MAKING ULTRACOLD MOLECULES WITH CONFINEMENT

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(Cold Molecules, KITP, 21.03.2013)

Acknowledgements

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DFG

CORINF Correlated Multielectron Dynamics in Intense Laser Fields

Bundesministerium für Bildung und Forschung

FCI Fonds der Chemischen Industrie

cost

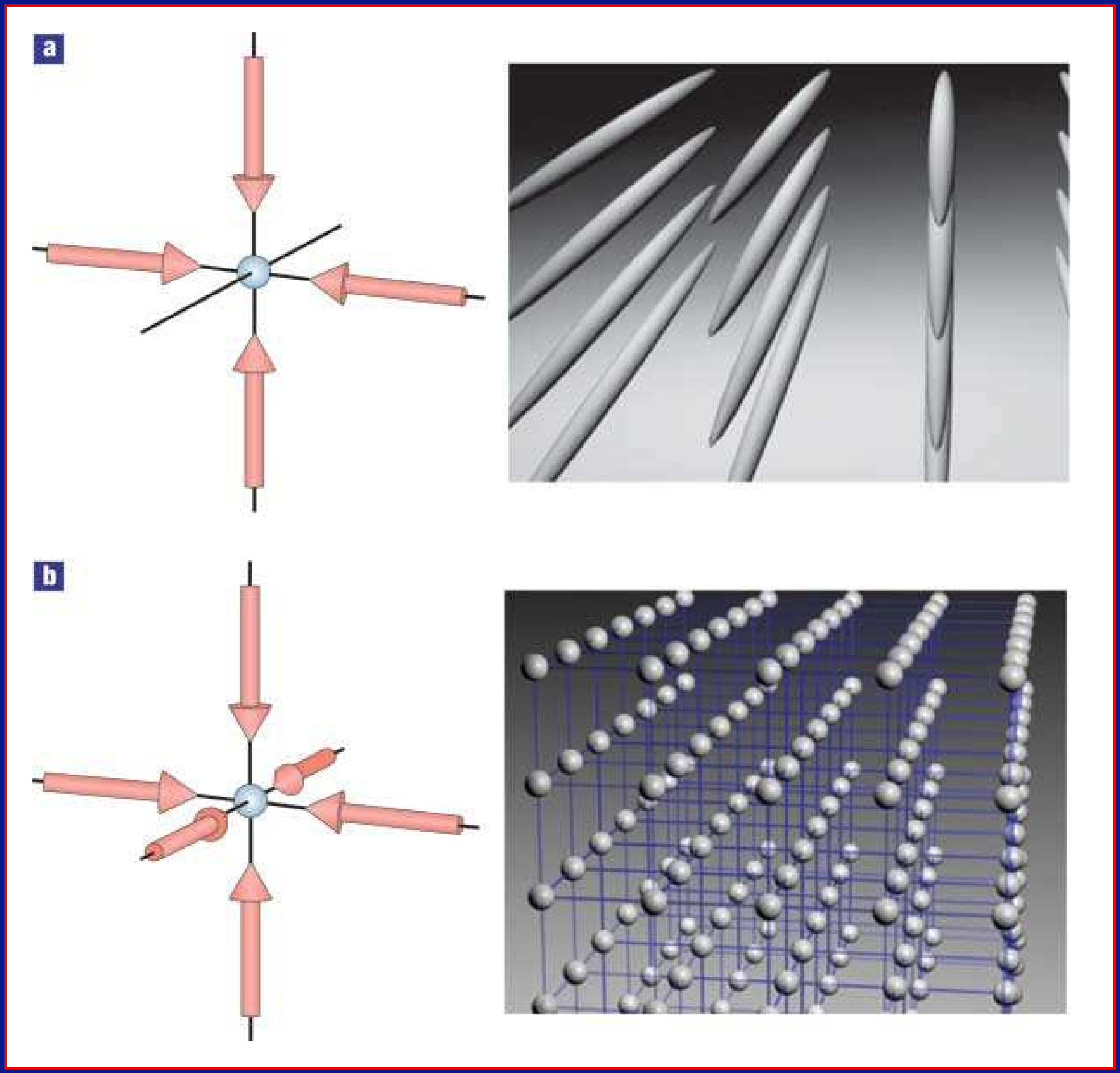
DAAD Deutscher Akademischer Austausch Dienst German Academic Exchange Service wandel durch austausch. change by exchange.

Stifterverband für die Deutsche Wissenschaft

Overview

- Motivation: coming from the few-body side.
- Influence of confinement.
- Bridge to many-body models: microscopic parameters.
- Confinement-induced resonances: resolving the puzzle.
- Few particles in 1D ptical lattices.
- Brief summary and outlook.

Optical lattices: physics on a lattice



[reproduced from I. Bloch, *Nature Physics* **1**, 23 (2005)]

Counterpropagating lasers:

$\longrightarrow$ standing light field.

Trap potential varies as

$$U_{\mathrm{lat}} \sin^2(\vec{k}\vec{r})$$

with

$k = \frac{2\pi}{\lambda}$

λ: laser wavelength.

$$U_{\mathrm{lat}} \propto I\,\alpha(\lambda)$$

with

laser intensity I and

atomic polarizability α.

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Required: Full understanding of few-body systems in optical lattices (static and dynamic properties).

Ultracold gases for quantum information: questions

Central issue: reliability of the mapping?

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   Do we simulate what we think we simulate?

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How are the atom-atom interactions usually modelled?

