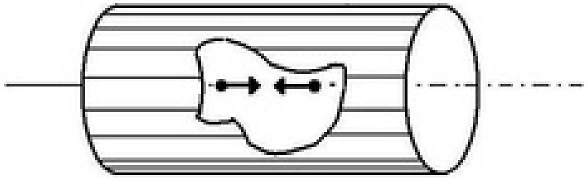
BLTP JINR two-core Intel processor Xenon 5160 with 3GHz frequency

Atom-atom CIRs



$$\left([-\frac{\hbar^2}{2\mu}\triangle_{\mathbf{r}} + \frac{1}{2}\mu(\omega_x^2 x^2 + \omega_y^2 y^2)]\hat{I} + \hat{V}(r)\right)|\psi(\mathbf{r})\rangle = E|\psi(\mathbf{r})\rangle$$

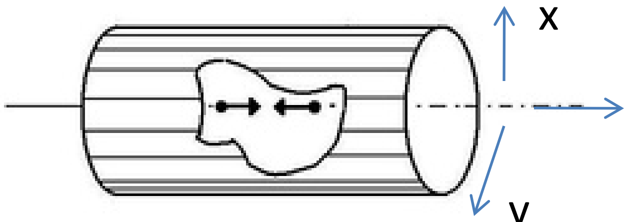
$$|\psi(\mathbf{r})\rangle = \sum_{\alpha} \psi_\alpha(\mathbf{r})|\alpha\rangle \ , \ \ \alpha = \{e, c = 1...\}$$

$$\hat{V}(r) = \begin{pmatrix} -V_e & \hbar\Gamma_1 & \hbar\Gamma_2 & \hbar\Gamma_3 \\ \hbar\Gamma_1 & -V_1 + \delta\mu_1(B - B_1) & 0 & 0 \\ \hbar\Gamma_2 & 0 & -V_2 + \delta\mu_2(B - B_2) & 0 \\ \hbar\Gamma_3 & 0 & 0 & -V_3 + \delta\mu_3(B - B_3) \end{pmatrix} \quad r < \bar{a}$$

$$\psi_e(\mathbf{r}) = (\exp\{ik_0 z\} + f_e \exp\{ik_0 \mid z \mid\})\,\Phi_0(x, y) \ , \ \ \psi_c(\mathbf{r}) \to 0$$

four coupled 3D Schrödinger-like equations

Atom-atom CIRs

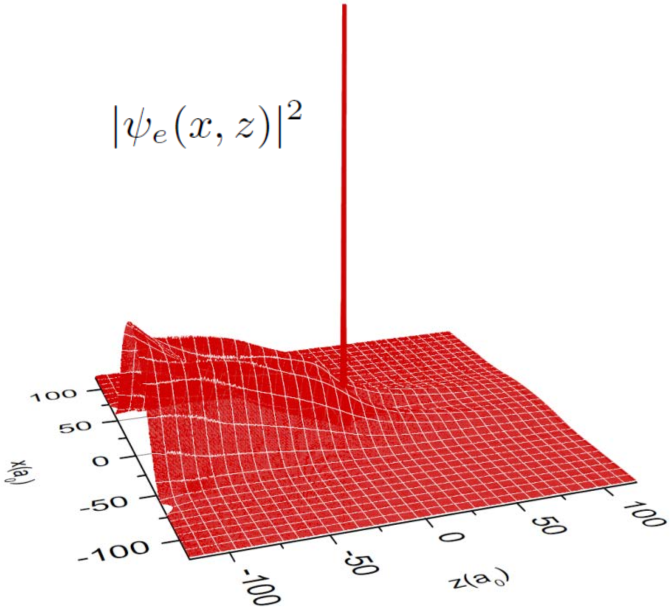


$$\left([-\frac{\hbar^2}{2\mu}\triangle_{\mathbf{r}} + \frac{1}{2}\mu(\omega_x^2 x^2 + \omega_y^2 y^2)]\hat{I} + \hat{V}(r)\right)|\psi(\mathbf{r})\rangle = E|\psi(\mathbf{r})\rangle$$

$$\sum_{p=1}^{3} R_{n-p}\hat{I}\mathbf{u}_{n-p} + \left(\hat{A}_n + \hat{W}_n + \hat{V}_n - E\hat{I}\right)\mathbf{u}_n + \sum_{p=1}^{3} R_{n+p}\hat{I}\mathbf{u}_{n+p} = 0, \quad (n = 1, 2, ..., N_r - 3),$$

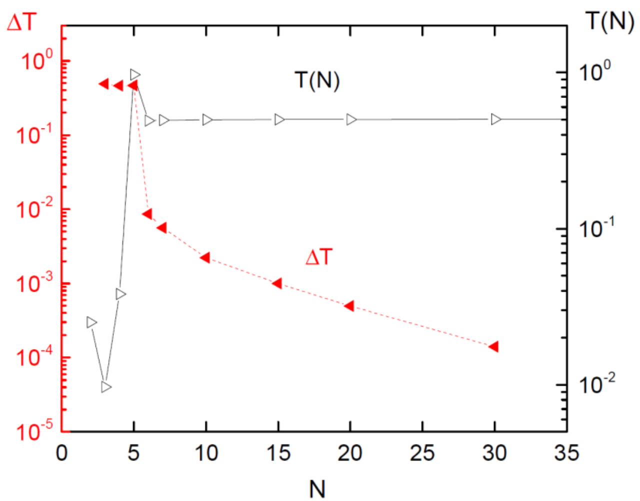
$$\mathbf{u}_n + \hat{B}_n\mathbf{u}_{n-1} = \mathbf{g}_n \quad (n = N_r - 2, N_r - 1, N_r).$$

$|\psi_e(x, z)|^2$



convergence of the npDVR

$$T = |1 + f_e|^2$$



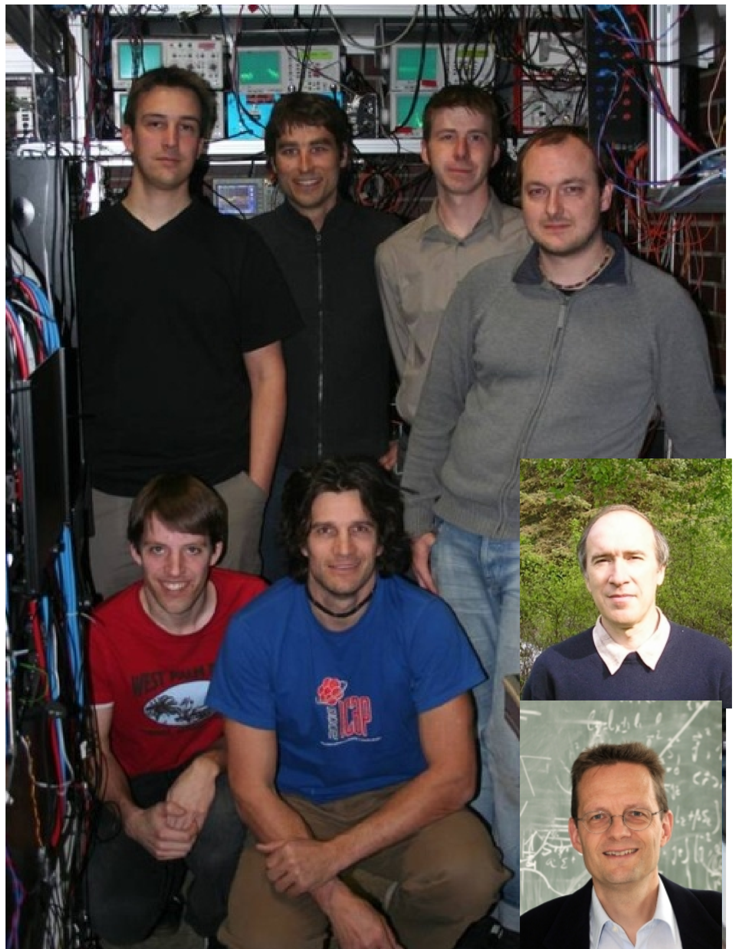
PRL **104,** 153203 (2010) PHYSICAL REVIEW LETTERS week ending 16 APRIL 2010

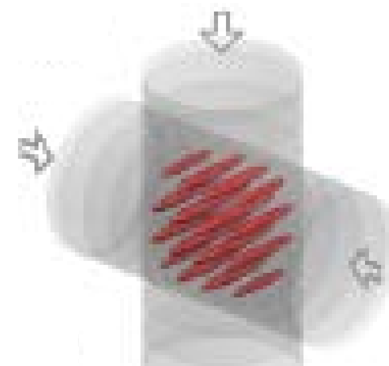
Confinement-Induced Resonances in Low-Dimensional Quantum Systems

Elmar Haller,[1] Manfred J. Mark,[1] Russell Hart,[1] Johann G. Danzl,[1] Lukas Reichsöllner,[1] Vladimir Melezhik,[2] Peter Schmelcher,[3] and Hanns-Christoph Nägerl[1]

[1]*Institut für Experimentalphysik and Zentrum für Quantenphysik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria*
[2]*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, 141980 Dubna, Russia*
[3]*Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany*
(Received 19 February 2010; published 14 April 2010)

