Low-Dimensional Few-Body Collisional Processes in Atom-Ion Traps

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Joint Institute for Nuclear Research, Dubna, Russia

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EFB24, Guildford UK, 6 September 2019

Outline

- Why it is interesting: confinement-induced resonances (CIRs) in hybrid atom-ion systems
- Problem: Ω ≈ 2MHz >> ω ≈ 100kHz >> ω ≈ 10kHz
- Method: ion (classical) ← coupling → atom (quantum)

  3D Schrödinger ← splitting-up approach in 2D DVR

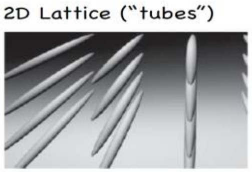
  3 coupled classical Hamiltonian eqs. ← Störmer-Verlet

- Results: CIRs in Li – Yb

- CIRs in two-center confined problem in pseudo-potential approach
-

Why it is interesting

- ultracold atoms



optical traps

Why it is interesting

- ultracold atoms

2D Lattice ("tubes")

optical traps

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)

Quantum simulation with fully controlled few-body systems

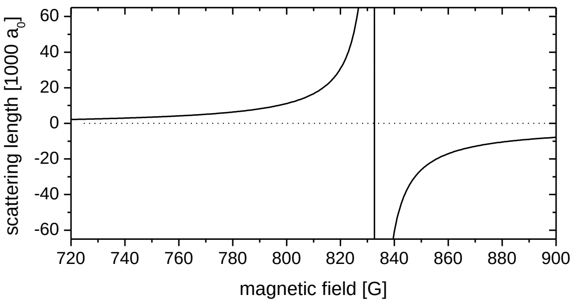
control over: quantum states, particle number, interaction

- 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)
- ...

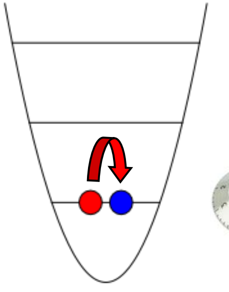
Experiments with deterministically prepared quantum systems

- control interparticle interaction

2 interacting particles in a 1D potential



magnetic Feshbach resonance



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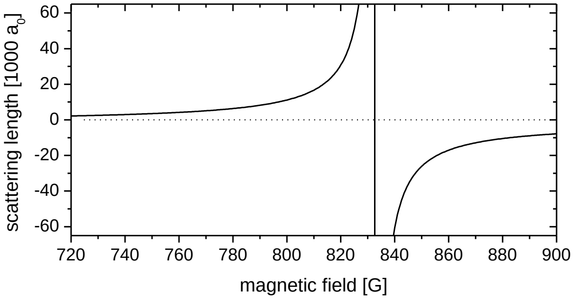

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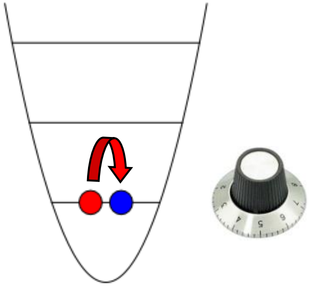
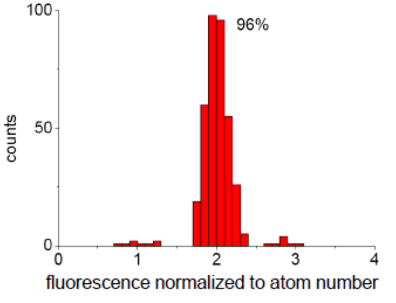


- control over quantum states and particle number with long lifetime



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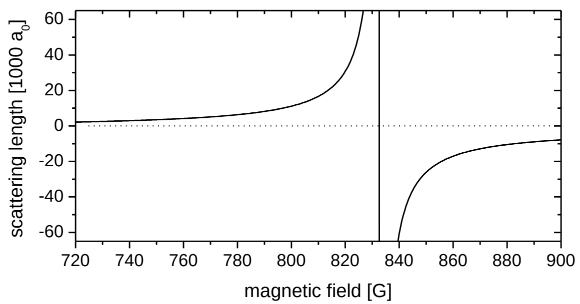

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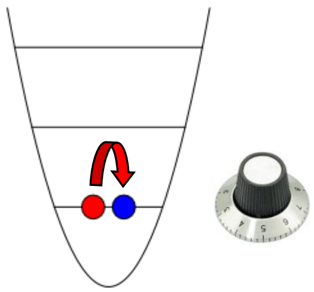

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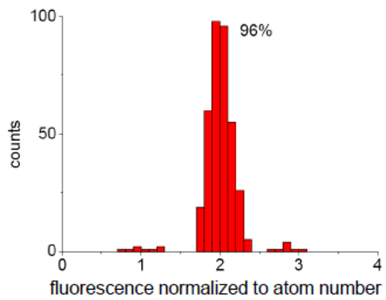


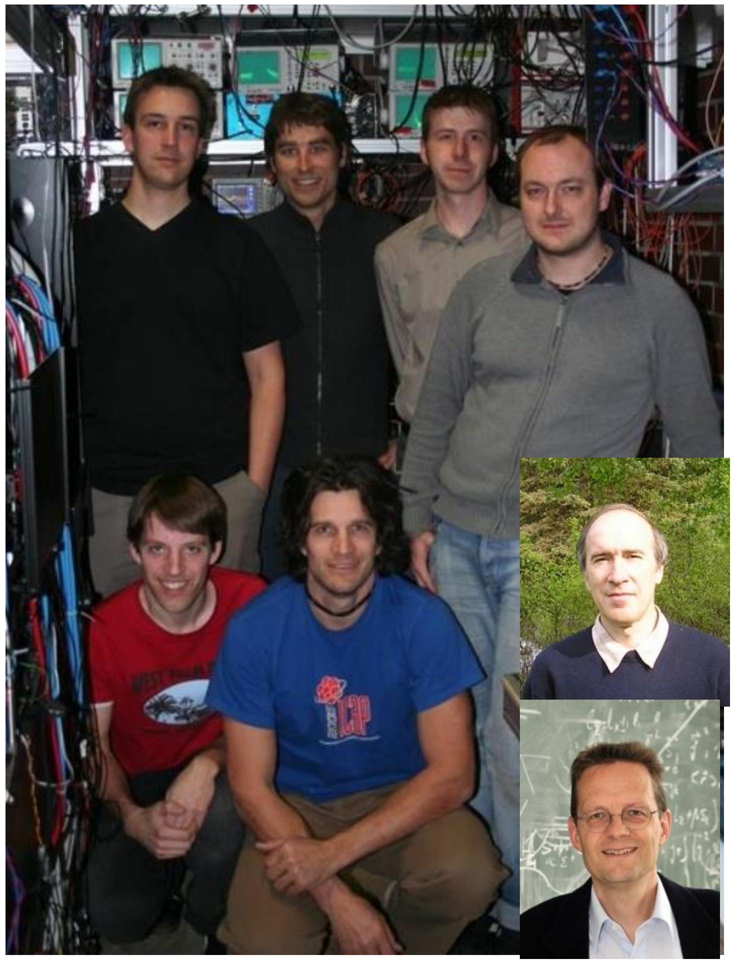
quantum simulation with fully controlled few-body systems

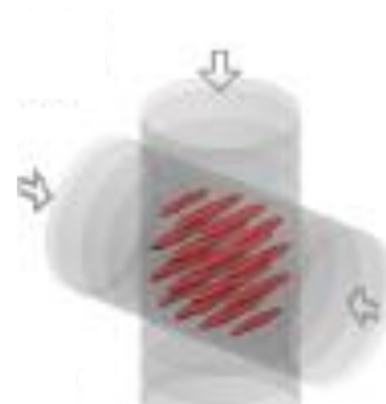
G.Zürn et. al. Phys. Rev. Lett. 108, 075303 (2012)

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)

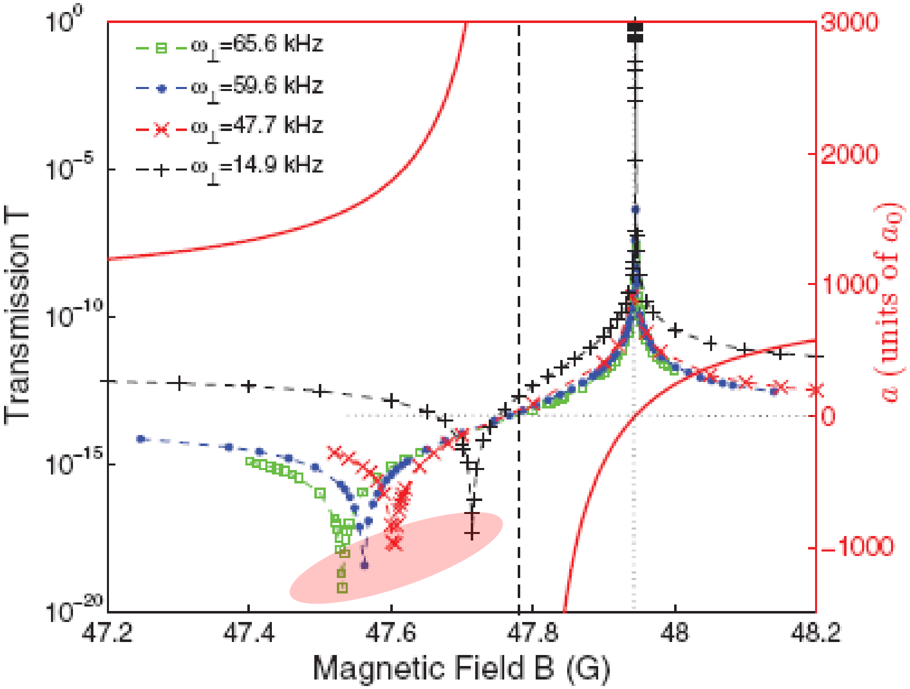




Shifts and widths of Feshbach resonances in atomic waveguides

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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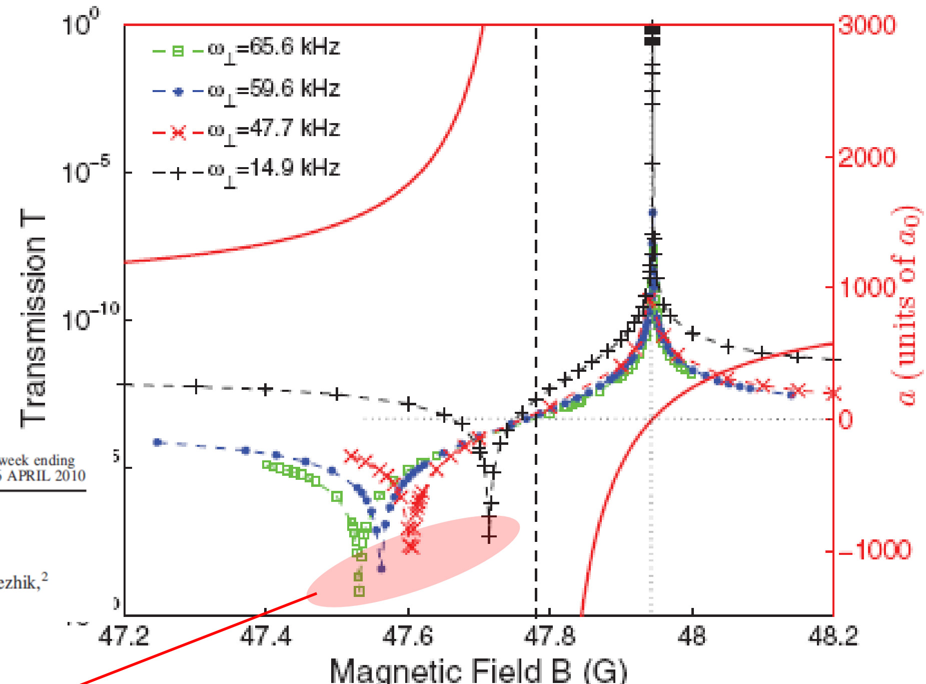