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Concept (cf. nuclear or solid-state physics):

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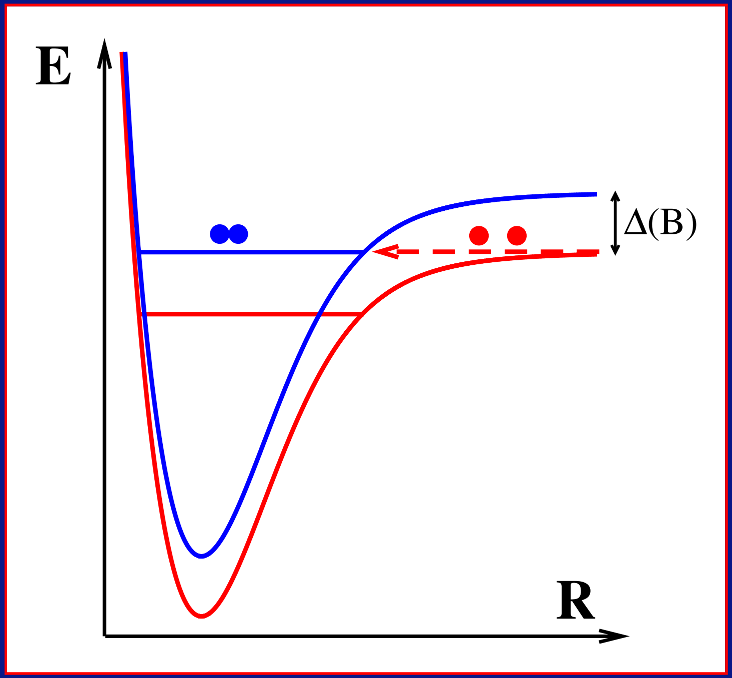
Note: V_{pseudo} is counterintuitive: long-range behaviour described by δ function!!!

Magnetic Feshbach resonances



Simple picture:

Only **2 channels**:

– open (continuum) channel,

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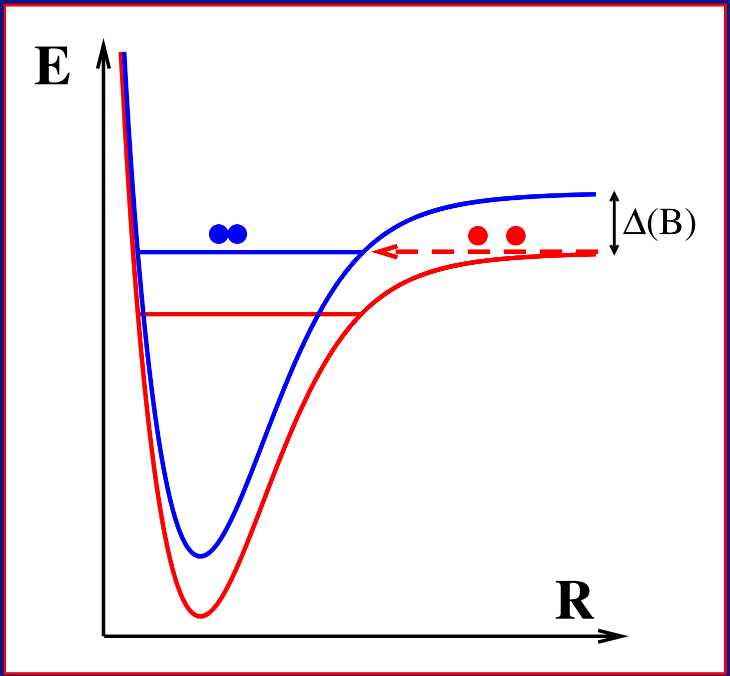

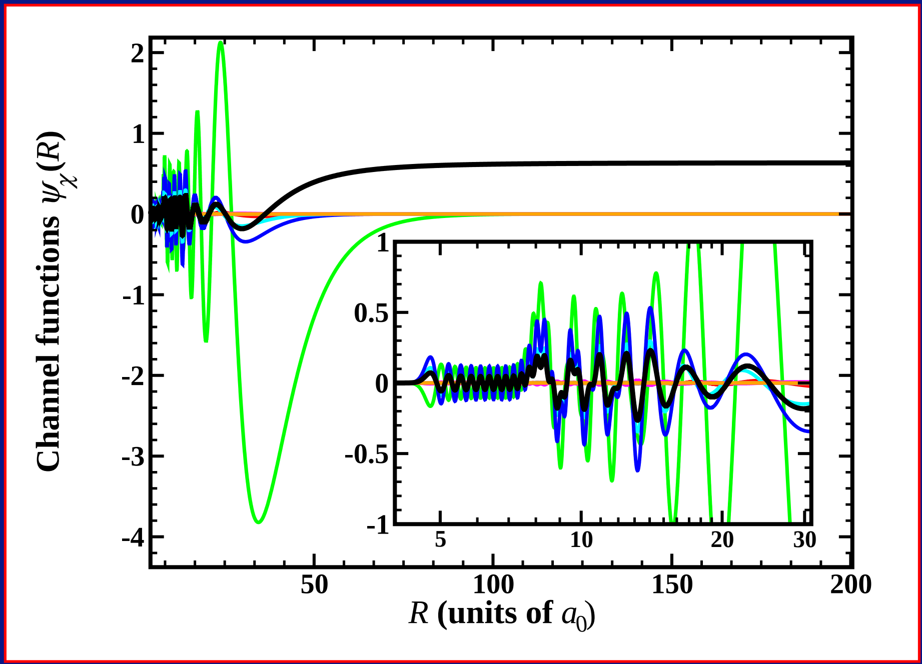

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Multichannel reality:

Example ^{6}Li-^{87}Rb : **8 coupled channels**,

— very different length scales involved,

— high quality molecular potential curves required.

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Influence of lattice (confinement) on magnetic Feshbach resonances?

Magnetic Feshbach resonances (MFRs) in a harmonic trap

- Description as coupled single open and closed channels ($|\Psi\rangle = C|\mathrm{open}\rangle + \mathrm{A}|\mathrm{closed}\rangle$)
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$$a(E,B) = a_{\mathrm{bg}}\left(1 - \frac{\Delta B}{B - B_0 + \delta B - E/\mu}\right)$$

in contrast to a previously suggested form

$$a(E,B) = a_{\mathrm{bg}}\left(1 - \frac{\Delta B\left(1 + (k a_{\mathrm{bg}})^2\right)}{B - B_0 + \delta B + (k a_{\mathrm{bg}})^2 \Delta B - E/\mu}\right)$$