Elmar Haller –>
Outstanding Doctoral Thesis in AMO Physics Recipients for 2011

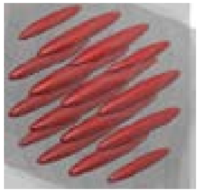


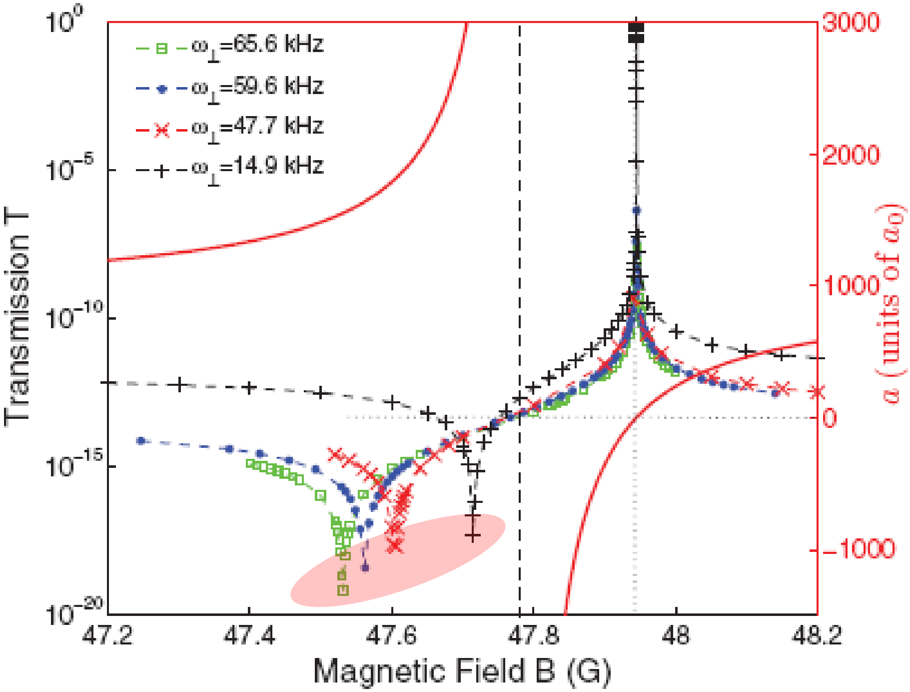


Shifts and widths of Feshbach resonances in atomic waveguides

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

$$a_\perp = \sqrt{\hbar/(m\omega_\perp)}$$





d-wave FR at 47.8G develops in waveguide as depending on $\omega_\perp$ minimums and stable maximum of transmission coefficient T

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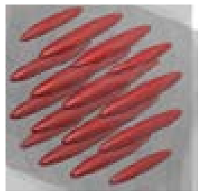

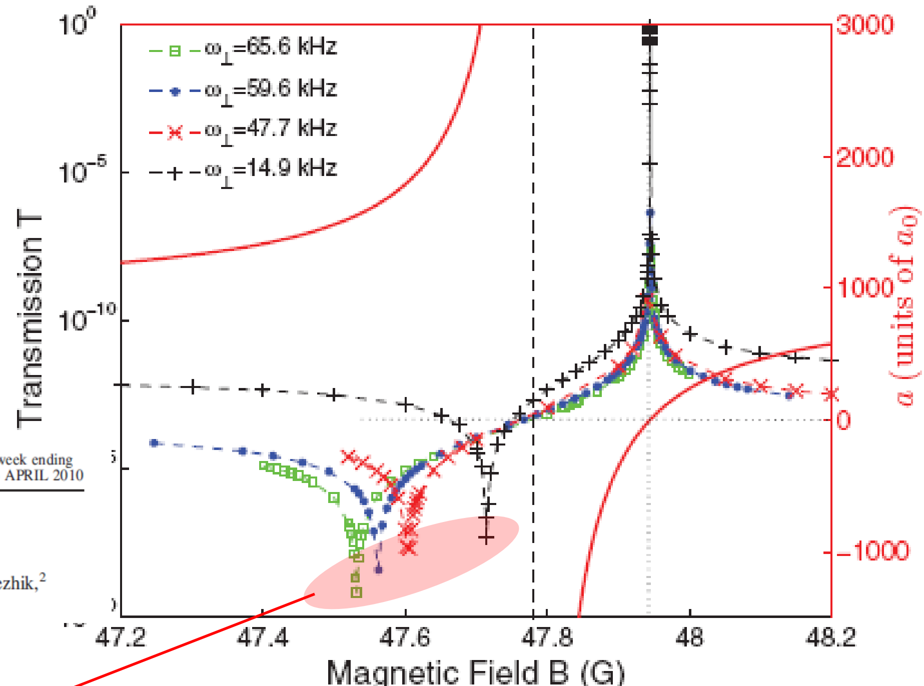

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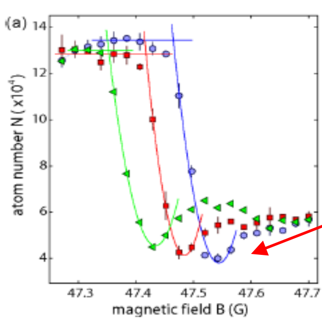

experiment

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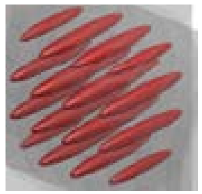

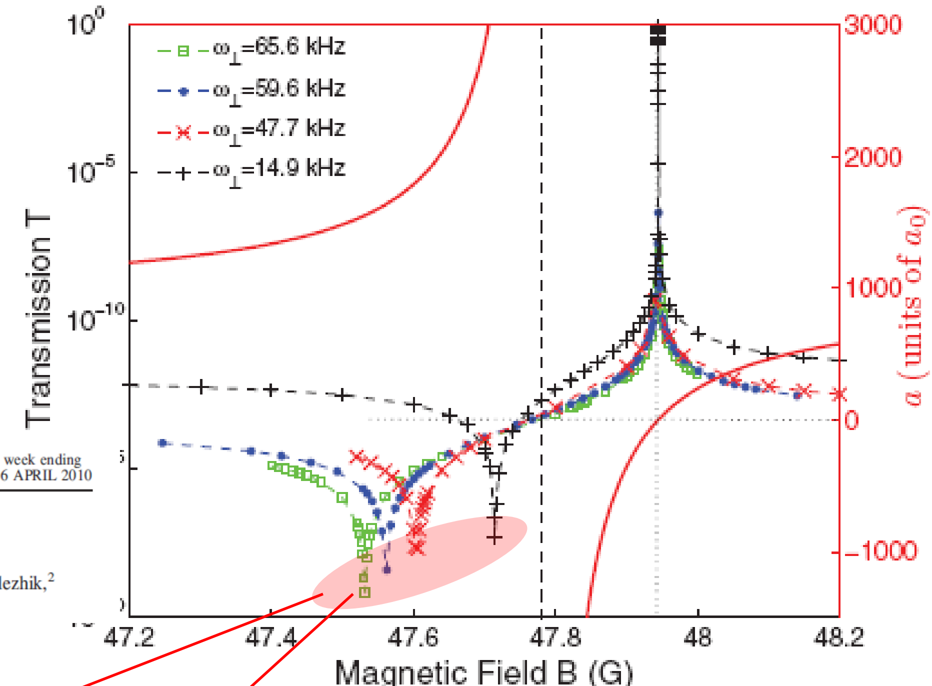

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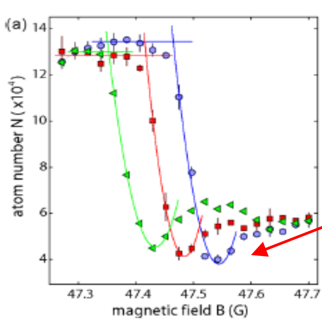
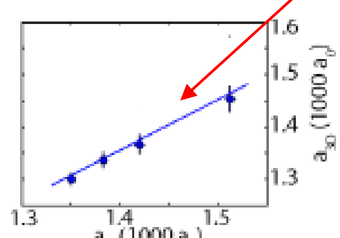


experiment

theory

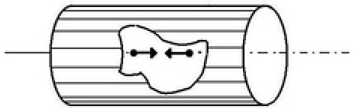


Olshanii formula

$$a_\perp = 1.46\, a_{3D}$$

works !

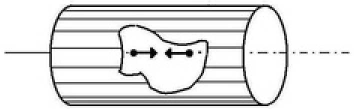
Atom-atom CIRs



$$\left(-\frac{1}{\mu}\nabla_r^2 + \mu\omega_\perp^2\rho^2 + \frac{C_{12}}{r^{12}} - \frac{1}{r^6}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$r^{*2} = \frac{\sqrt{2\mu C_6}}{\hbar} \quad E^* = \frac{\hbar^2}{2\mu(r^*)^2}$$

Atom-atom CIRs



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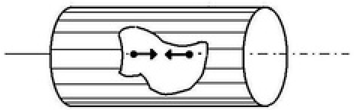
modern atomic traps $\omega_\perp = 2\pi \times (10 - 100)\mathrm{kHz}$

Atom-atom CIRs



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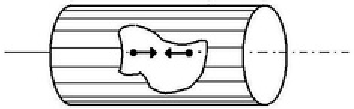
modern atomic traps $\omega_\perp = 2\pi \times (10 - 100)\mathrm{kHz}$

permit to work only within long-wavelength limit (LWL)

$E \ll E^*$

Atom-atom CIRs



$$\left(-\frac{1}{\mu}\nabla_r^2 + \mu\omega_\perp^2\rho^2 + \frac{C_{12}}{r^{12}} - \frac{1}{r^6}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$r^{*2} = \frac{\sqrt{2\mu C_6}}{\hbar} \qquad E^* = \frac{\hbar^2}{2\mu(r^*)^2}$$

modern atomic traps $\omega_\perp = 2\pi \times (10 - 100)\mathrm{kHz}$

permit to work only within long-wavelength limit (LWL)

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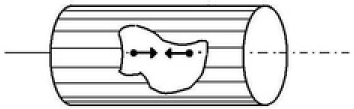

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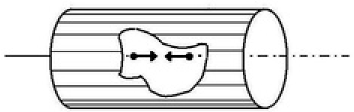

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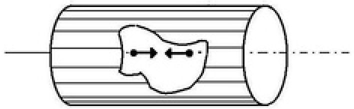

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quasi-1D Schrödinger eq. (M. Olshanii, PRL (1998))

$$\left(-\frac{1}{\mu}\frac{d^2}{dz^2} + g_{1D}\delta(z)\right)\psi(z) = E\psi(z)$$

$$g_{1D} = \frac{2a_{3D}}{\mu a_\perp^2[a_\perp + \zeta(1/2)a_{3D}]} = \frac{2k}{\mu}\frac{\mathrm{Re}[f^+ + f^-]}{\mathrm{Im}[f^+ + f^-]}$$

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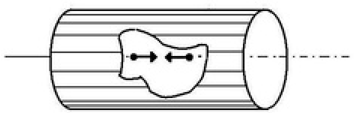