PRL 104, 153203 (2010) PHYSICAL REVIEW LETTERS week ending 16 APRIL 2010

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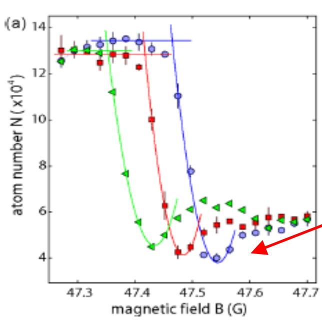

experiment

Shifts and widths of Feshbach resonances in atomic waveguides

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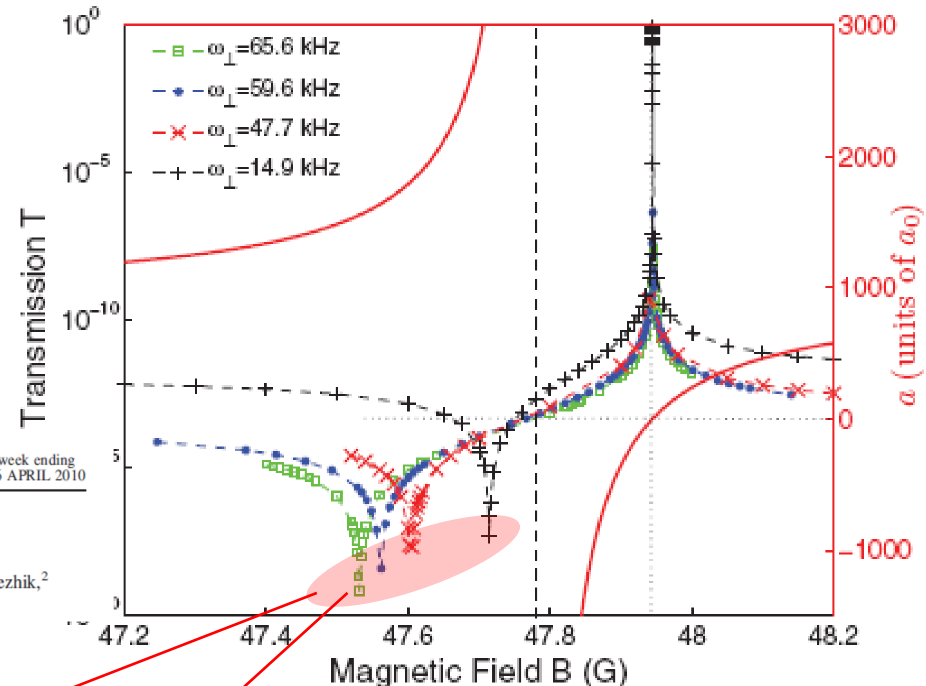

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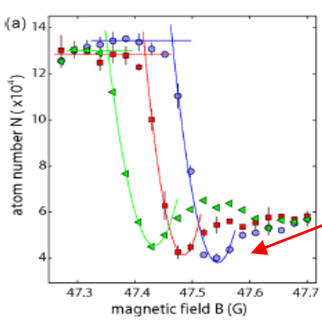
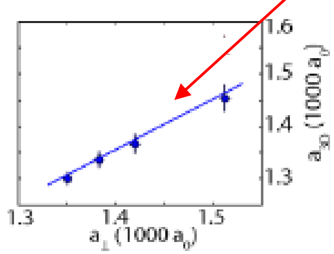


experiment

theory



theory prediction (M.Olshanii PRL (1998))

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

works !

Why it is interesting

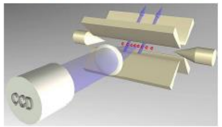
- ultracold atoms

2D Lattice ("tubes")

optical traps

- cold ions

Trapped ions:
Arrays of interacting spins



RF Paul traps

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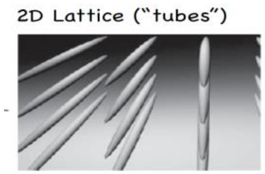

optical traps

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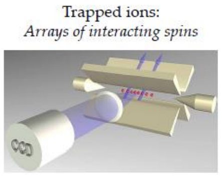
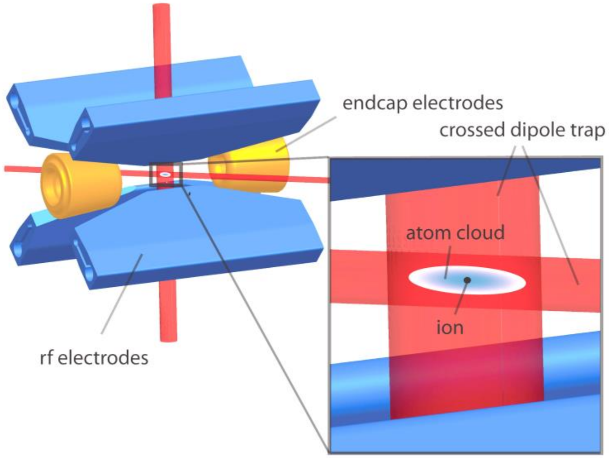


RF Paul traps

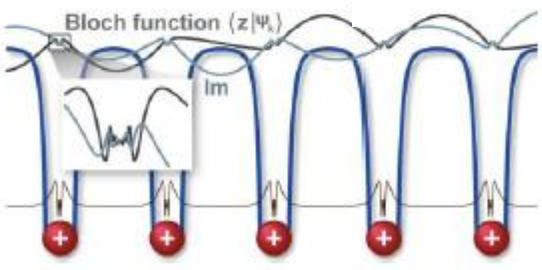
- last few years: hybrid systems ``atom+ion''



new quantum systems with different energy and length scales with respect to ultracold atoms and molecules

Why it is interesting

quantum simulation with cold atoms and ions



Ion crystal + atoms: Fröhlich model

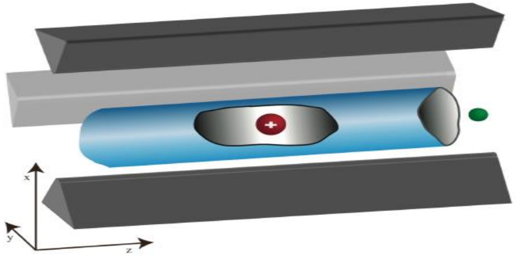
U. Bissbort *et al.*, PRL 111, 080501 (2013)

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 ?

Resonant Processes in Hybrid Atom-Ion Systems



^{6}Li - ^{174}Yb^{+} confined system

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

$$H_i^{trap}(\mathbf{p}_i, \mathbf{r}_i, t) = \frac{\mathbf{p}_i^2}{2m_i} + U(\mathbf{r}_i, t) \qquad U(\mathbf{r}_i, t) = \frac{m_i\omega_i^2}{2}\left(z_i^2 - \frac{x_i^2 + y_i^2}{2}\right) + \frac{m_i\Omega_{rf}^2}{2} q\cos(\Omega_{rf}t)\left(\frac{y_i^2}{2} - \frac{x_i^2}{2}\right)$$

$$\hat{H}_a(\hat{\mathbf{r}}_a, t; \mathbf{r}_i) = -\frac{\hbar^2}{2m_a}\nabla_a^2 + \frac{m_a\omega_\perp^2}{2}(\hat{x}_a^2 + \hat{y}_a^2) + V_{ai}(\hat{\mathbf{r}}_a, \mathbf{r}_i(t))$$

$$V_{ai}(\hat{\mathbf{r}}_a, \mathbf{r}_i(t)) \simeq -\frac{C_4}{r^4}, \quad r(t) \equiv |\hat{\mathbf{r}}_a - \mathbf{r}_i(t)| \to \infty$$

three scales:

$$\Omega_{rf} = 2\pi \times 2\text{MHz} \quad \gg \quad \omega_i = 2\pi \times 63\text{kHz} \quad \gg \quad \omega_\perp = 2\pi \times (1 - 100)\text{kHz}$$

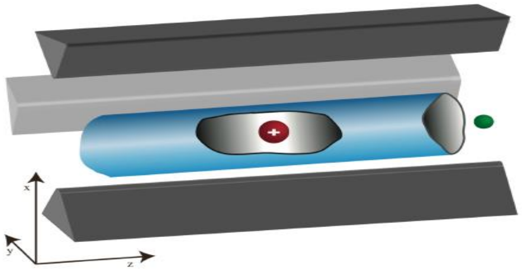
Resonant Processes in Hybrid Atom-Ion Systems: Static Approximation

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

“static” ion

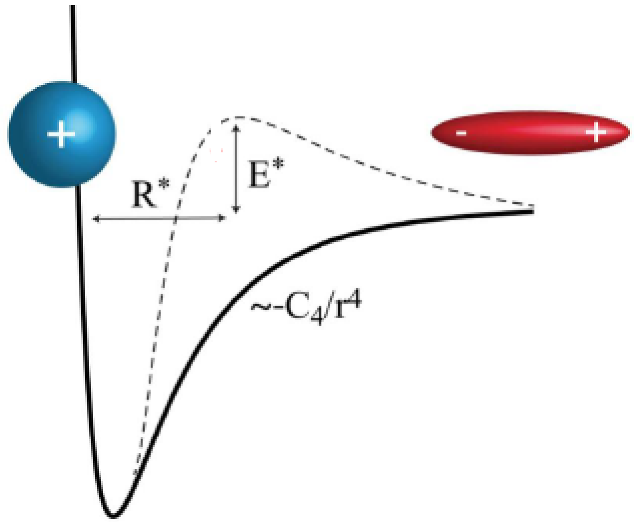
$m_I \gg m_A$

^{6}Li - ^{174}Yb$^+$



$$\left(-\frac{1}{m_A}\nabla_r^2 + m_A\omega_\perp^2\rho^2 + \frac{C_{12}}{r^{12}} - \frac{1}{r^4}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

atom-ion interaction $\frac{C_{12}}{r^{12}} - \frac{C_4}{r^4}$ $R^* = \frac{\sqrt{2\mu C_4}}{\hbar}$ $E^* = \frac{\hbar^2}{2\mu(R^*)^2}$



Resonant Processes in Hybrid Atom-Ion Systems: Static Approximation

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2D Eq. (1) is integrated at fixed energy E with subsequent extracting the amplitude $f^{\pm}(k,\omega_\perp)$ from $\psi(z,\rho)$ at $z \to \pm\infty$

$$T(k,\omega_\perp) = |1 + f^{+}(k,\omega_\perp)|^2 \to 0$$

$$g_{1D}(k,\omega_\perp) = \frac{2k}{m_A}\frac{\mathtt{Re}[f^{+}(k,\omega_\perp) + f^{-}(k,\omega_\perp)]}{\mathtt{Im}[f^{+}(k,\omega_\perp) + f^{-}(k,\omega_\perp)]} \to \pm\infty$$

confinement-induced resonance (CIR)

parameterize quasi-1D scattering in waveguide-like traps

Atom-ion CIR ?