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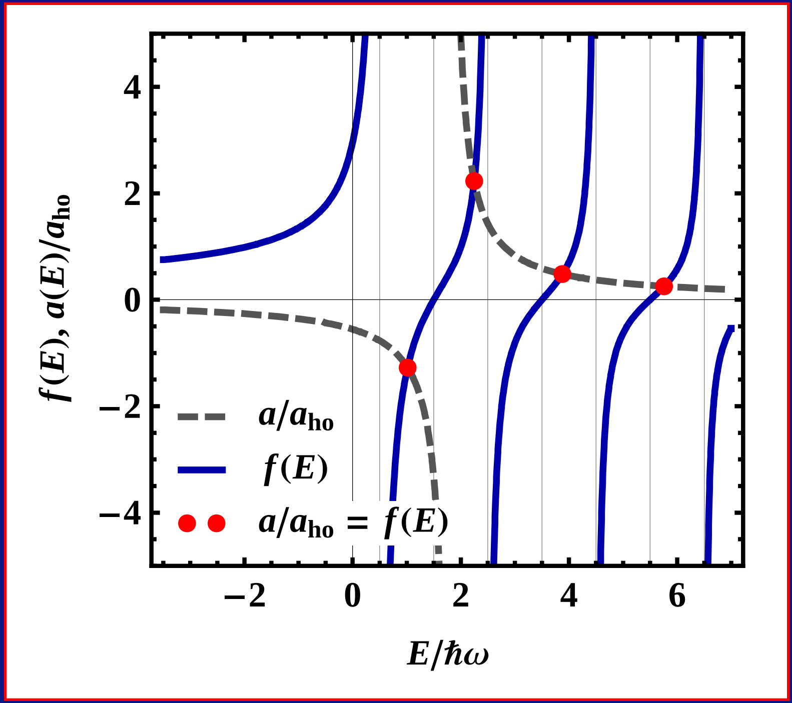

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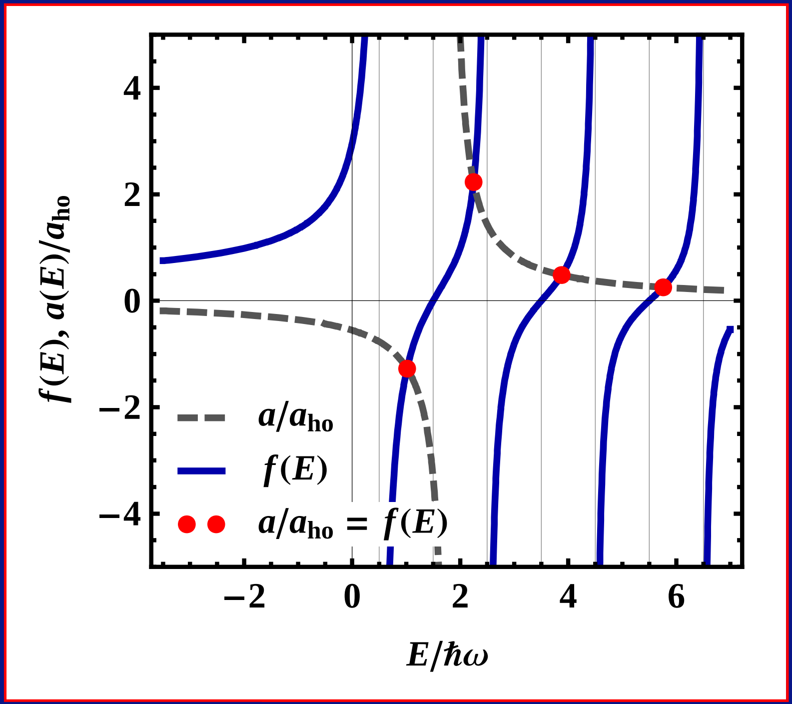

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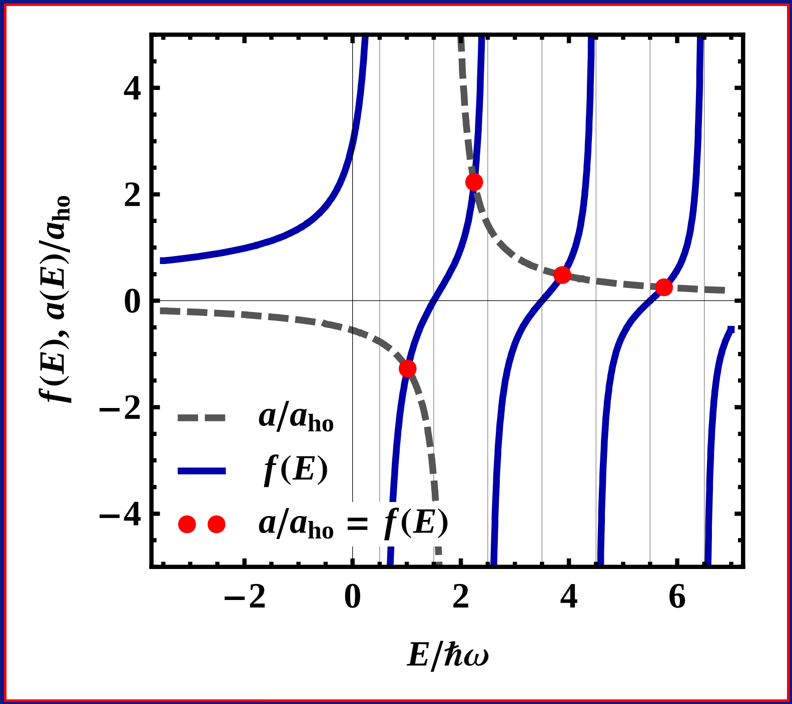
3. derive the admixture of the closed channel