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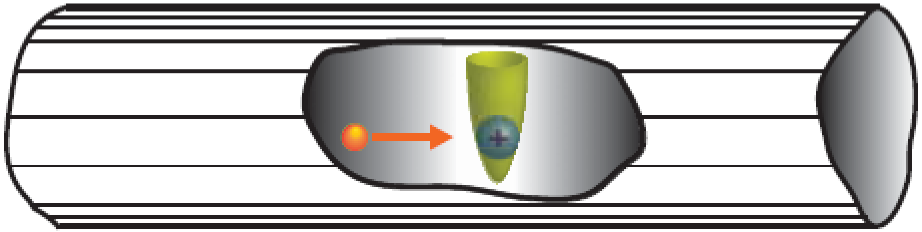
CIR : $\frac{a_\perp}{a_{3D}} = -\zeta(1/2) = 1.4603$

Confined ultracold atom-ion collisions



atom-ion Hamiltonian in confined geomery

$$\hat{H} = -\frac{\hbar^2}{2m_A}\nabla_A^2 + \frac{1}{2}m_A\omega_\perp^2(x_A^2 + y_A^2)$$
$$-\frac{\hbar^2}{2m_I}\nabla_I^2 + \frac{1}{2}m_I\omega^2|\mathbf{r}_I|^2 + V(|\mathbf{r}_A - \mathbf{r}_I|)$$

long-range atom-ion polarization interaction

$$V(|\mathbf{r}_A - \mathbf{r}_I|) \to -\frac{C_4}{|\mathbf{r}_A - \mathbf{r}_I|^4}$$

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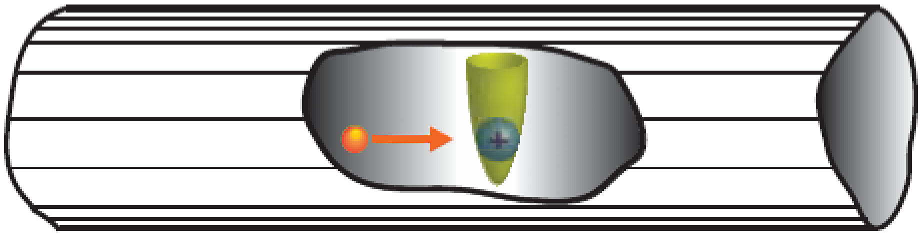

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^{6}Li-^{171}Yb^{+}

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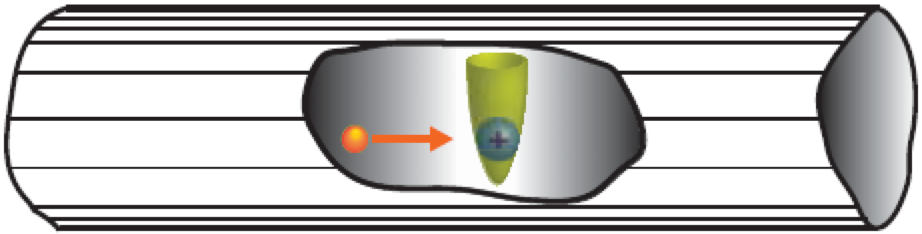

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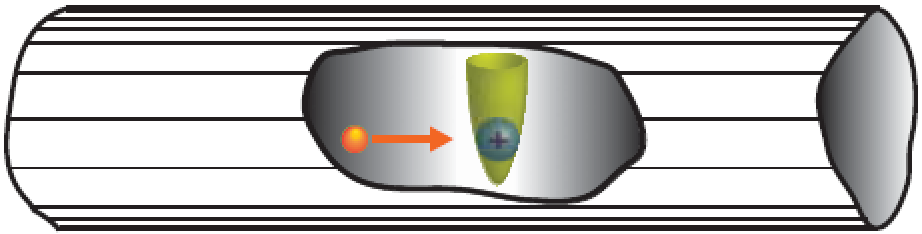

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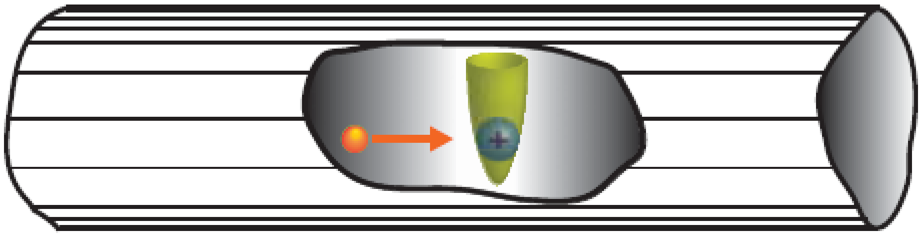

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Confined ultracold atom-ion collisions

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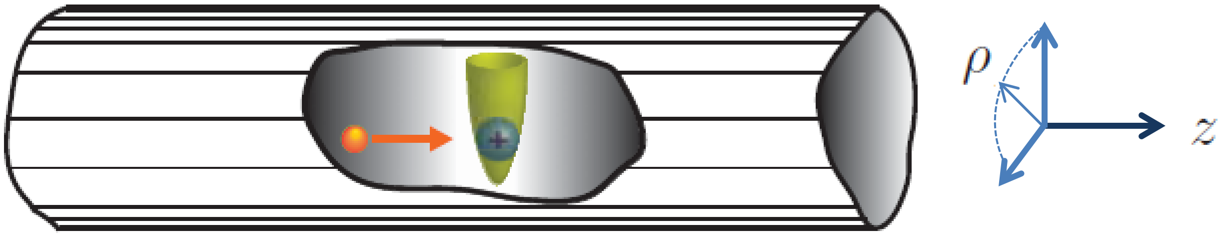

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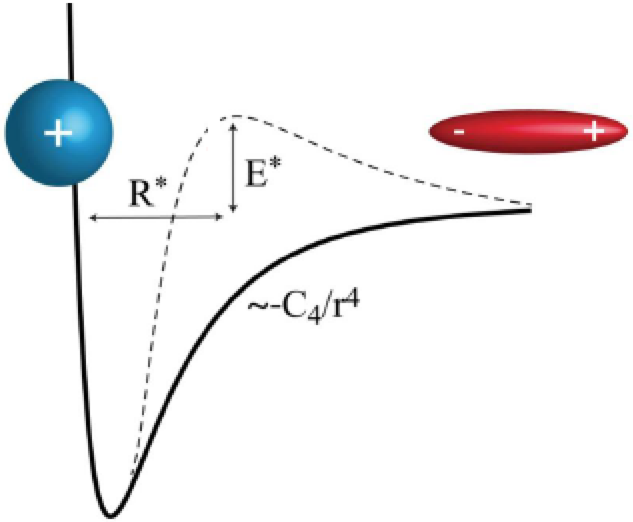

Confined ultracold atom-ion collisions

"static" ion
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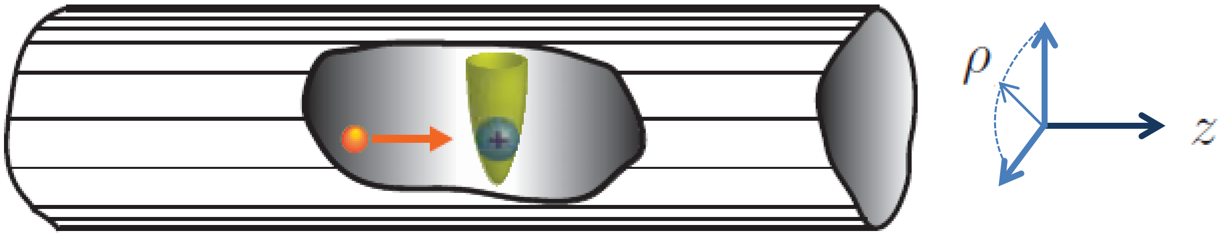

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Confined ultracold atom-ion collisions

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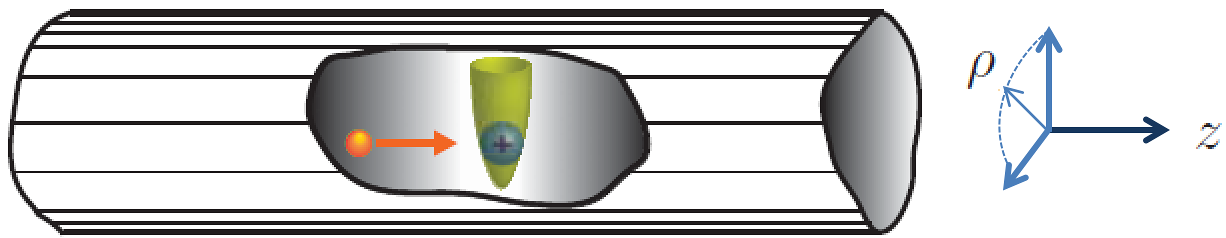

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$$\psi(z,\rho) = [\exp(ikz) + f^{\pm}(k,\omega_\perp)\exp(ik|z|)]\varphi_0(\rho)$$

Confined ultracold atom-ion collisions

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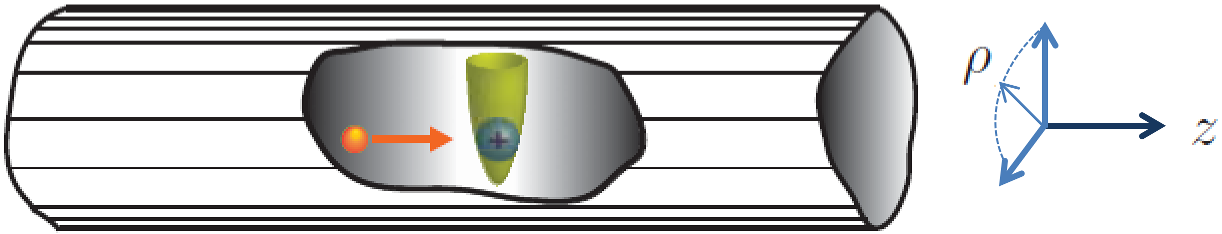

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$\varphi_0(\rho)$ – the ground state of 2D harmonic oscillator,
$k = \sqrt{m_A E_\parallel}/\hbar$ – the wave-number defined by $E_\parallel = (E - \hbar\omega_\perp)$