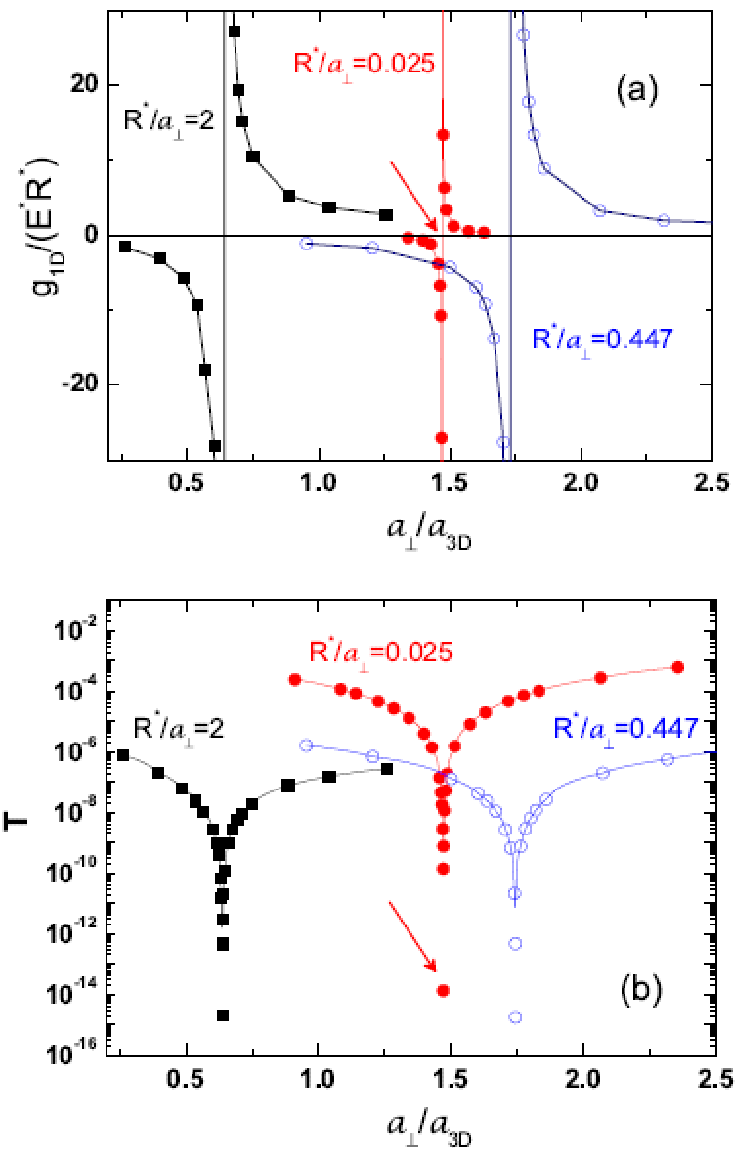
$$g_{1D} \to \pm\infty \,?$$

zero-energy limit + LWL

$\Rightarrow \; R^* \ll a_\perp$

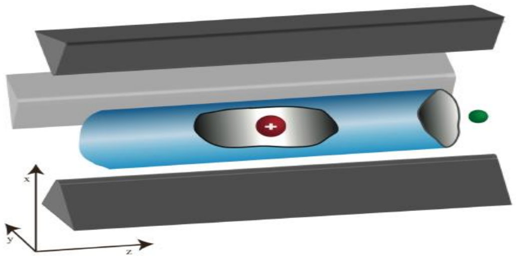
good "candidate" : $R^*/a_\perp = 0.025$

atom-ion CIR: $a_\perp/a_{3D} = 1.46$!!



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

Resonant and Heating/Cooling Processes in Hybrid Atom-Ion Systems



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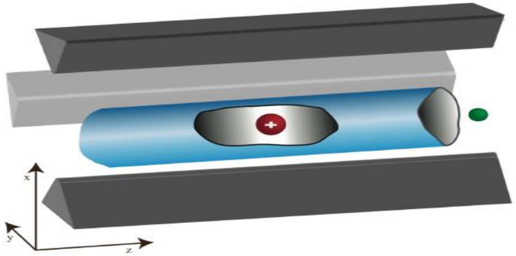

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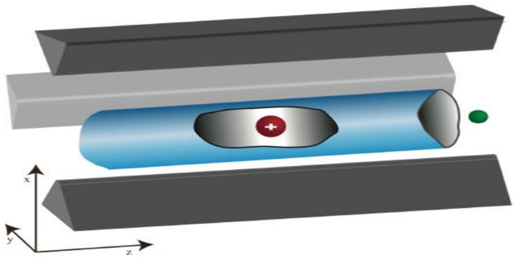

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quantum **classical**

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atoms in optical waveguide-like traps

Method

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

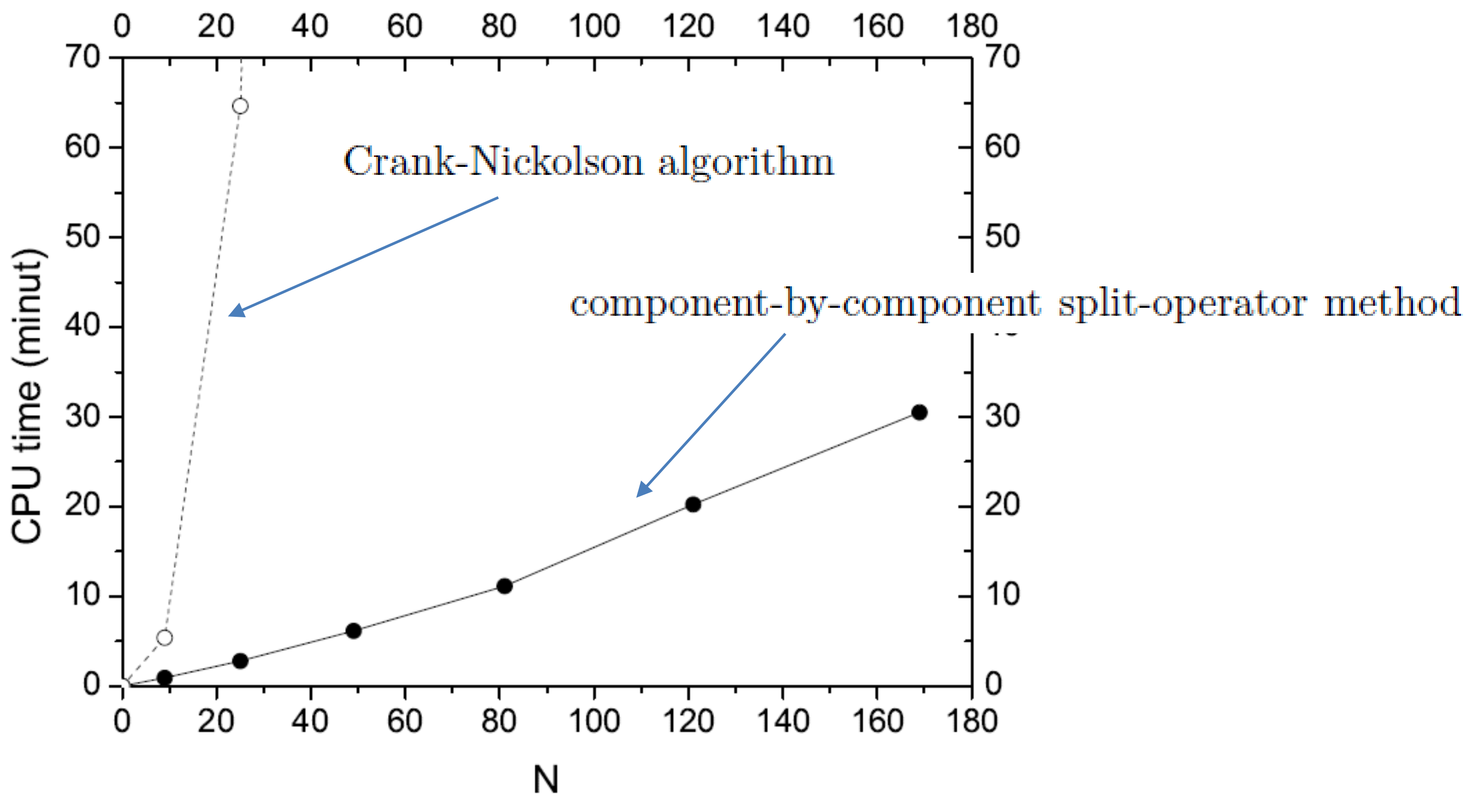
1D DVR: J.C.Light et al J.Chem.Phys. 1985

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

- 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

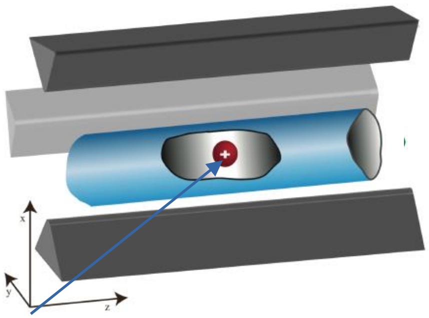
economic computational scheme



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

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

ion in Paul trap



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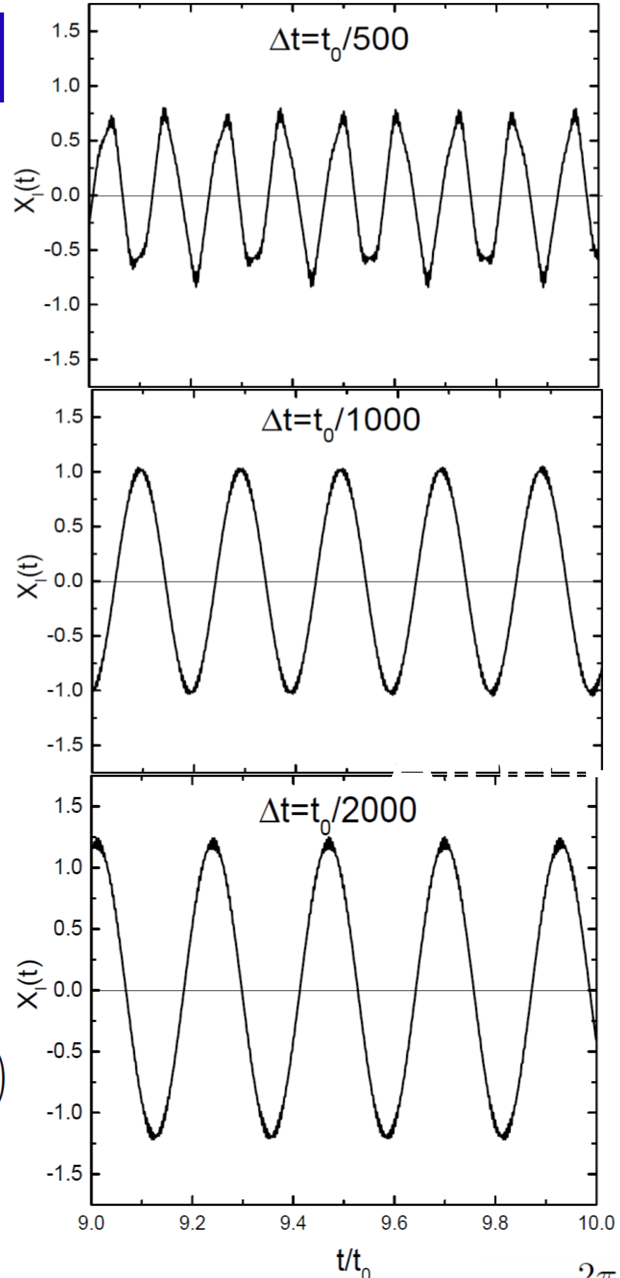