$$\frac{A}{C} \propto \frac{f(E) - a_{\text{bg}}/a_{\text{ho}}}{\sqrt{f'(E)}}$$



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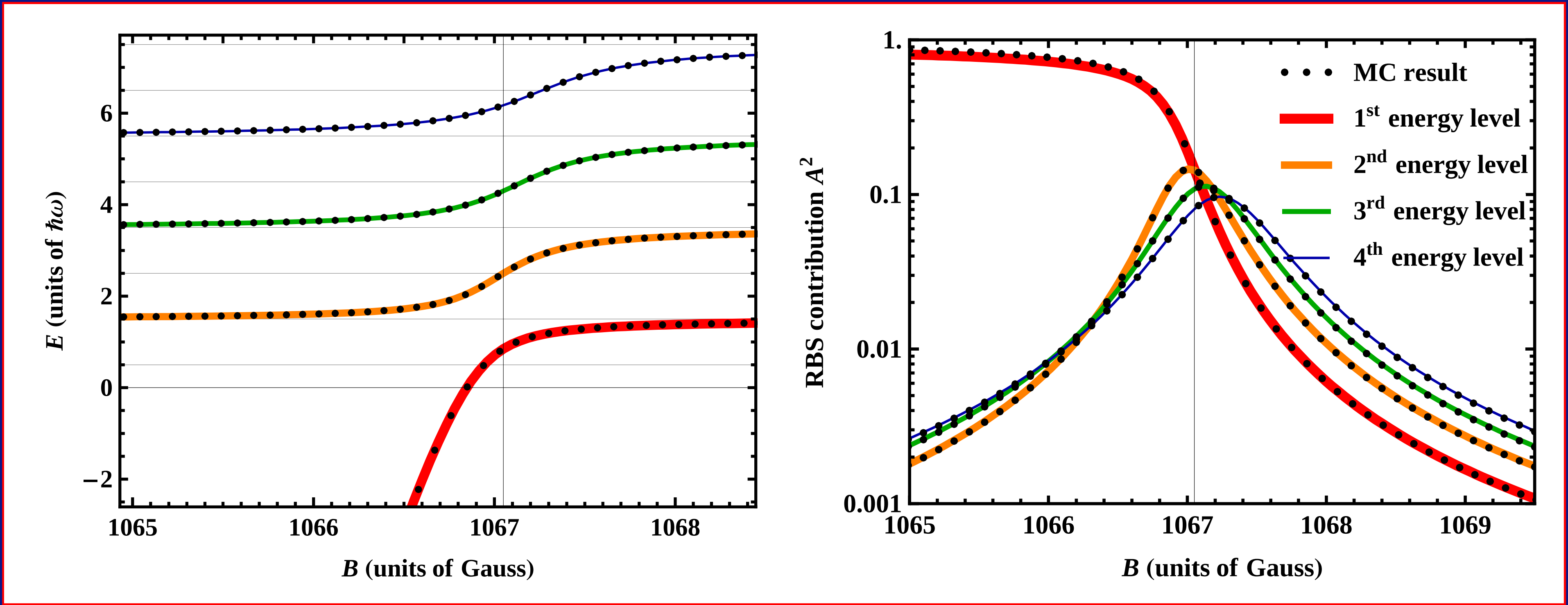
How good is the model?

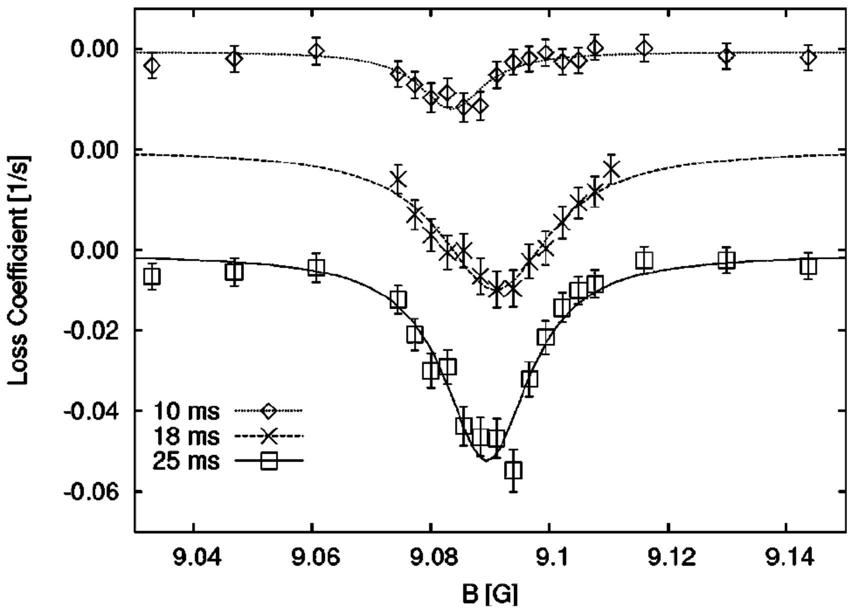
Comparison with full coupled-channel calculations for ^{6}Li-^{87}Rb in a 200 kHz trap:

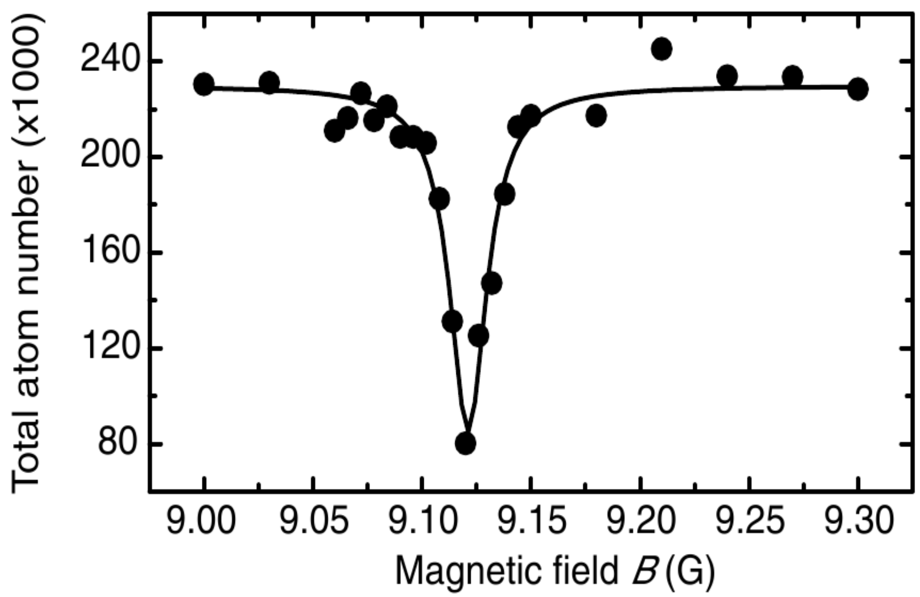


- **Energy deviation** $< 0.003\,\hbar\omega$.
- **Closed-channel admixture deviation** $< 0.1\%$.