Confined ultracold atom-ion collisions

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$$T(k,\omega_\perp) = |1 + f^+(k,\omega_\perp)|^2$$

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parameterize quasi-1D scattering in waveguide-like traps

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confinement-induced resonance (CIR)

parameterize quasi-1D scattering in waveguide-like traps

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zero-energy limit: $(E,k) \Rightarrow 0$

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atom-ion interaction: $C_{12} \longleftrightarrow a_{3D}$

confining trap: $\omega_\perp \longleftrightarrow a_\perp$

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s-wave scattering length in free-space $a_{3D} = -f_0(C_{12}, k \rightarrow 0)$

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Confined ultracold atom-ion collisions

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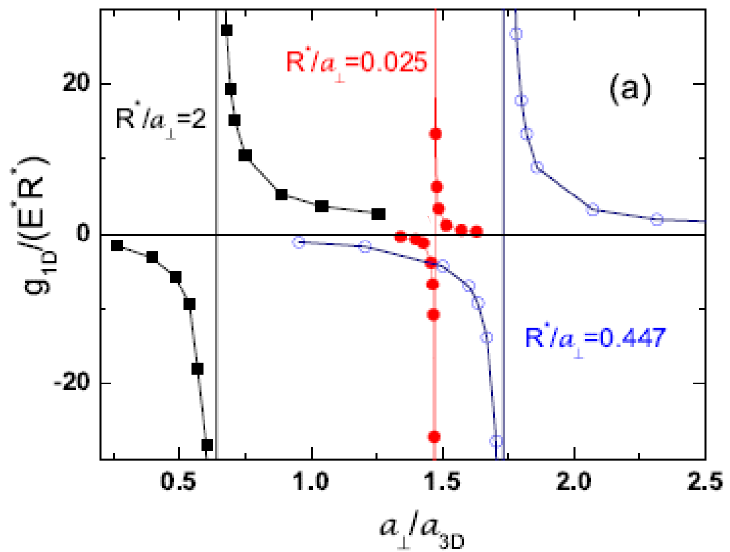

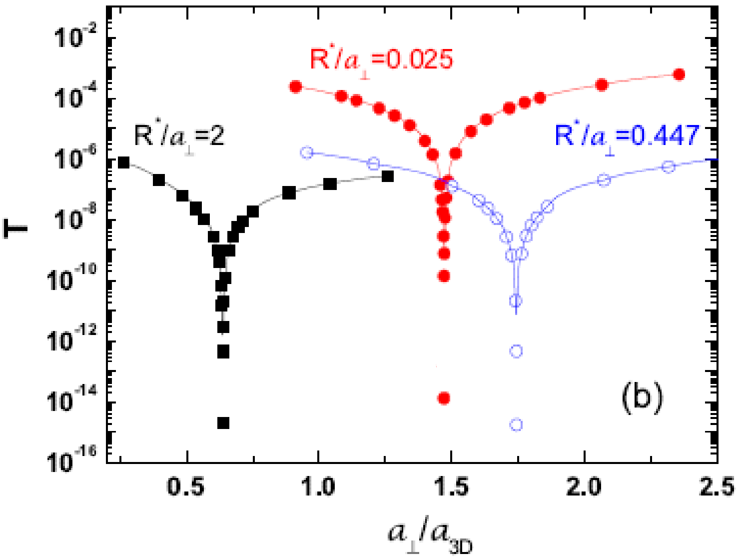

atom-ion pair ^{6}Li-^{171}Yb$^+$

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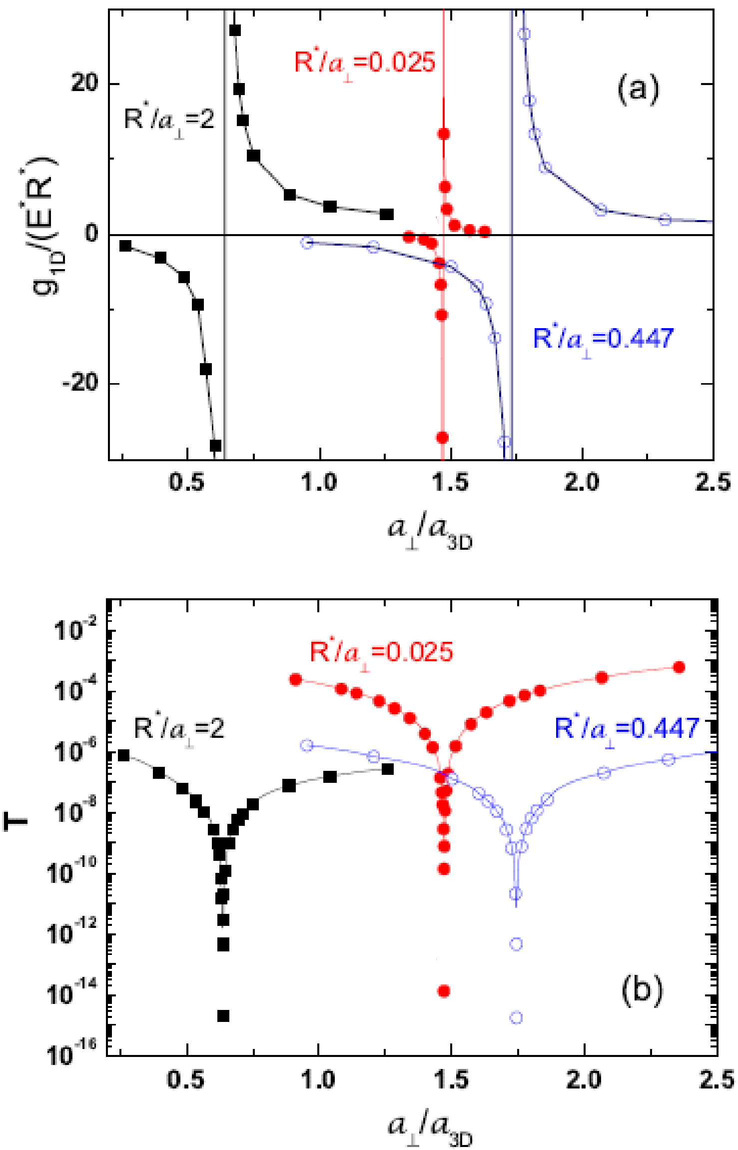

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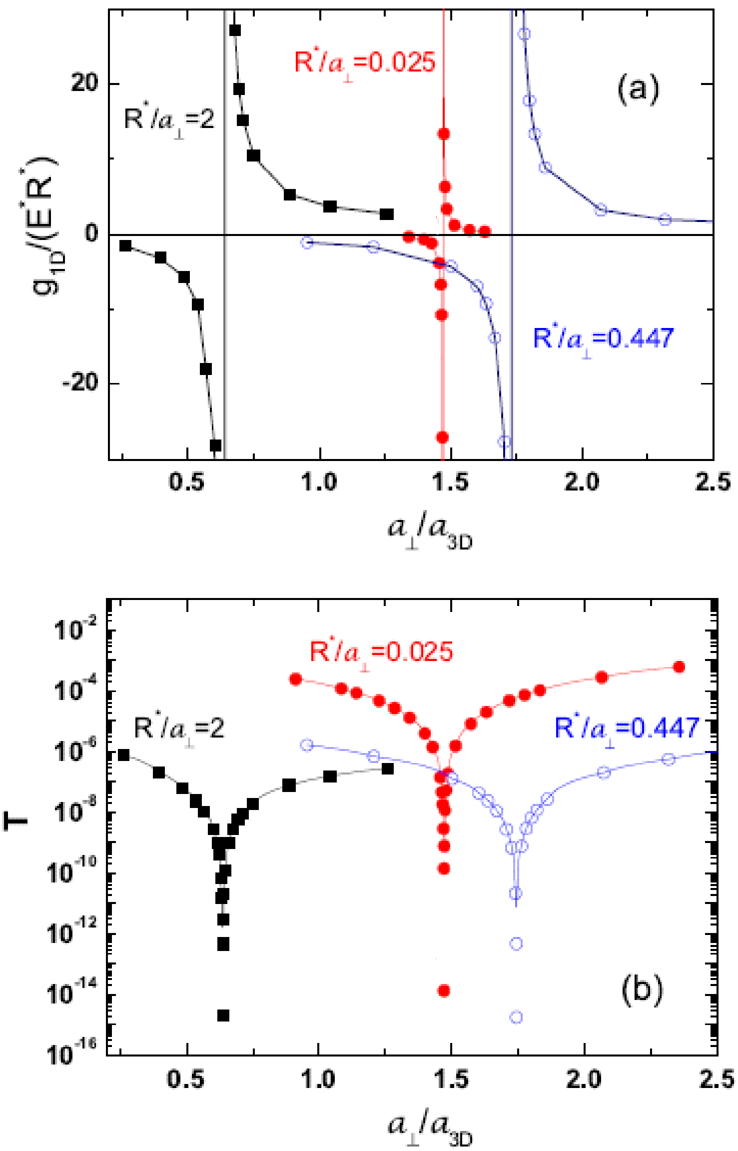

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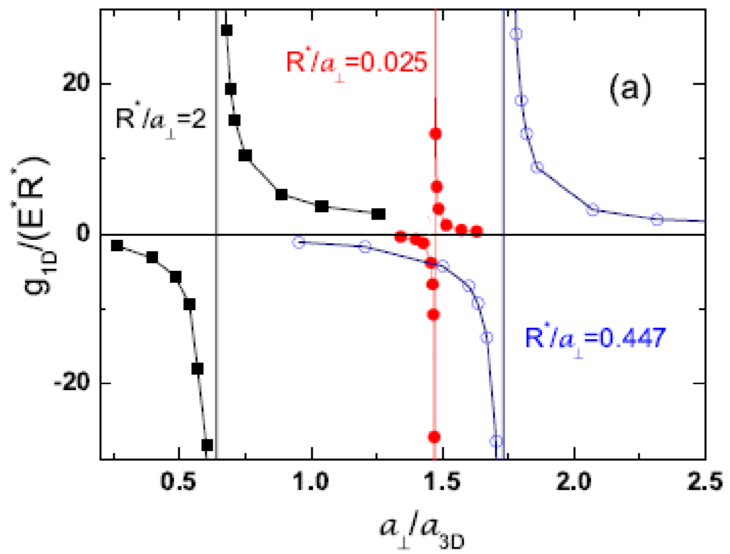