$$t_0 = \frac{2\pi}{\omega_\perp}$$

2-order Störmer-Verlet

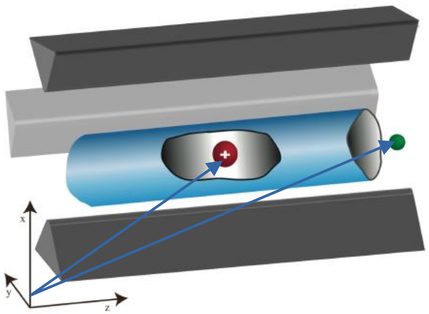
$$\mathbf{p}(t_n + \frac{\Delta t}{2}) = \mathbf{p}(t_n) - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{r}_I}[H_I(\mathbf{p}_I(t_n + \frac{\Delta t}{2}), \mathbf{r}_I(t_n))],$$

$$\mathbf{r}(t_{n+1}) = \mathbf{r}(t_n) + \frac{\Delta t}{2}\{\frac{\partial}{\partial \mathbf{r}_I}[H_I(\mathbf{p}_I(t_n + \frac{\Delta t}{2}), \mathbf{r}_I(t_n))] + \frac{\partial}{\partial \mathbf{r}_I}[H_I(\mathbf{p}_I(t_n + \frac{\Delta t}{2}), \mathbf{r}_I(t_{n+1}))]\},$$

$$\mathbf{p}(t_{n+1}) = \mathbf{p}(t_n + \frac{\Delta t}{2}) - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{r}_I}[H_I(\mathbf{p}_I(t_n + \frac{\Delta t}{2}), \mathbf{r}_I(t_{n+1}))]$$

$$\mathbf{r}_I(t=0) = p_{I,y}(t=0) = 0$$
$$p_{I,x}(t=0) = \sqrt{2M_I E_\perp}$$
$$p_{I,z}(t=0) = \sqrt{2M_I E_\parallel}$$

Quantum-Quasiclassical Approach for Atom-Ion Systems



$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}_A,t) = H_A(\mathbf{r}_A,t)\Psi(\mathbf{r}_A,t)$$

$$H_A(\mathbf{r}_A,t) = -\frac{\hbar^2}{2m_A}\nabla_A^2 + \frac{m_A\omega_\perp^2}{2}(x_A^2+y_A^2) + V_{AI}(\mathbf{r}_A,\mathbf{r}_I(t))$$

$$V_{AI}(\mathbf{r}_A,\mathbf{r}_I(t)) \simeq -\frac{C_4}{r^4}$$

$$\frac{d}{dt}\mathbf{p}_I = -\frac{\partial}{\partial \mathbf{r}_I}H_I(\mathbf{p}_I,\mathbf{r}_I)$$

$$\frac{d}{dt}\mathbf{r}_I = \frac{\partial}{\partial \mathbf{p}_I}H_I(\mathbf{p}_I,\mathbf{r}_I).$$

$$H_I(\mathbf{p}_I,\mathbf{r}_I) = H_I^{trap}(\mathbf{p}_I,\mathbf{r}_I) + \langle\Psi(\mathbf{r}_A,t)|V_{AI}(\mathbf{r}_A,\mathbf{r}_I(t))|\Psi(\mathbf{r}_A,t)\rangle$$

$$H_I^{trap}(\mathbf{p}_I,\mathbf{r}_I,t) = \frac{\mathbf{p}_I^2}{2M_I} + U(\mathbf{r}_I,t). \qquad U(\mathbf{r}_I,t) = \frac{M_I\omega_I^2}{2}\left(z_I^2 - \frac{x_I^2+y_I^2}{2}\right) + \frac{M_I\Omega_{rf}^2}{2}q\cos(\Omega_{rf}t)\left(\frac{y_I^2}{2}-\frac{x_I^2}{2}\right)$$

$$\Psi(\mathbf{r}_A,t=0) = N\varphi_0(\rho_A)exp\{-\frac{(z_A-z_0)^2}{2a_z^2}\}exp\{ikz_A\}$$

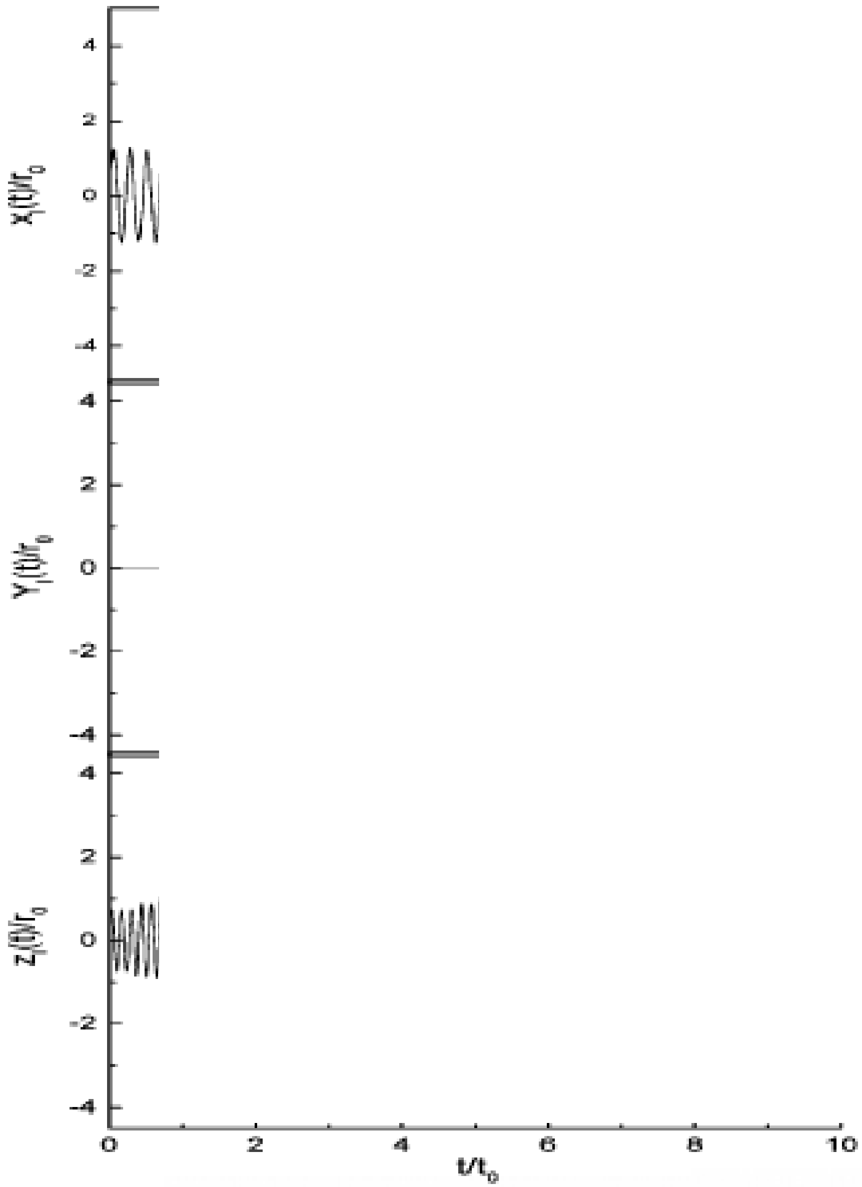
$$\mathbf{r}_I(t=0) = p_{I,y}(t=0) = 0$$