Explaining a long-standing discrepancy

- Resonances of $a \propto f(E)$ are located at $E_{\rm res}^{(n)} = \hbar\omega(2n + \frac{1}{2}) \Rightarrow$ thus NOT at bare resonance position $B_R = B_0 - \delta B$, but at
$$B = B_{\rm res}^{(n)} = B_0 - \delta B + E_{\rm res}^{(n)}/\mu \, .$$
- This explains the disagreement of experimentally observed MFR positions of ^{87}Rb; predicted shift of 0.034 Gauss in good agreement with experimental results.





weak dipole trap, M. Erhard *et al.*
Phys. Rev. A **69** 032705 (2004)

tight optical trap, A. Widera *et al.*
Phys. Rev. Lett. **92** 160406 (2004).

Many-body effects due to the molecular bound state

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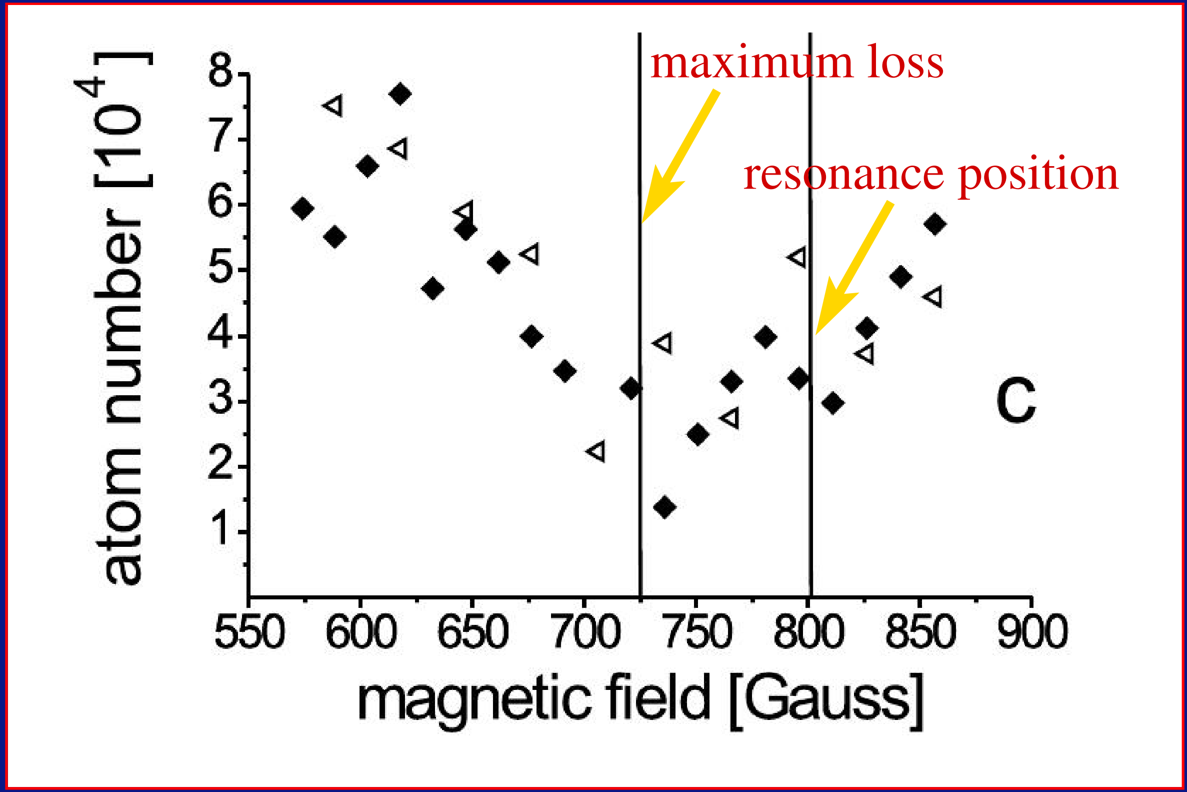
Experiment with ^{6}Li:

[Bourdel *et al.*
PRL **91**, 020402 (2003)]