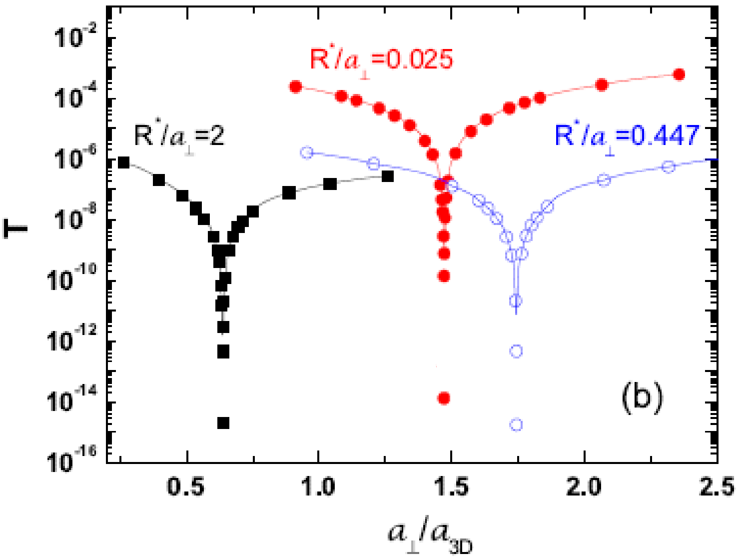

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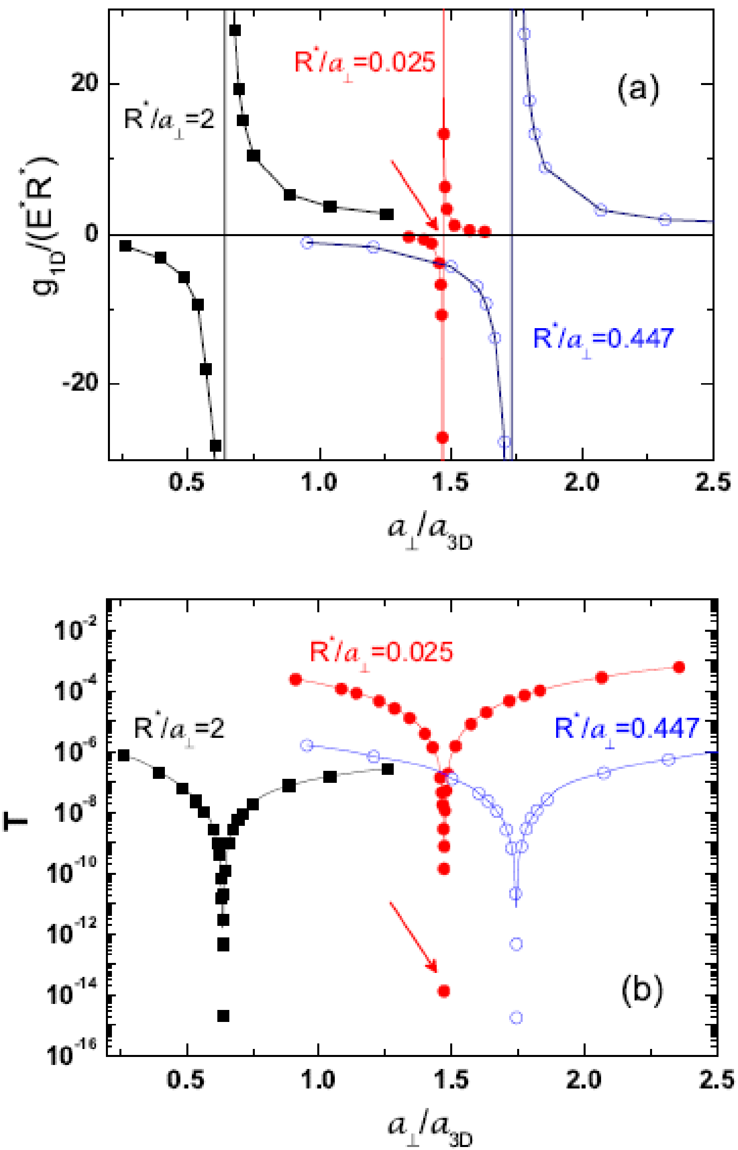

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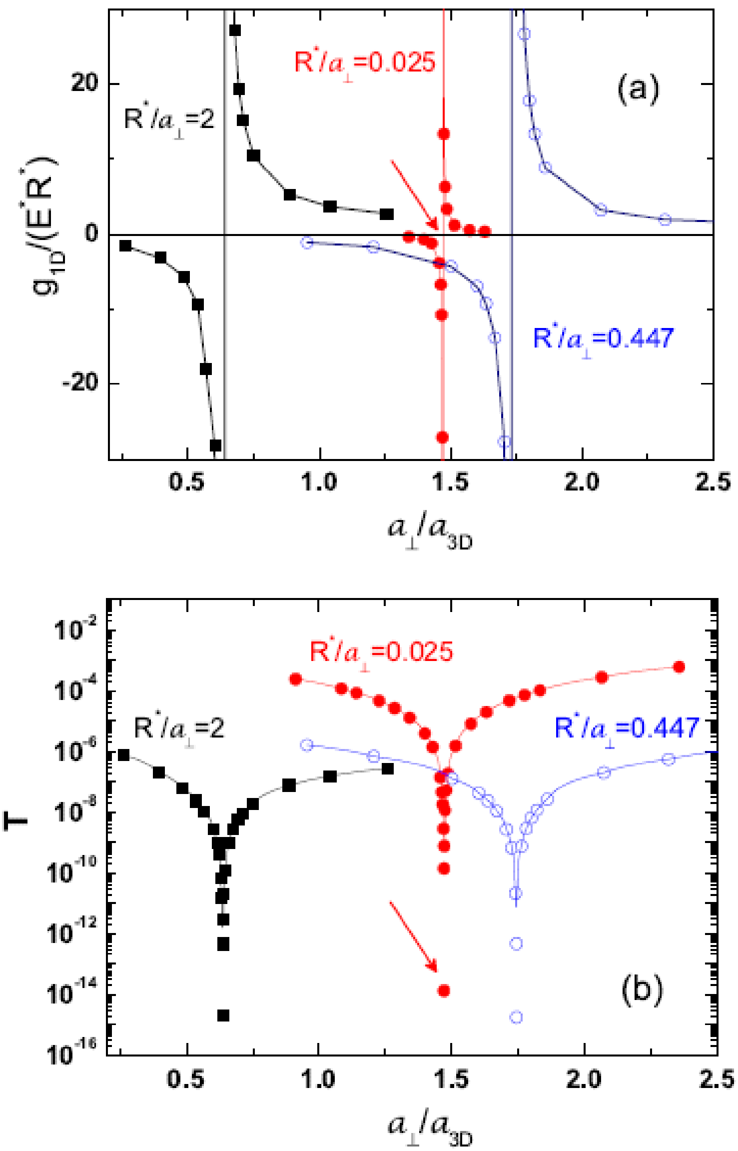

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what happens outside LWL

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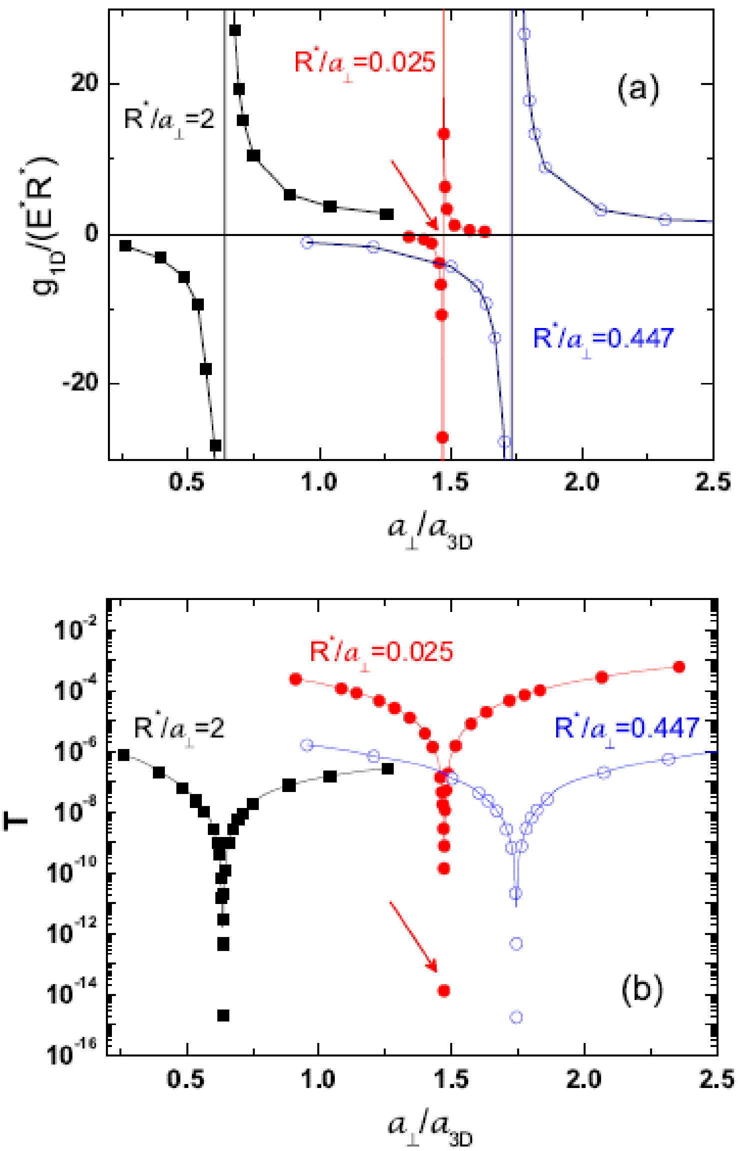