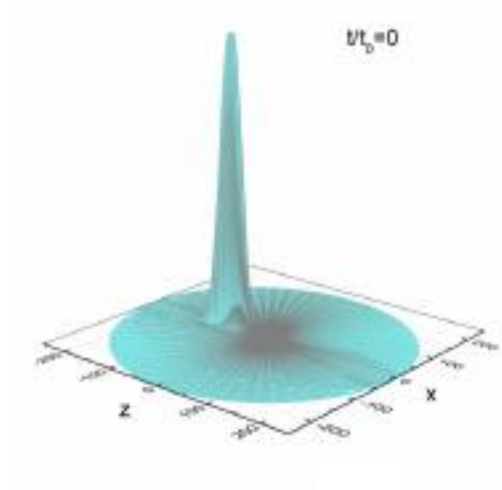
$$p_{I,x}(t=0) = \sqrt{2M_IE_\perp}$$

$$p_{I,z}(t=0) = \sqrt{2M_IE_\parallel}$$

ion

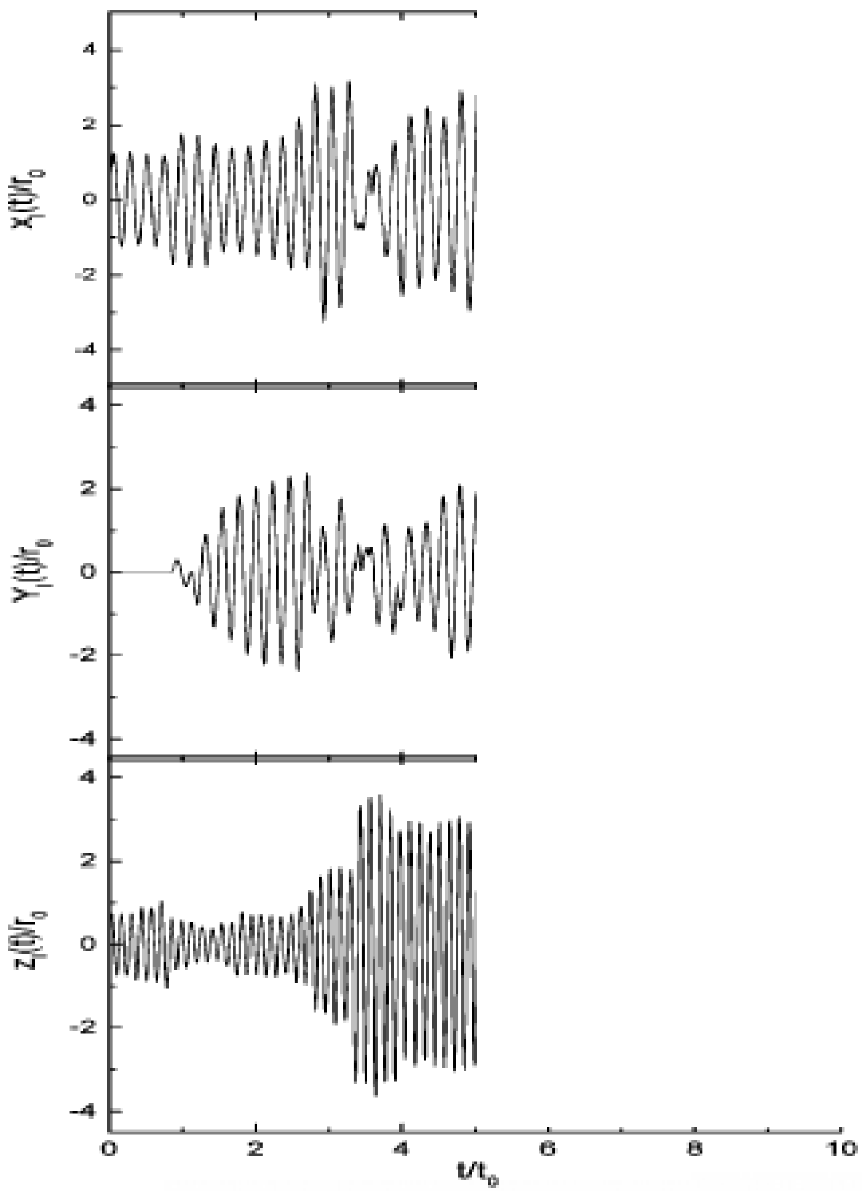
atom

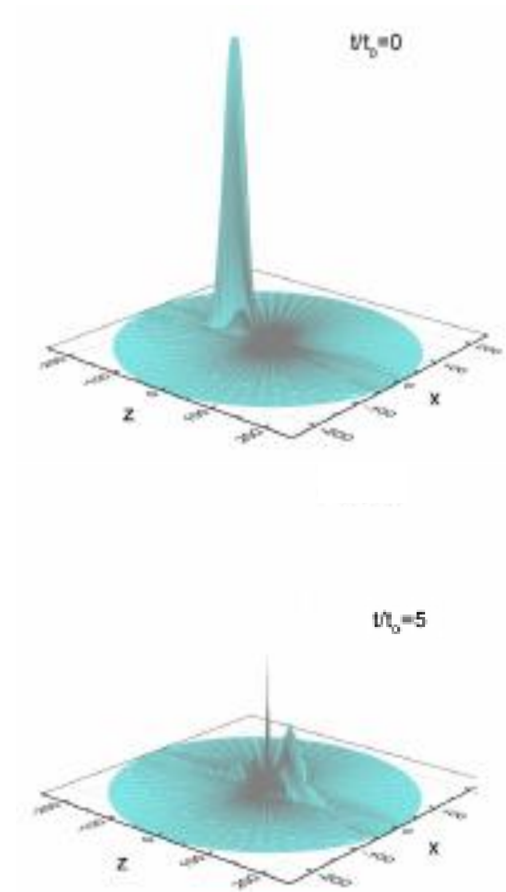




$t_0 = \frac{2\pi}{\omega_\perp}$

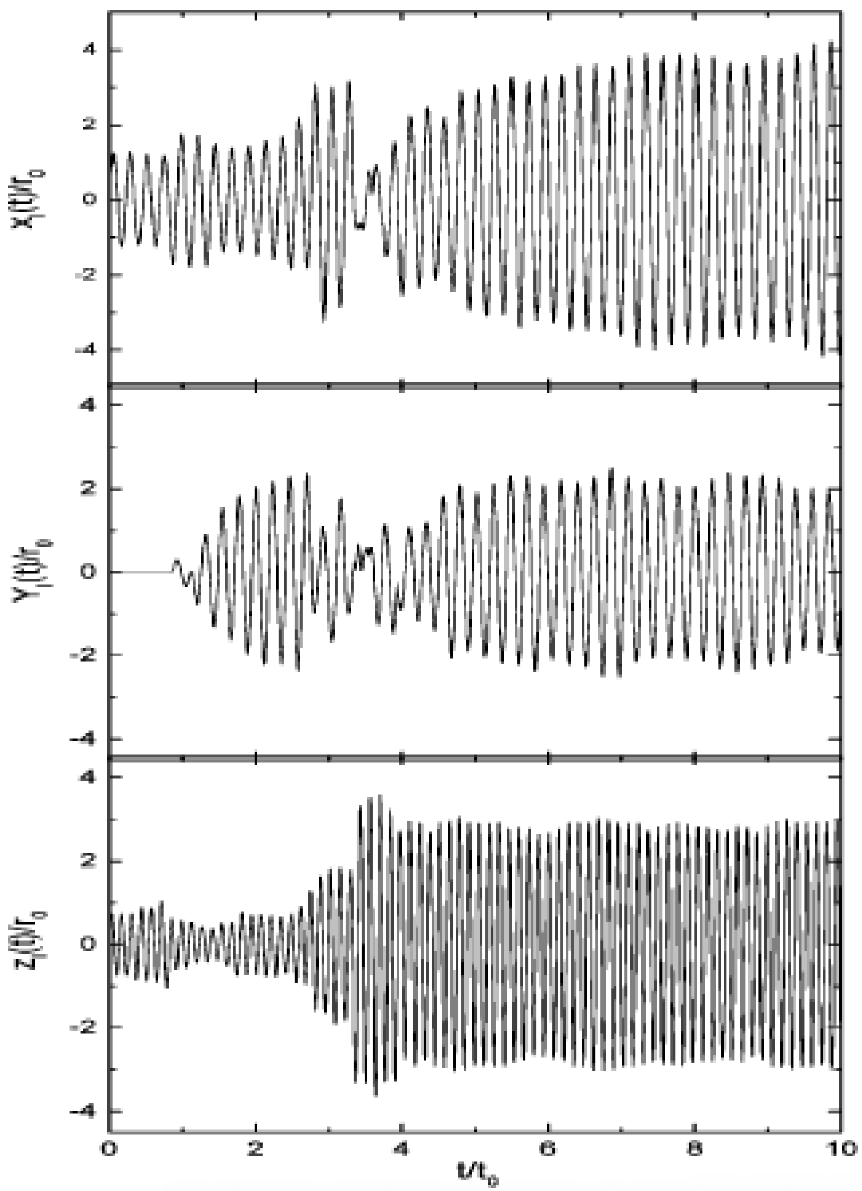
ion **atom**



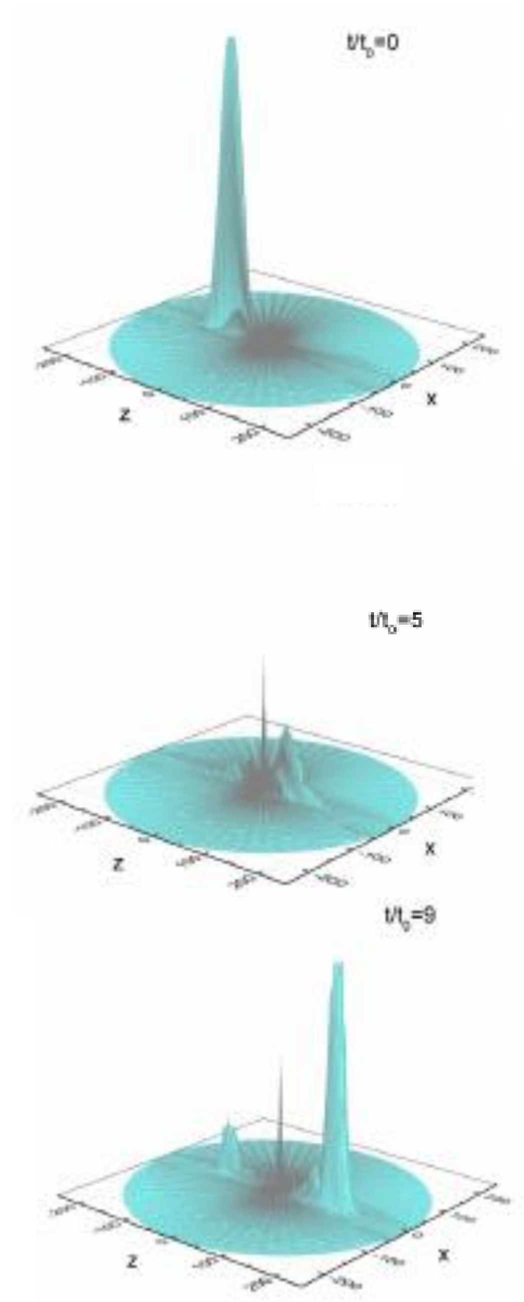


$$t_0 = \frac{2\pi}{\omega_\perp}$$

ion

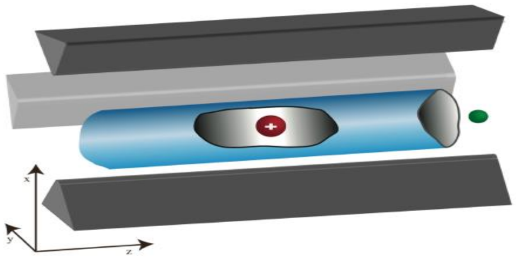


atom



$t_0 = \frac{2\pi}{\omega_\perp}$

Scattering Observables



$$\Psi(\mathbf{r}_A, t=0) = N\varphi_0(\rho_A) exp\{-\frac{(z_A - z_0)^2}{2a_z^2}\} exp\{ikz_A\}$$

$$= N\varphi_0(\rho_A)\chi(z_A - z_0) exp\{ikz_A\} \ ,$$

$$| \psi(t \to +\infty) > \underset{z_A \to +\infty}{\longrightarrow} | \psi(t)^+ >= (1 + f^+(k)) N\varphi_0(\rho_A)\tilde{\chi}(z_A - (z_0 + vt)) exp\{ikz_A\}$$

$$\underset{z_A \to -\infty}{\longrightarrow} | \psi(t)^- >= f^-(k) N\varphi_0(\rho_A)\tilde{\chi}(-z_A - (z_0 + vt)) exp\{-ikz_A\}$$

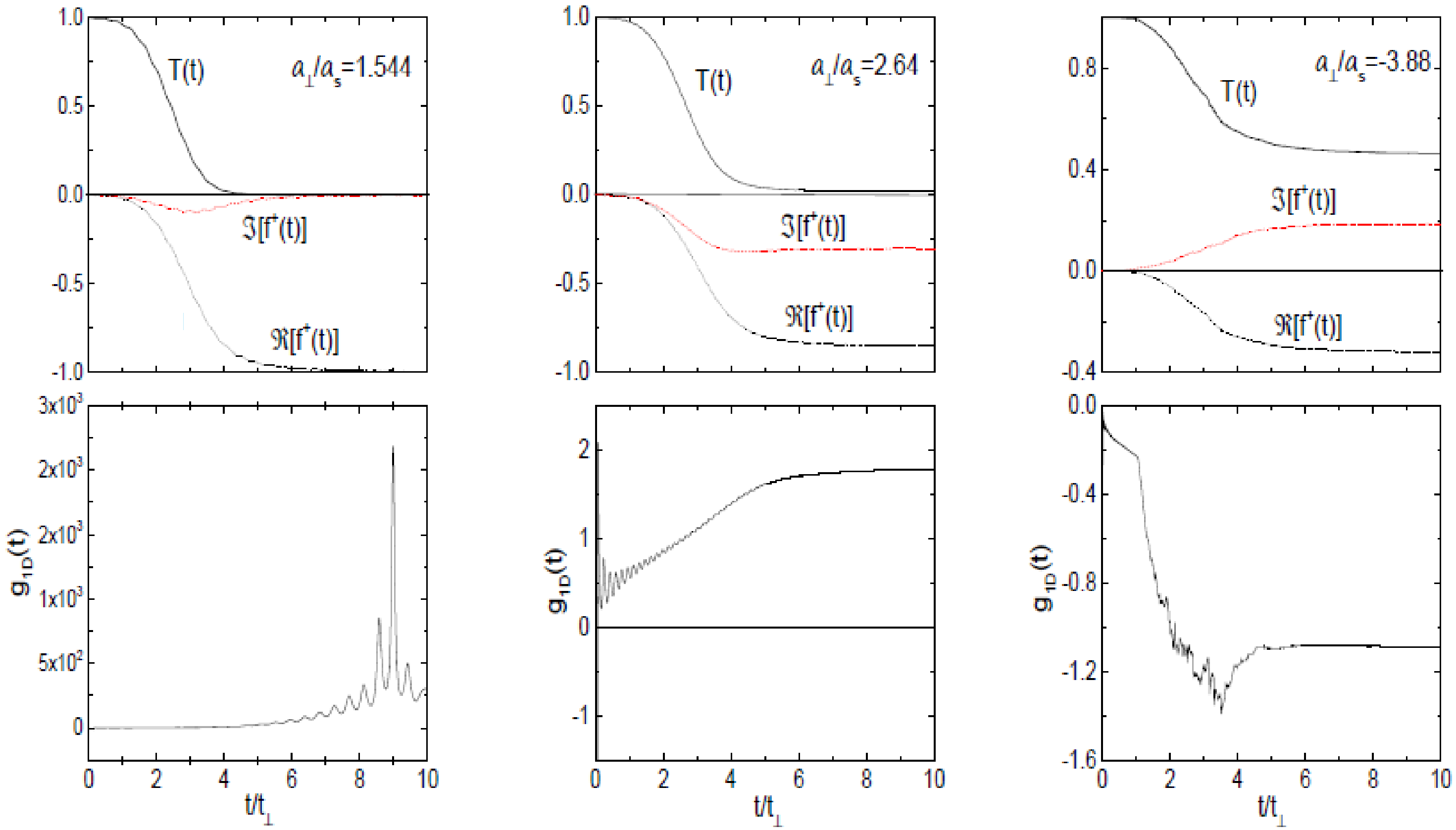
in the absence of atom-ion interaction $(V_{AI}(r,t) = 0)$ at large times $t \to +\infty$