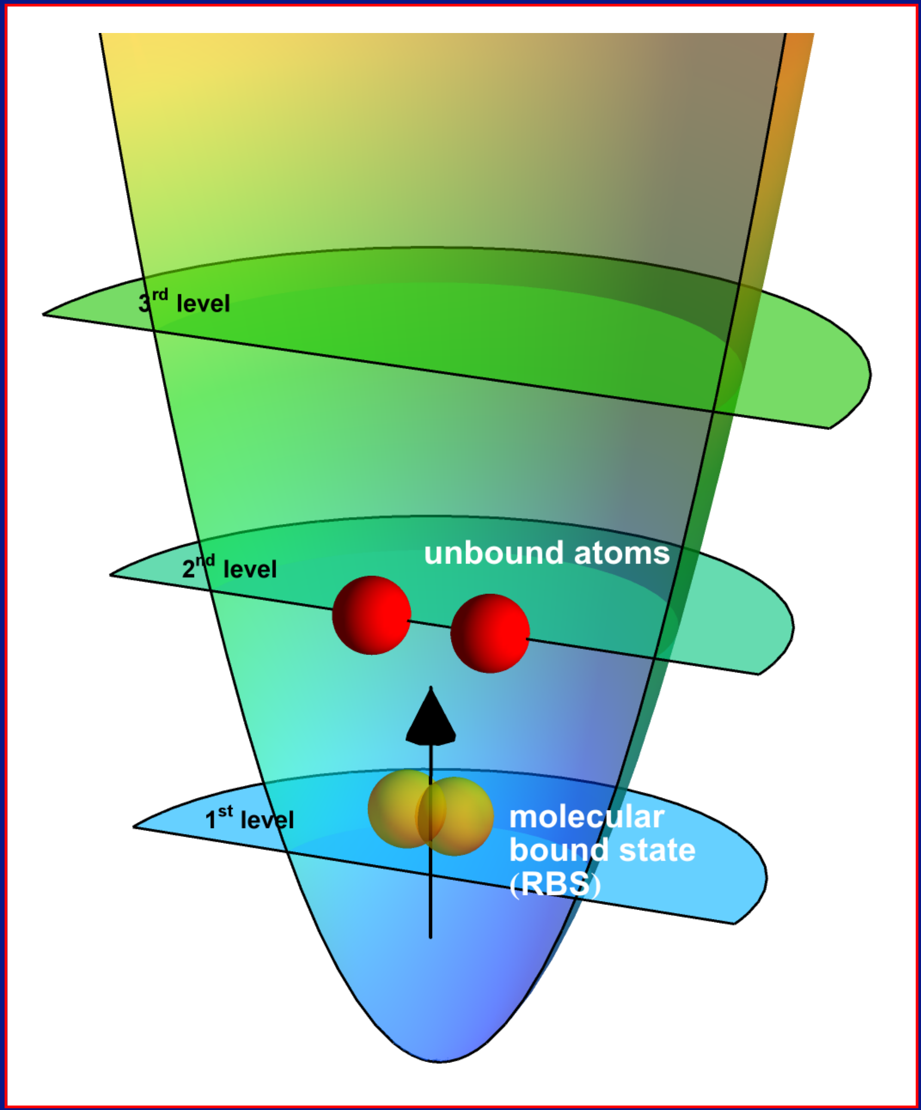
found shift $\approx$ **−80 G**

our prediction: **−80.8 G**

[*Phys. Rev. A* **83**
030701(R) (2011)]



Another aspect of the resonant-bound-state (RBS) admixture



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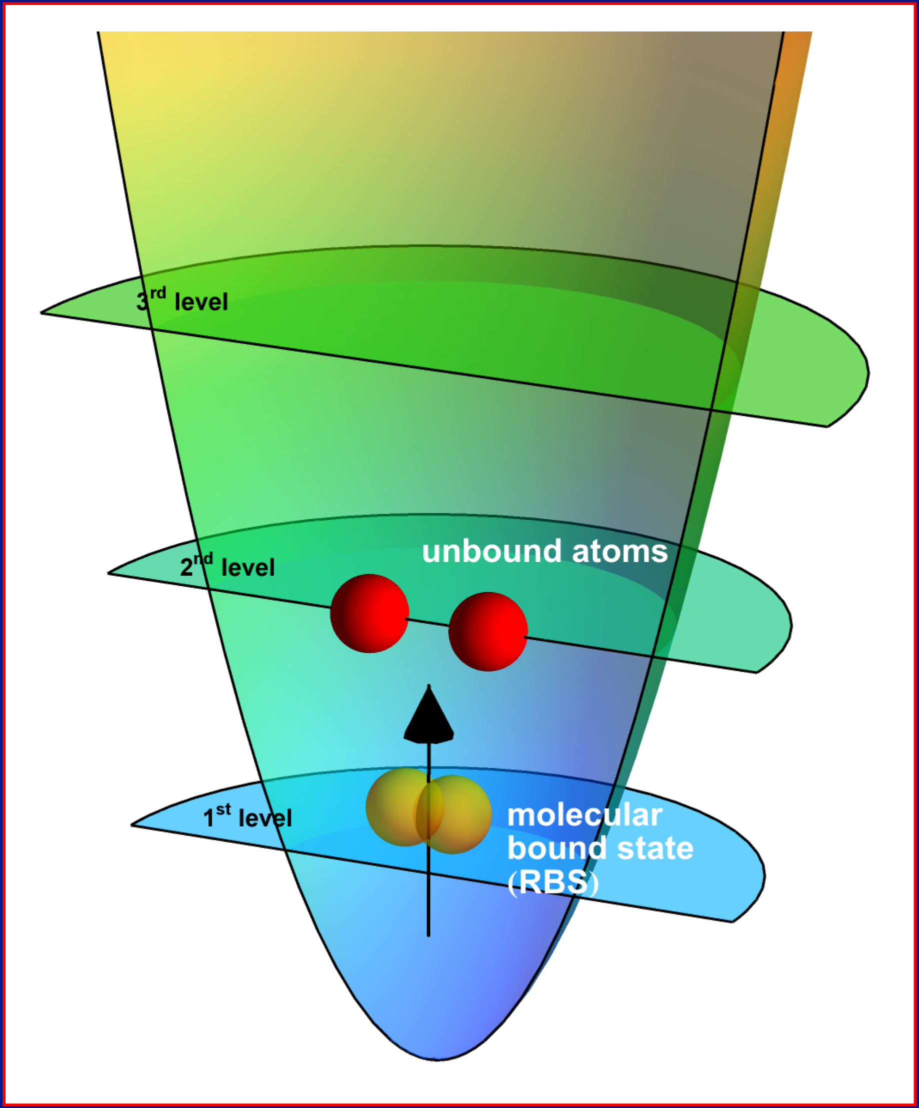