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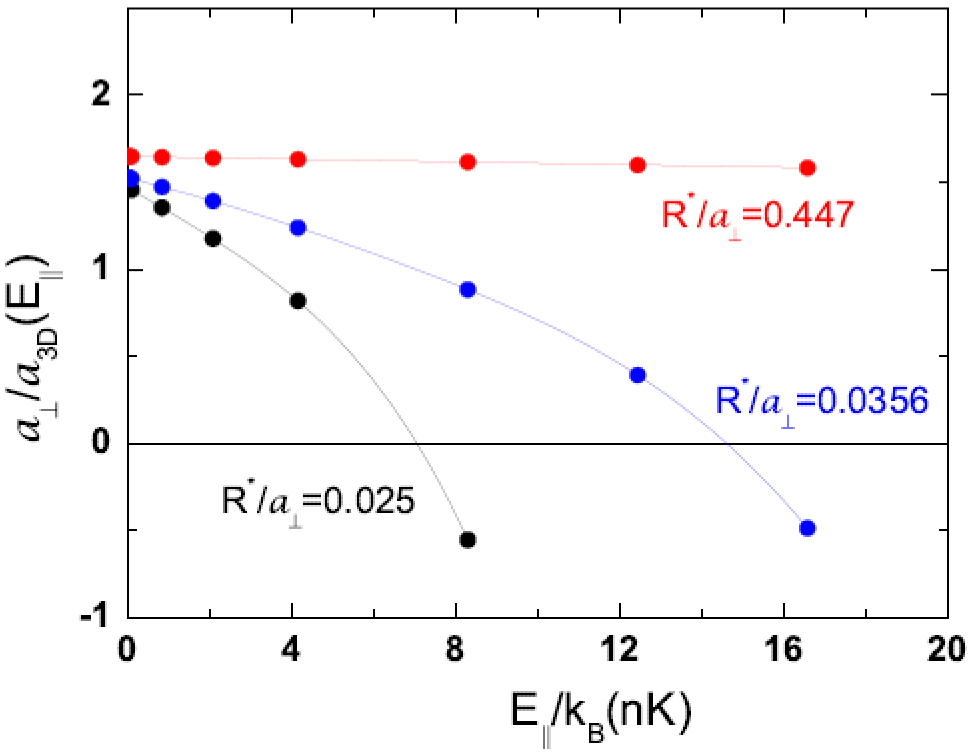

atom-ion pair ^{6}Li-^{171}Yb^{+}

numerical integration of 2D Schrödinger eq.

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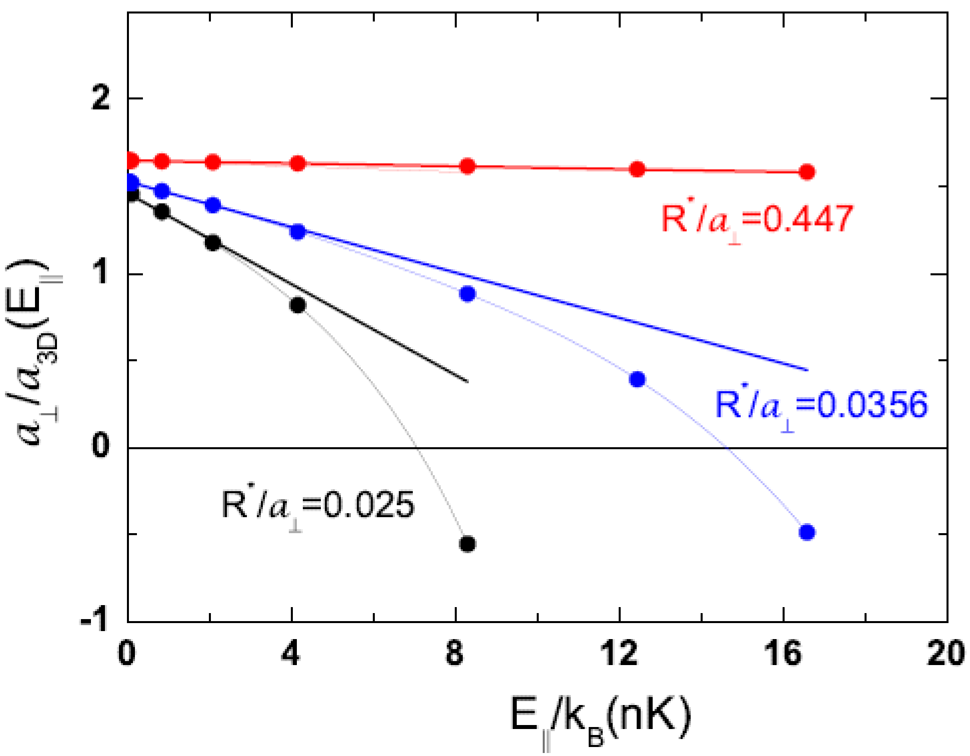

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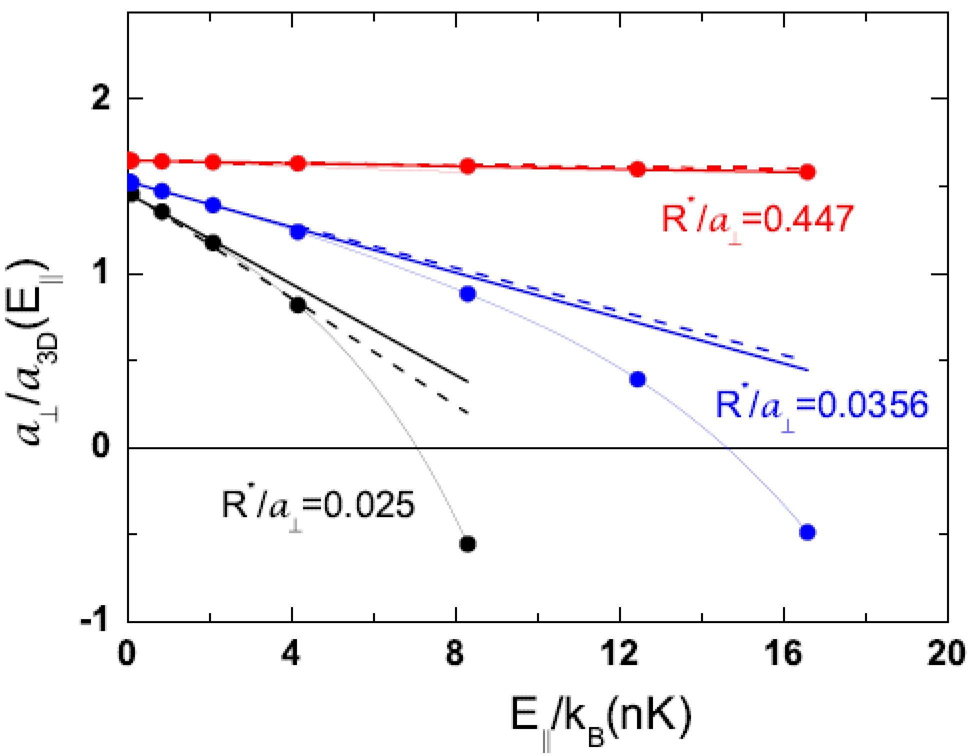

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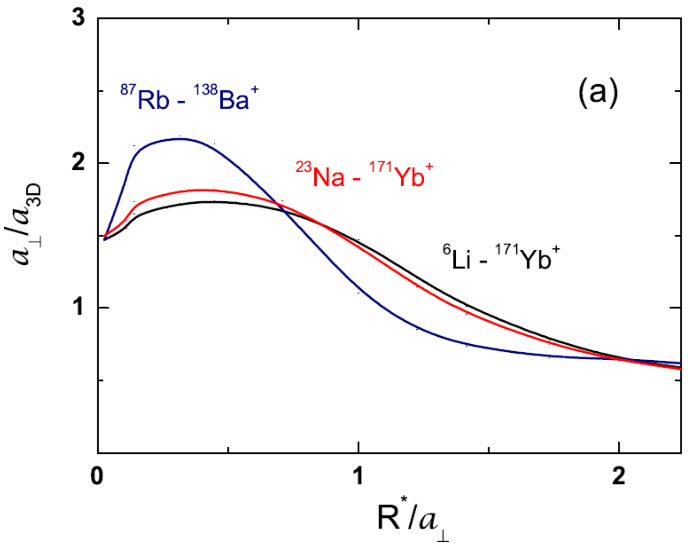

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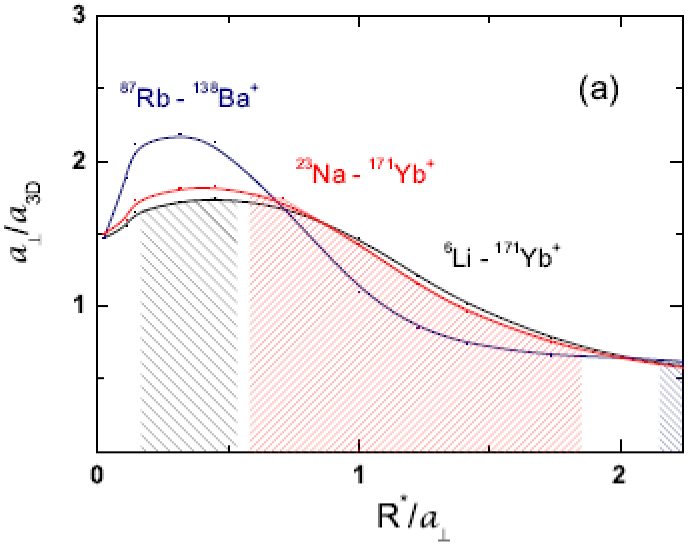