$$| \psi^{(0)}(t \to +\infty) > \underset{z_A \to +\infty}{\longrightarrow} | \psi^{(0)+} >= N\varphi_0(\rho_A)\tilde{\chi}(z_A - (z_0 + vt)) \exp\{ikz_A\}$$

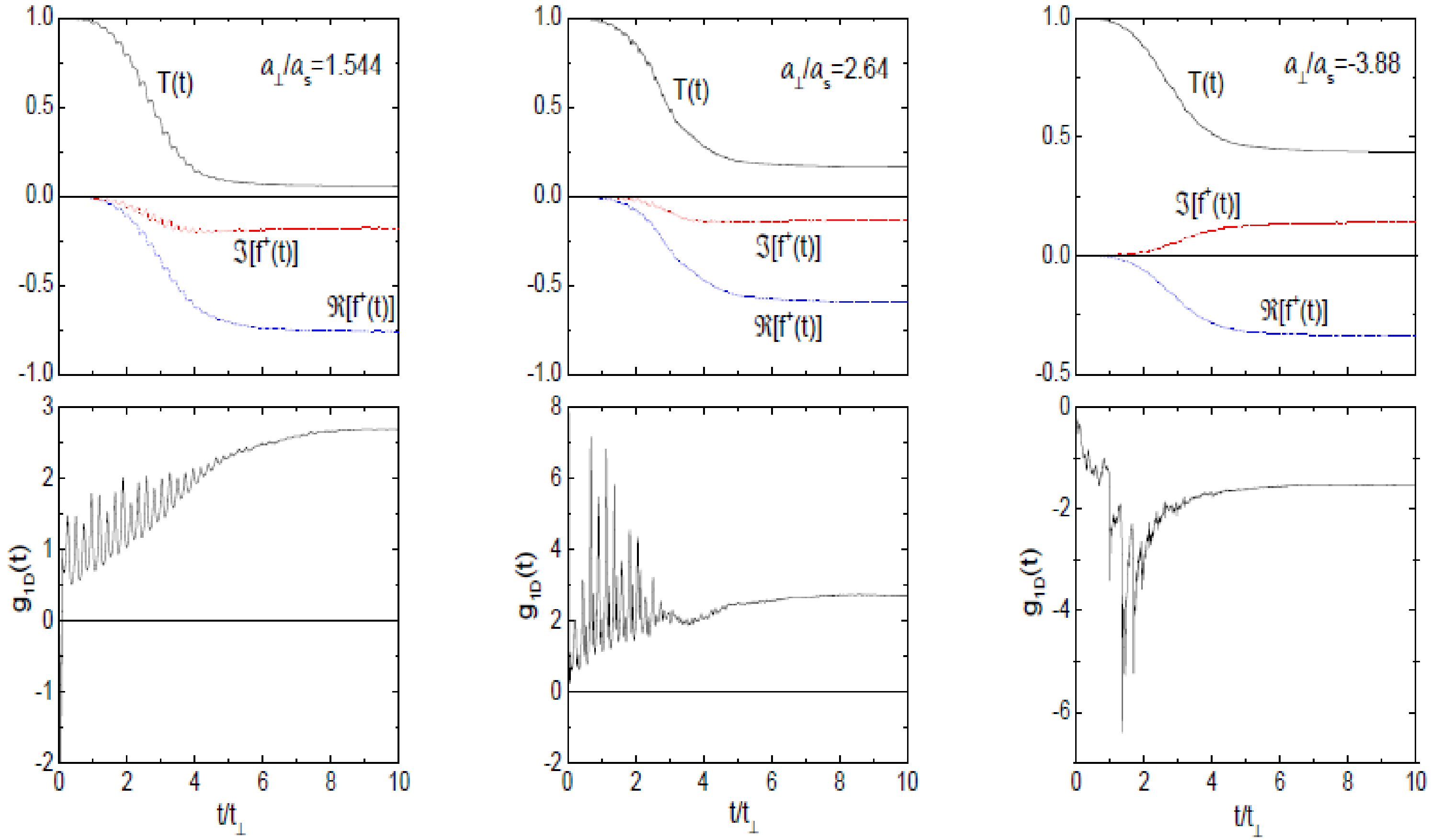
$$< \psi^{(0)}(t) \mid \psi(t) > \underset{t \to +\infty}{\longrightarrow} (1 + f^+(k))$$

$$T(k) = |1 + f^+(k)|^2 \ , \ \ R(k) = 1 - |1 + f^+(k)|^2$$

$$g_{1D} = \lim_{k \to 0} \frac{k}{m_a} \frac{\Re\{f^+(k)\}}{\Im\{f^+(k)\}}$$

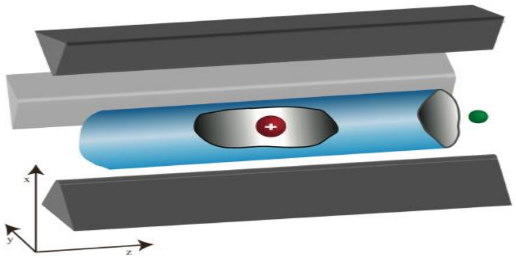


ion in rest $E_\perp = E_\parallel = 0$



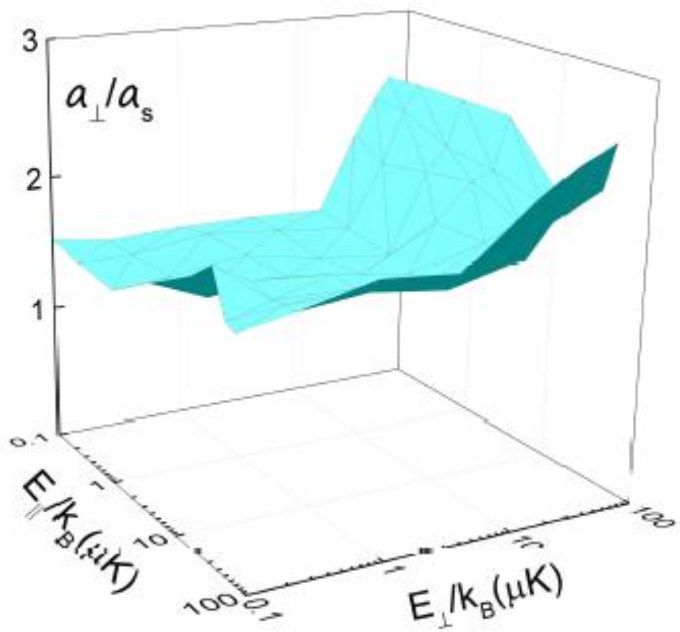
$$E_\perp = E_\| = 4.25\mu K$$

Impact of Ion Motion on CIR

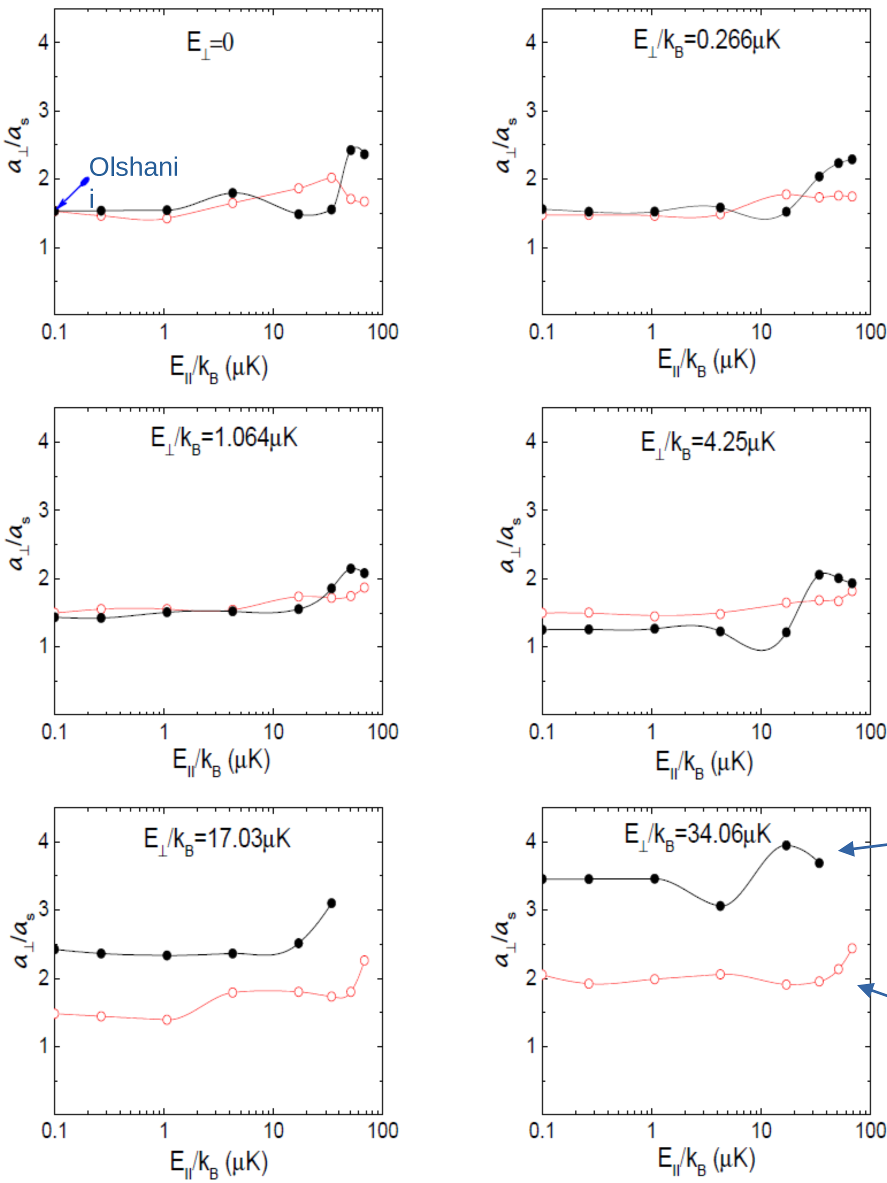


secular time-independent ion trap

$$U_{sec}(\mathbf{r}_i) = \frac{m_i}{2}\left[\omega_{xy}^2(x_i^2 + y_i^2) + \omega_z^2 z_i^2\right]$$