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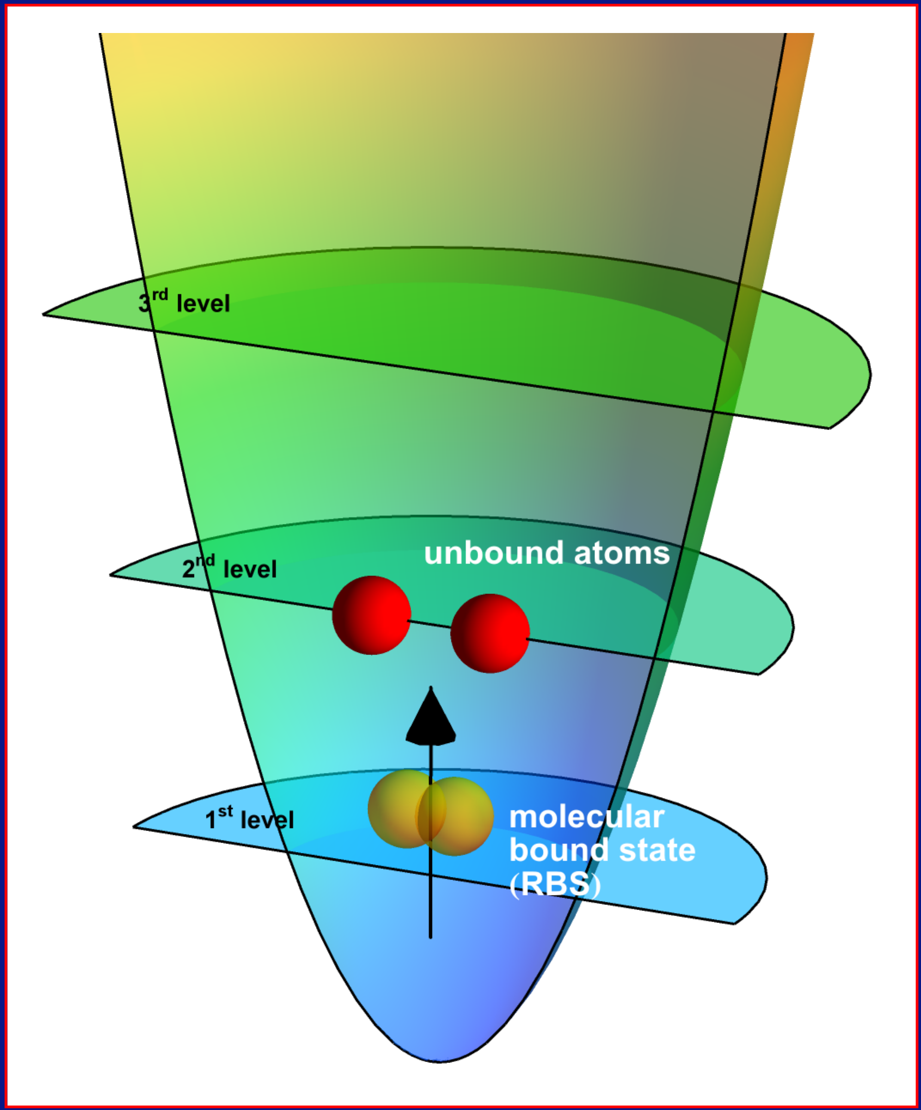

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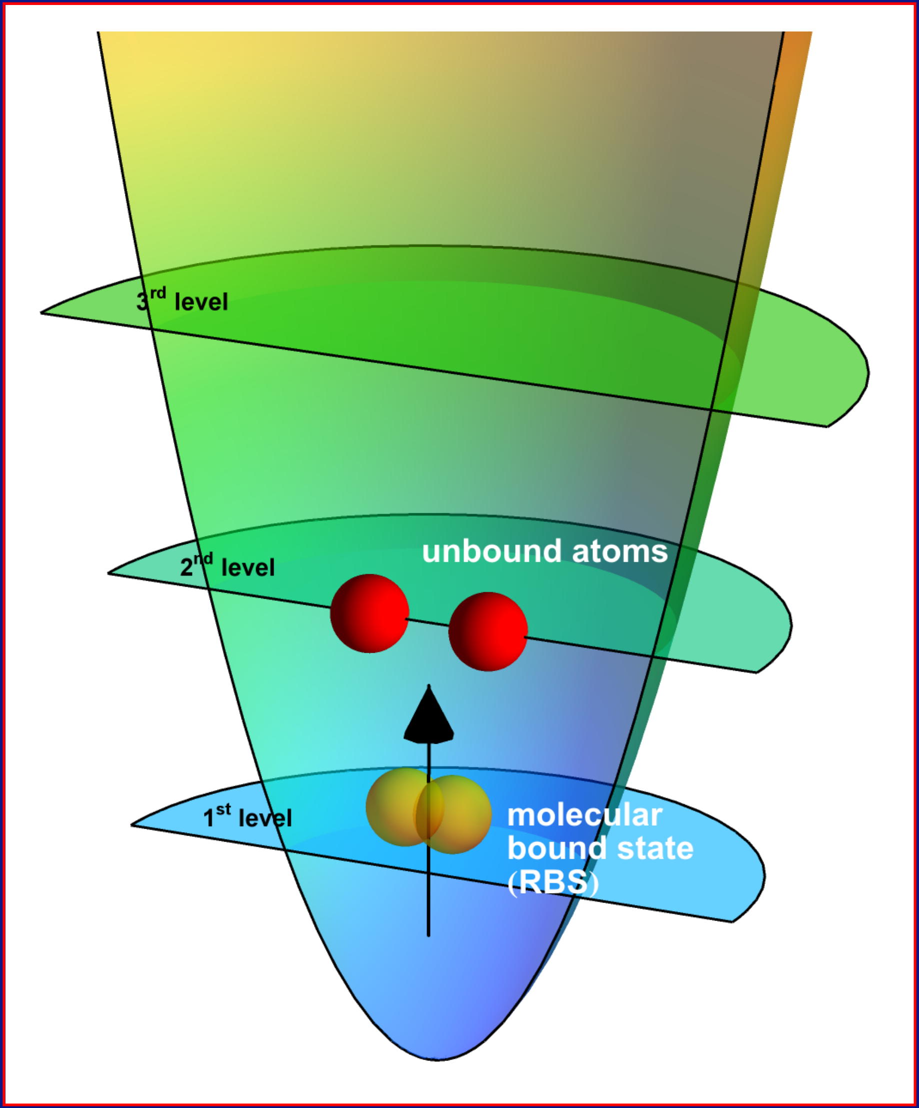

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- Experiment by Rempe *et al.* [PRL 99, 033201 (2007)] with ^{87}Rb: $g \sim 0.004 \Rightarrow$ very weak coupling $\Rightarrow$ RBS admixture visible in the experiment

RBS admixture and dissociation

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1. start with unbound atoms in ground state