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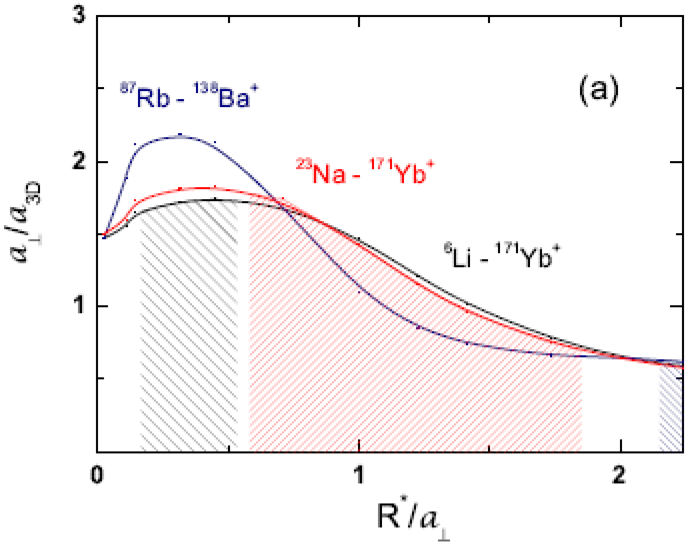

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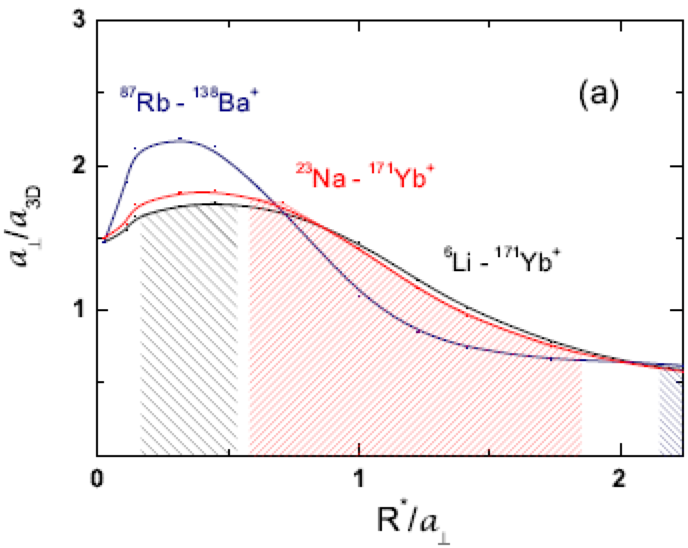

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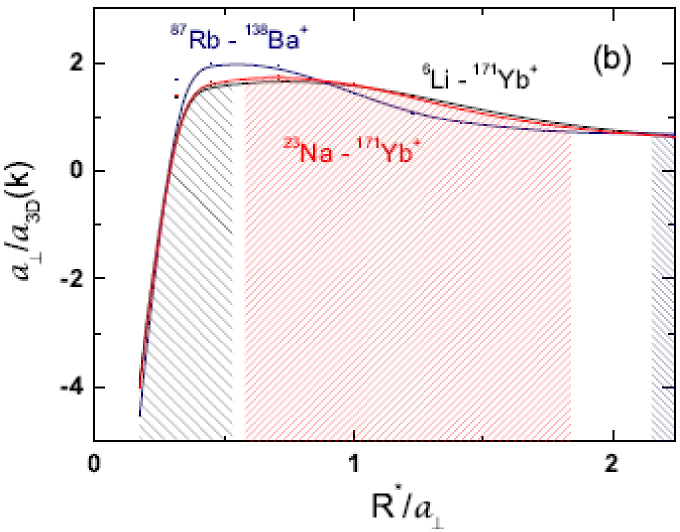
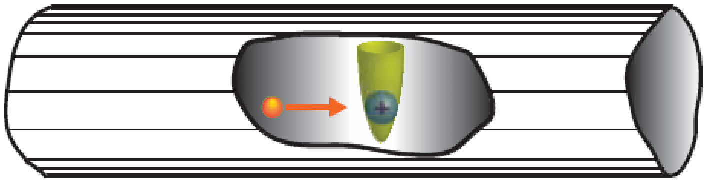


strong dependence of CIR position on the ratio $R^*/a_\perp$ and isotope-like effect

(b) $a_\perp/a_{3D}(k)$ in points of CIR at finite colliding energy $E_\parallel/E^* = 0.117$ corresponds to $E_\parallel/k_B = 1\mu$K (^{6}Li-^{171}Yb$^+$), $6n$K (^{87}Rb-^{138}Ba$^+$), $80n$K (^{23}Na-^{171}Yb$^+$)

Impact of Ion Micromotion-Induced Heating



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Paul trap

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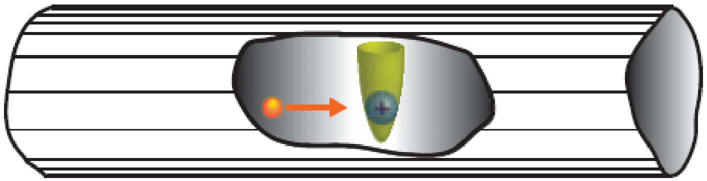

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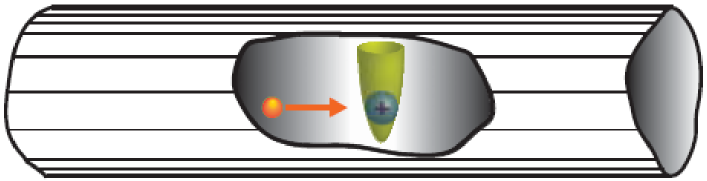

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atom in rest - ion moving with V_I

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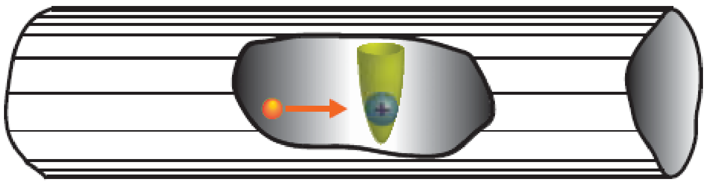

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by change the frame of reference, where
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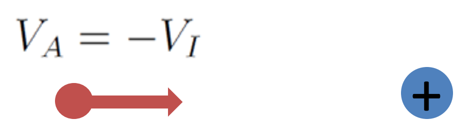

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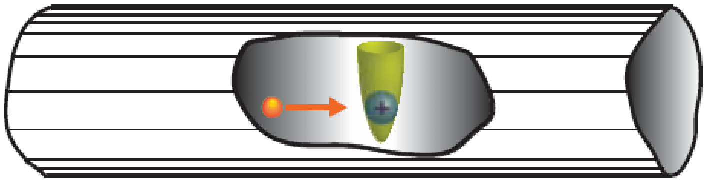
quasi-classical treatment of ion micromotion

Impact of Ion Micromotion-Induced Heating



$$H(t) = \frac{p_i^2}{2m_i} + \frac{p_a^2}{2m_a} + \boxed{\frac{1}{8} m_i \Omega^2 r_i^2 \left(a + 2q\cos(\Omega t)\right)} + V_{dw}(r_a) - \frac{C_4}{(r_i - r_a)^4}$$

Paul trap

confined atom can be cooled to $E_A/k_B = m_A \langle V_A^2 \rangle /(2k_B) \sim$ few nK

due to micromotion ion can be cooled to $E_I/k_B = m_I \langle V_I^2 \rangle /(2k_B) \sim$ few 10μK

because $E_I \gg E_A$ we have $V_A = 0$ and $V_I \neq 0$:

atom in rest - ion moving with V_I

by change the frame of reference, where the atom is moving with $V_A = -V_I$ and the ion is in rest ($V_I = 0$) we return to our model

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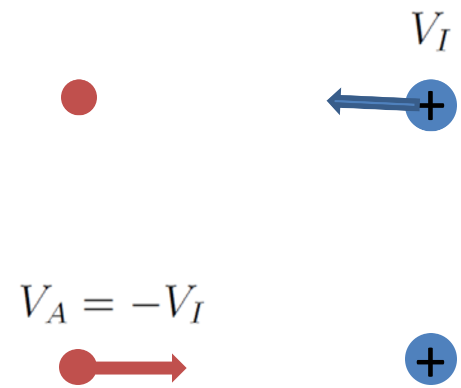

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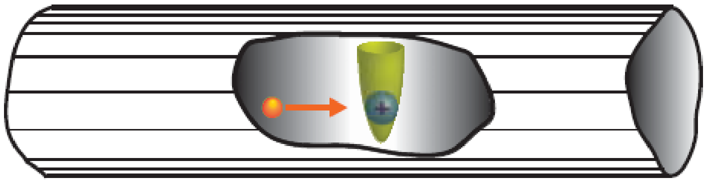

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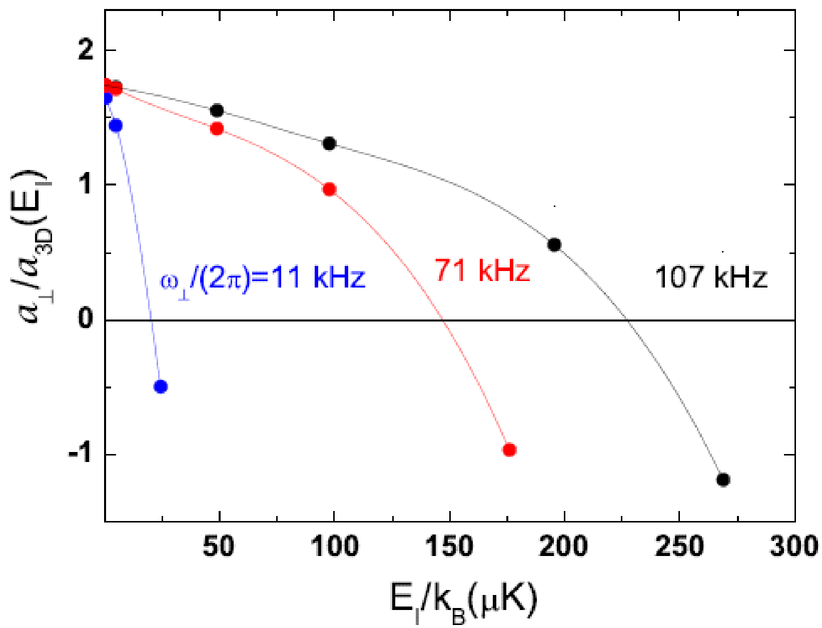