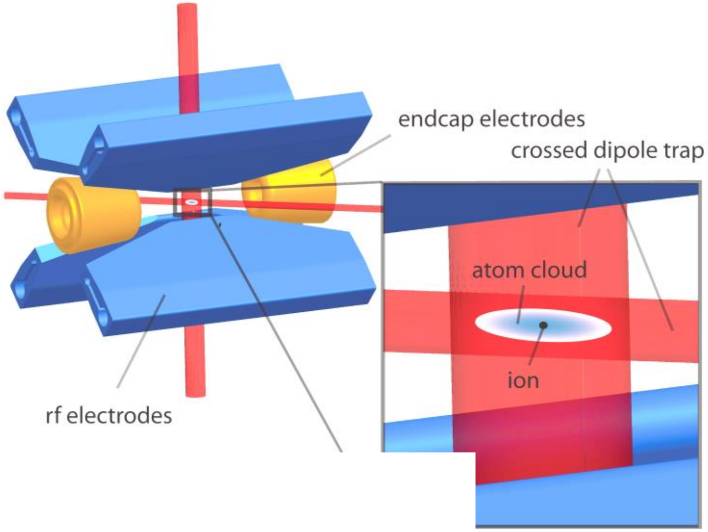
position of the atom-ion CIR is fixed quite well near the constant value $a_\perp/a_s \simeq 1.5$ in the square domain $E_\perp/k_B, E_\parallel/k_B \leq 10\mu$K. In other words, in the secular harmonic trap approximation (19) the position of the CIR is stabilised near the value obtained in the static approximation for the ion (independent of the ion mean energy) if the ion transversal and longitudinal initial energies do not exceed the value of 10μK.



$$U(\mathbf{r}_I, t) = \frac{M_I \omega_I^2}{2}\left(z_I^2 - \frac{x_I^2 + y_I^2}{2}\right) + \frac{M_I \Omega_{rf}^2}{2} q \cos(\Omega_{rf} t)\left(\frac{y_I^2}{2} - \frac{x_I^2}{2}\right)$$

secular time-independent ion trap ($\Omega_{rf} = 0$)

Conclusion & Outlook (I)



- quantum-quasiclassical approach for quantitative treatment of hybrid atom-ion systems

- strong dependence of CIR position on transverse $E_\perp$ and longitudinal $E_\parallel$ ion energy is found in the region $E_\perp, E_\parallel \geq 10\mu K$ for Li-Yb$^+$

- for $E_\perp, E_\parallel \leq 10\mu K$ CIR position coincides with well known value $\frac{a_\perp}{a_s} = 1.46$

- developed method will be used for finding optimal conditions for heating/cooling Li-Yb$^+$

- full quantum consideration is needed for atom-ion with comparable masses

V.S. Melezhik, Z. Idziaszek, A. Negretti, arXiv:1908.01151 (submitted to PRA)

Confinement Induced Resonances in Two-Center Problem

SARA SHADMEHRI , VLADIMIR S. MELEZHIK

BOGOLIUBOV LABORATORY OF THEORETICAL PHYSICS, JINR,DUBNA

S. Shadmehri, V.S. Melezhik, PRA 99, 032705 (2019)

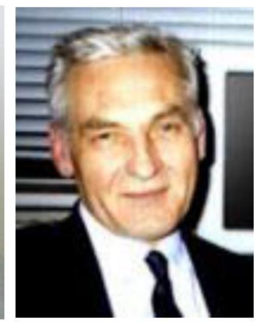
H_2^+

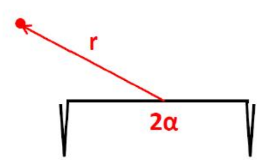
И. В. КОМАРОВ
Л. И. ПОНОМАРЕВ
С. Ю. СЛАВЯНОВ

СФЕРОИДАЛЬНЫЕ
И КУЛОНОВСКИЕ
СФЕРОИДАЛЬНЫЕ
ФУНКЦИИ

Под редакцией В. С. Булдырева

ИЗДАТЕЛЬСТВО «НАУКА»
ГЛАВНАЯ РЕДАКЦИЯ
ФИЗИКО-МАТЕМАТИЧЕСКОЙ ЛИТЕРАТУРЫ
Москва 1976





И. В. КОМАРОВ
Л. И. ПОНОМАРЕВ
С. Ю. СЛАВЯНОВ

СФЕРОИДАЛЬНЫЕ И КУЛОНОВСКИЕ СФЕРОИДАЛЬНЫЕ ФУНКЦИИ

Под редакцией В. С. Булдырева

ИЗДАТЕЛЬСТВО «НАУКА»
ГЛАВНАЯ РЕДАКЦИЯ
ФИЗИКО-МАТЕМАТИЧЕСКОЙ ЛИТЕРАТУРЫ
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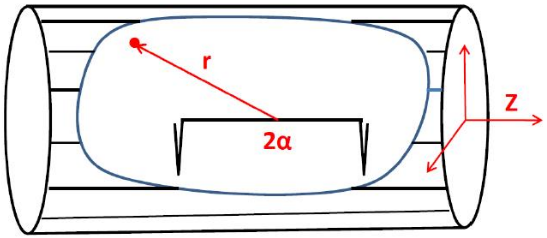
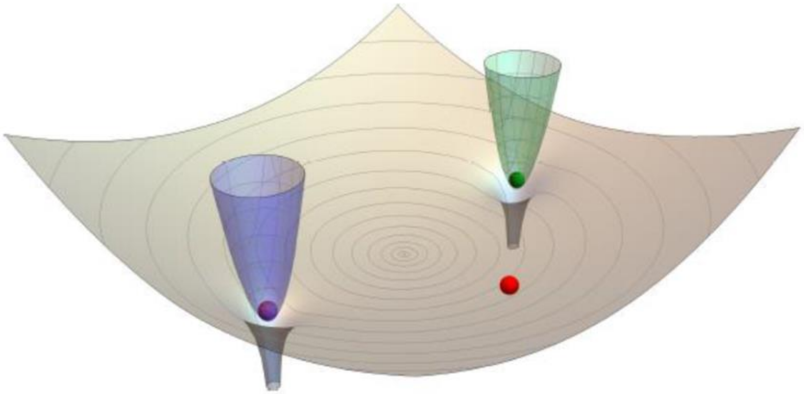


Study the Interaction of a *Single Atom* with *two Trapped Stationary Impurities* (ions or Rydberg atoms)

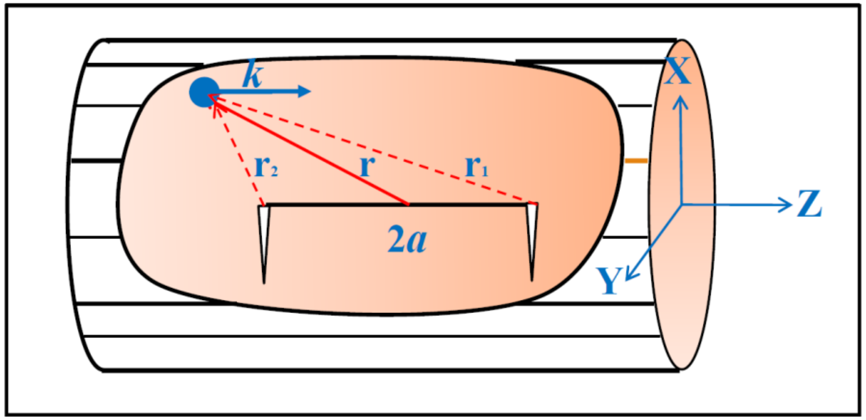
Study the Discrete Spectrum†



† M. SROCZY´NSKA, T. WASAK, K. JACHYMSKI, T. CALARCO, AND Z. IDZIASZEK, PHY. REV. A. 98(1), 012708 (2018).

Our Project

Study the *Scattering States*

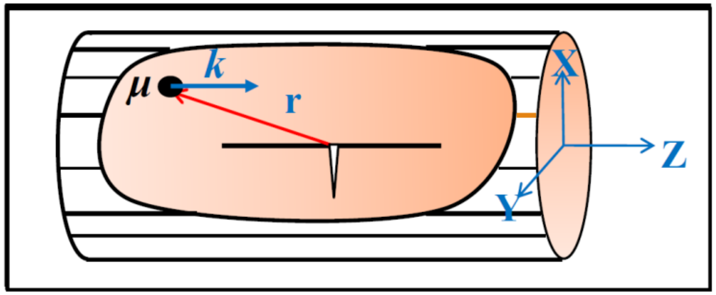


S. Shadmehri, V.S. Melezhik, PRA 99, 032705 (2019)

$$H_{3D} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + H_{\perp} + V_{3D}(\vec{r})$$

$$H_{\perp} = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}\mu\omega_{\perp}^2\rho^2$$

$$a_{\perp} = \sqrt{\frac{\hbar}{\mu\omega_{\perp}}}$$



Huang-Fermi Pseudopotential

$$V_{3D}(\vec{r}) = g_{3D}\delta(\vec{r})\frac{\partial}{\partial r}(r.)$$

$$g_{3D} = \frac{2\pi\hbar^2 a_{3D}}{\mu}$$

$$\hbar\omega_{\perp} < E = \frac{\hbar^2 k_z^2}{2\mu} + \hbar\omega_{\perp} < 3\hbar\omega_{\perp}$$

Asymptotic Wave Function

$$\psi(z,\rho) \xrightarrow{|z|\to\infty} \{e^{ik_z z} + f_{even}e^{ik_z|z|} + f_{odd}\,sign(z)e^{ik_z|z|}\}\phi_{0,0}(\rho)$$

$$\psi(z,\rho) = \sum_{n=0}^{\infty}\psi_n(z)\phi_n(\rho)$$

$$f_{odd} = 0 \quad , \quad f_{even} = -\frac{1}{1 + ik_z a_{1D}}$$

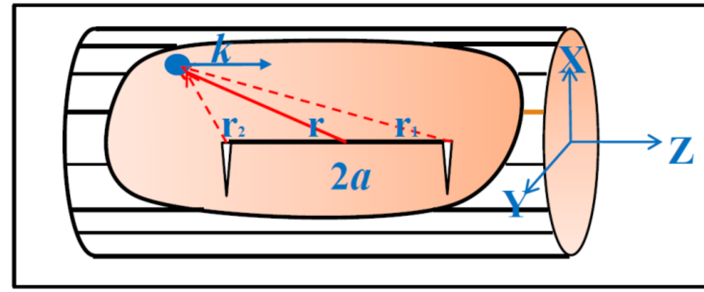
One-Dimensional Scattering Length

$$a_{1D} = -\frac{a_{\perp}^2}{2a_{3D}}\left(1 - C\frac{a_{3D}}{a_{\perp}}\right)$$

$$C = -\varsigma(1/2) = 1.4603$$

M. OLSHANII, PHYS. REV. LETT. 81, 938 (1998).
V. DUNJKO, M. G. MOORE, T. BERGEMAN, AND M. OLSHANII, ADVANCES IN ATOMIC, MOLECULAR, AND OPTICAL PHYSICS 60, 461 (2011).

$$H_{3D} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + H_\perp + V_{3D}(\vec{r})$$



$$H_\perp = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}m\omega_\perp^2\rho^2$$

$$V_{3D}\psi = g_{3D}\delta(\vec{r})\frac{\partial}{\partial r}(r\psi)$$

$\Downarrow$

proper generalization: (?)

$$V_{3D}\psi = \frac{1}{2}g_{3D}\left[\delta(\vec{r}_1)\frac{\partial}{\partial r_1}(r_1\psi) + \delta(\vec{r}_2)\frac{\partial}{\partial r_2}(r_2\psi)\right]$$

PHYSICAL REVIEW A **98**, 012708 (2018)

Trap-induced shape resonances in an ultracold few-body system of an atom and static impurities

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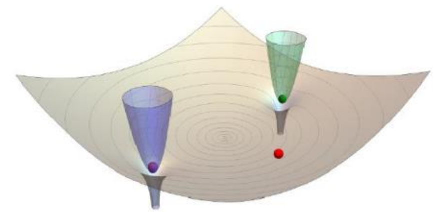
[1]*Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL-02-093 Warsaw, Poland*
[2]*Institute for Theoretical Physics III & Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany*
[3]*Institute for Complex Quantum Systems & Center for Integrated Quantum Science and Technology (IQST), Universität Ulm, Albert-Einstein-Allee 11, D-89075 Ulm, Germany*



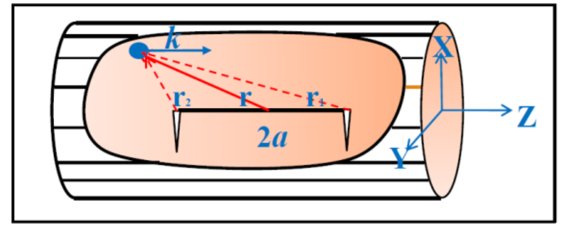
$$V_{3D}\psi = \frac{1}{2} g_{3D} \left[\delta(\vec{r}_1) \frac{\partial}{\partial r_1}(r_1 \psi) + \delta(\vec{r}_2) \frac{\partial}{\partial r_2}(r_2 \psi) \right] \longrightarrow 1/a \longrightarrow \infty$$

...but the even states for $a = 0$ do not approach the results obtained by Busch* for a single impurity. In the limit $a \rightarrow 0$, our model in terms of two separate regularized delta potentials is no longer valid.

*T. BUSCH, B. ENGLERT, K. RZĄŻEWSKI, AND M. WILKENS, FOUND. PHYS. 28, 549 (1998).

$$H_{3D} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + H_\perp + V_{3D}(\vec{r})$$

$$H_\perp = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \varphi^2}\right) + \frac{1}{2}m\omega_\perp^2\rho^2$$



Alternative Regularization

$$V_{3D}\psi = \frac{1}{2} \times \frac{1}{2} g_{3D}\left[\delta(\vec{r}_1)\frac{\partial^2}{\partial r_1 \partial r_2}(r_1 r_2 \psi) + \delta(\vec{r}_2)\frac{\partial^2}{\partial r_2 \partial r_1}(r_1 r_2 \psi)\right]$$

removes the difficulty at $a \longrightarrow 0$

satisfies the Bethe-Peierls Contact Condition on the scattering centers:

$$\psi(\vec{r}) = A\left(\frac{1}{r} - \frac{1}{a_{3D}}\right) + \mathcal{O}(r) \qquad as\ r \longrightarrow 0$$

$$\psi(\vec{r}) = \psi(z, \rho) = \sum_{n=0}^{\infty} \psi_n(z)\phi_n(\rho)$$

$$\psi_0(z) \xrightarrow{|z| \to \infty} \{e^{ikz} + f_e e^{ik|z|} + f_o sign(z) e^{ik|z|}\}$$

$$f_e = -\frac{\cos^2(ka) - ka\sin(2ka)}{\frac{1}{2}\left(1 + e^{2ika}\right) - ika_\perp\left[\frac{a_\perp}{2a_{3D}} + \frac{1}{4}\left(\widetilde{\Lambda}(0,\epsilon) + \widetilde{\Lambda}\left(\frac{4a}{a_\perp},\epsilon\right)\right) - \frac{a}{a_\perp}\left(1 - \epsilon + e^{2ika} + \tilde{F}\left(\frac{4a}{a_\perp},\epsilon\right)\right)\right]}$$

$$f_o = -\frac{\sin^2(ka) + ka\sin(2ka)}{\frac{1}{2}\left(1 - e^{2ika}\right) - ika_\perp\left[\frac{a_\perp}{2a_{3D}} + \frac{1}{4}\left(\widetilde{\Lambda}(0,\epsilon) - \widetilde{\Lambda}\left(\frac{4a}{a_\perp},\epsilon\right)\right) - \frac{a}{a_\perp}\left(1 - \epsilon - e^{2ika} - \tilde{F}\left(\frac{4a}{a_\perp},\epsilon\right)\right)\right]}$$

$$\epsilon = -(a_\perp k/2)^2$$

$$\widetilde{\Lambda}(0,\epsilon) = \zeta(1/2\,, 1 + \epsilon)$$

$$\widetilde{\Lambda}\left(\frac{4a}{a_\perp},\epsilon\right) = -\frac{a_\perp}{2a} + \sum_{n=1}^{\infty}\frac{e^{-\frac{4a\sqrt{n+\epsilon}}{a_\perp}}}{\sqrt{n+\epsilon}}$$

$$\tilde{F}\left(\frac{4a}{a_\perp},\epsilon\right) = -\frac{a_\perp^2}{8a^2} + \sum_{n=1}^{\infty} e^{-\frac{4a\sqrt{n+\epsilon}}{a_\perp}}$$

$a \to 0$

$$f_e = -\frac{1}{1 + ik\left[-\frac{a_\perp^2}{2a_{3D}}\left(1 + \widetilde{\Lambda}(0,\epsilon)\frac{a_{3D}}{a_\perp}\right)\right]}$$

$$f_o = 0$$

effective 1D Schrödinger equation $$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dz^2} + V_{1D}\psi_0(z) = \frac{\hbar^2 k^2}{2m}\psi_0(z)$$

$$V_{1D} = \frac{1}{2}\left[g_{1D}^{+}\delta(z-a) + g_{1D}^{-}\delta(z+a)\right]$$

$$g_{1D}^{+} = i\frac{k\hbar^2}{m}e^{-ika}\frac{f_e/\cos(ka) + if_o/\sin(ka)}{1+f_e+f_o}$$

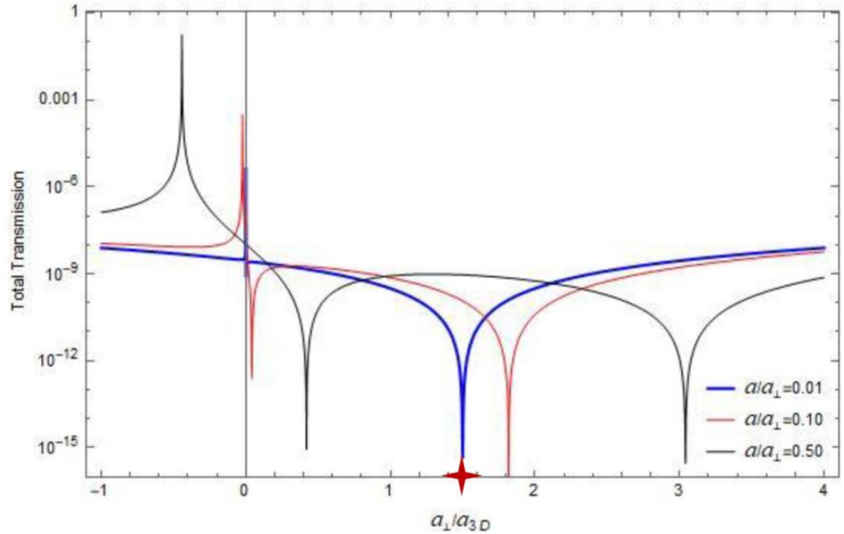
$$g_{1D}^{-} = i\frac{k\hbar^2}{m}e^{-ika}\frac{f_e/\cos(ka) - if_o/\sin(ka)}{e^{-2ika}+f_e-f_o}$$

CIR occurs at complete reflectance

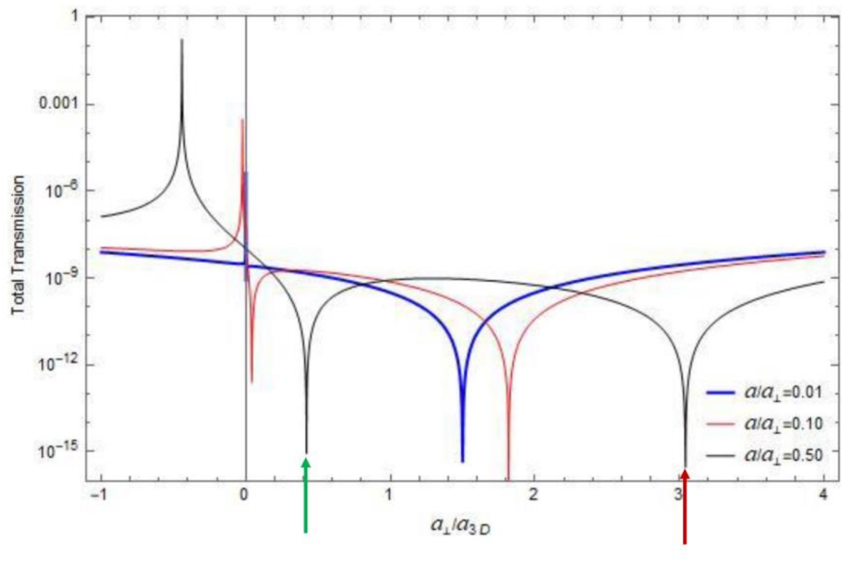
$T = |1 + f_e + f_o|^2 = 0 \longrightarrow$ divergent g_{1D}^{+}

$R = |f_e - f_o|^2 = 1 \xrightarrow{k \to 0}$ divergent g_{1D}^{-}

$T_{tot} = |1 + f_e + f_o|^2$



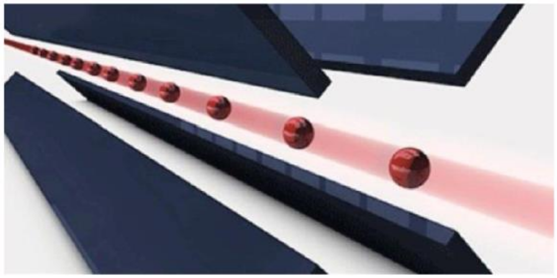
In the limit $a \to 0$
right minimum in T_{tot}
approaches the value
$a_\perp/a_{3D} = 1.46$



Total Transmission
1
0.001
10^{-6}
10^{-9}
10^{-12}
10^{-15}
-1
0
1
2
3
4
$a_\perp/a_{3D}$
$a/a_\perp$=0.01
$a/a_\perp$=0.10
$a/a_\perp$=0.50

Conclusion & Outlook (II)

- Study confined atomic scattering from two centers via pseudopotential approach
- A novel regularization operator in pseudopotential leading to consistent results at $a \to 0$
- Two CIRs due to the interplay between even and odd wave scattering
- Capable to be extended to the confined N-center problem
- Useful for constructing mean-field approaches with contact interactions



S. Shadmehri, V.S. Melezhik, PRA 99, 032705 (2019)

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