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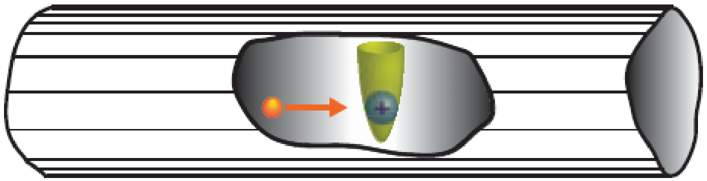

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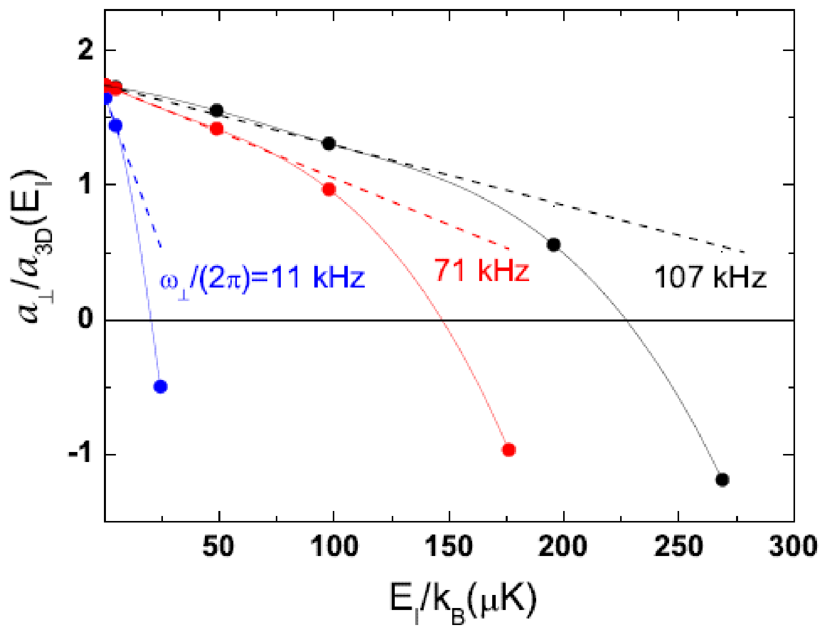
$$\frac{a_\perp}{a_{3D}(k)} = 1.4603 + \Delta(R^*/a_\perp) - 0.6531(\frac{m_A}{\mu})(\frac{E_\parallel}{\hbar\omega_\perp})$$



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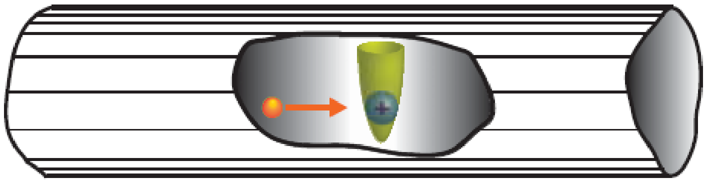

by measuring position of CIR ($a_\perp/a_{3D}(E_\parallel)$ at point where CIR appeares) energy $E_\parallel$ or temperature of confined atomic gas can be determined by calculated curve $a_\perp/a_{3D}(E_\parallel)$

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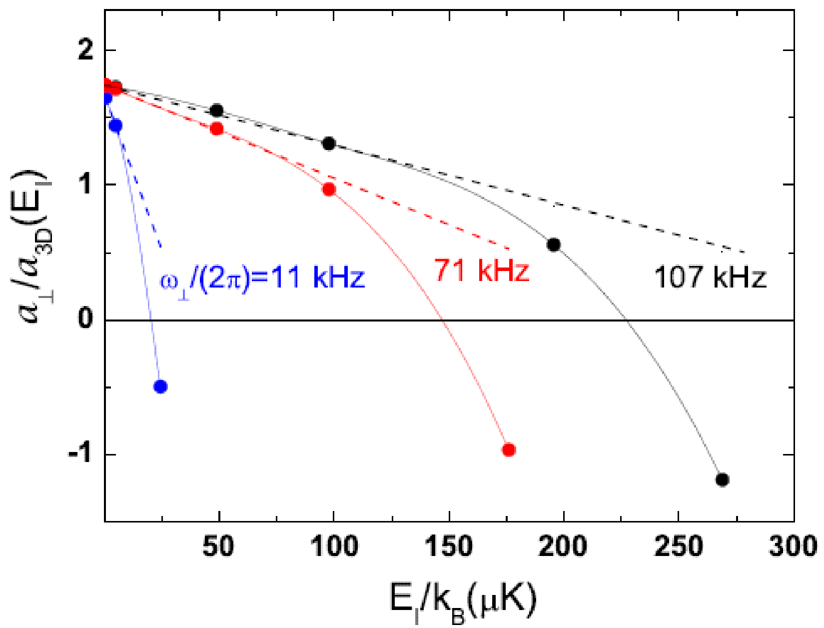
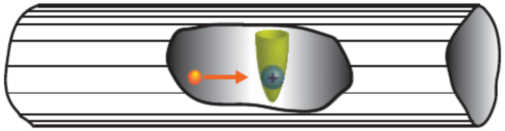


quasi-classical treatment of ion micromotion

Conclusion & Outlook



Our results can be used in current experiments for searching atom-ion CIRs with the aims:

- measuring the atom-ion scattering length $a_{3D}(k)$
- determining the temperature of the atomic gas in the presence of an ion impurity if a_{3D} is known
- tuning the effective atom-ion interaction in confined geometry :

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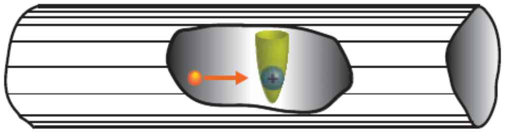

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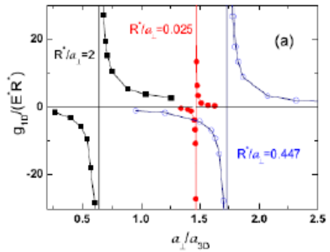
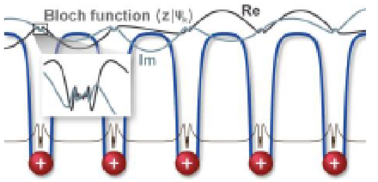
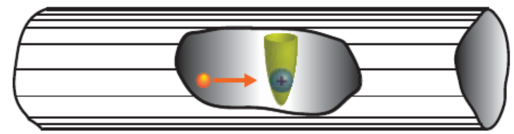
The manipulation of the atom-ion interaction could be exploited to control the atom-phonon coupling in a solid-state quantum simulator, to investigate more exotic quantum phases in low dimensional systems, where simultaneously a strongly correlated atom-atom and the atom-ion system is created





U. Bissbort *et al.*, PRL 111, 080501 (2013)

Conclusion & Outlook



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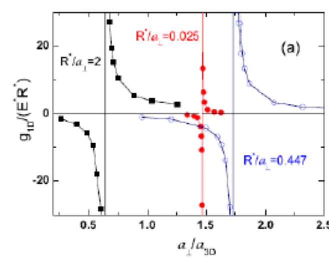
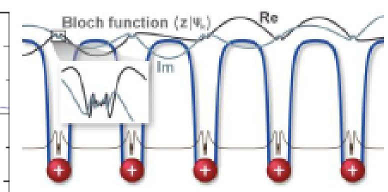
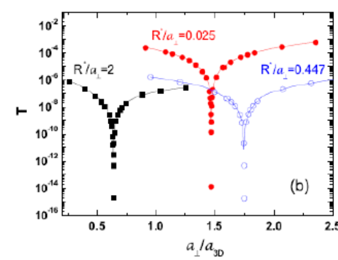




U. Bissbort *et al.*, PRL 111, 080501 (2013)

The complete reflection of the confined atom from the ion in the CIR can also be exploited to realise a device for triggering the confined atom flow, similarly to a single atom transistor

A. Micheli, A. J. Daley, D. Jaksch, and P. Zoller, PRL **93** (2004)



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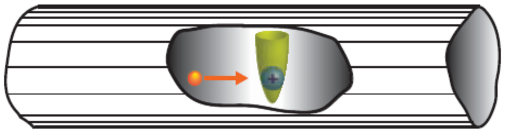

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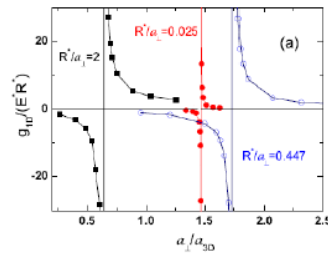

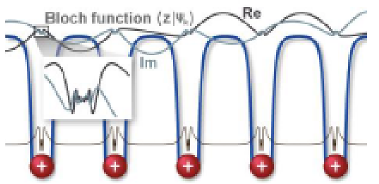

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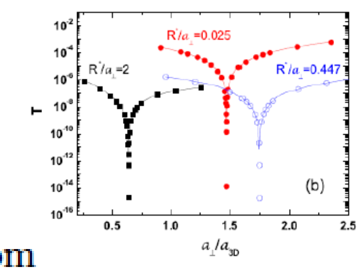

Current experimental set-ups permit to investigate the atom-atom CIRs only in "long wave-length limit" ($R^* \ll a_\perp$) and the atom-ion CIRs - in much more broader region ($R^* \gtrsim a_\perp$) .

Conclusion & Outlook

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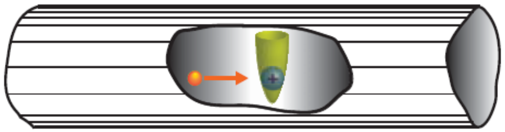

Actual problem: full quantum treatment of ion micromotion influence into CIRs

V.S. Melezhik and A. Negretti, Phys. Rev. A94, 022704 (2016)

V. S. Melezhik, EPJ Web of Conf. 108, 01008 (2016)

Collaboration:

Theory:

P. Schmelcher	Hamburg University, Germany
A. Negretti	Hamburg University, Germany
S. Saeidian	IASBS, Iran
P. Giannakeas	Purdue University, USA
Z. Idziaszek	Warsaw University, Poland

Experiment:

E. Haller	Innsbruck University, Austria
H.-C. Nägerl	Innsbruck University, Austria