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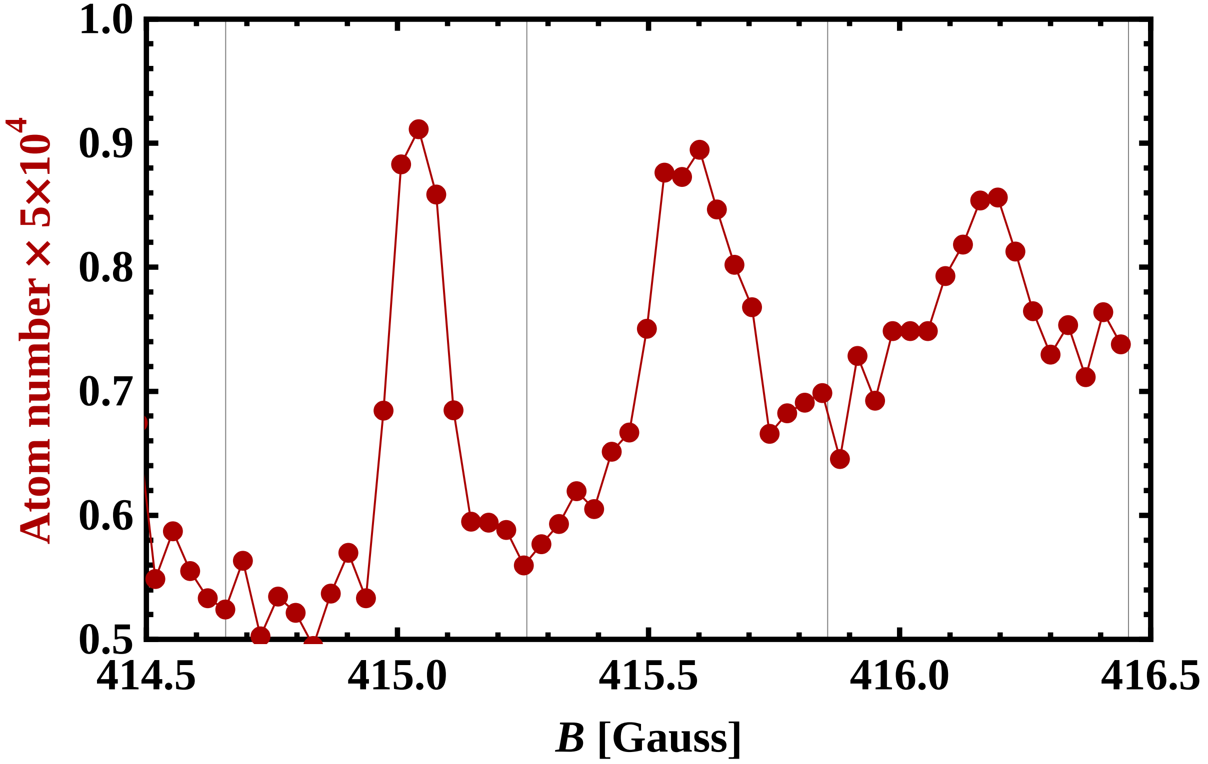
Dissociation of RBS vs. magnetic field at $\omega = 210\,\mathrm{kHz}$



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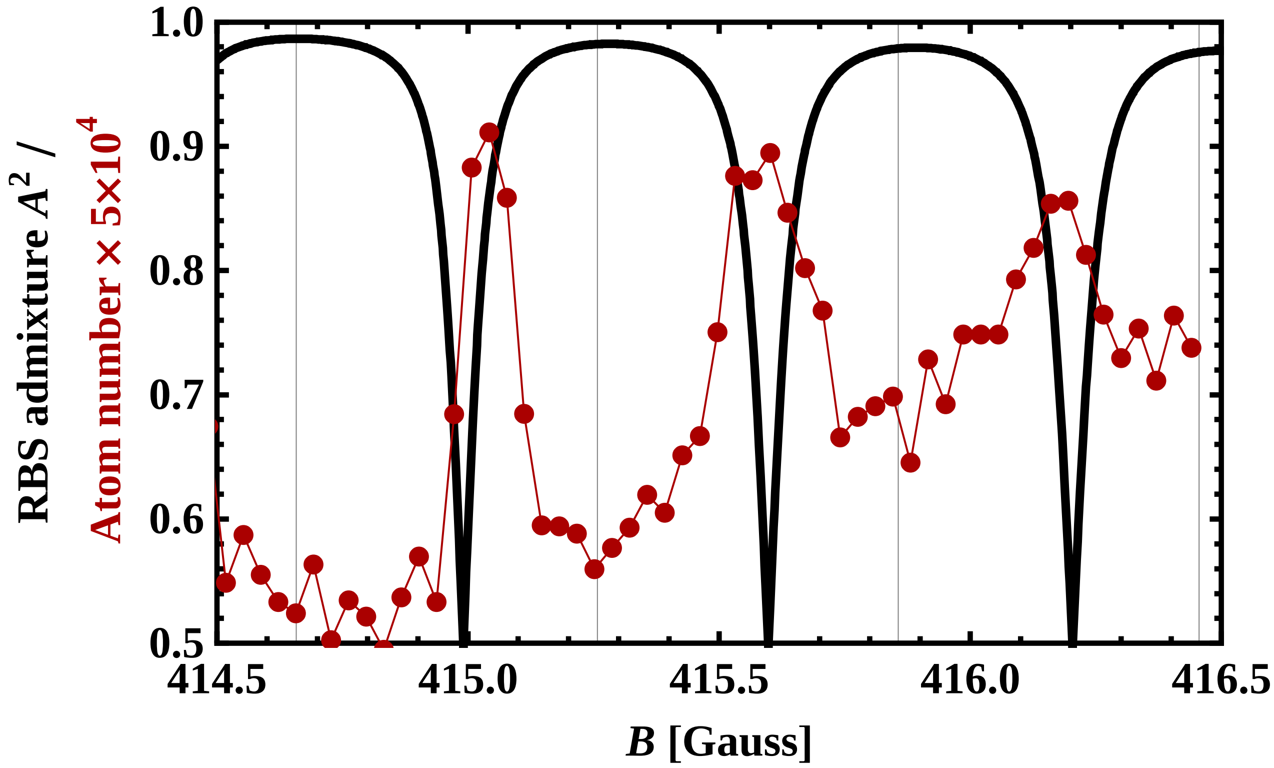

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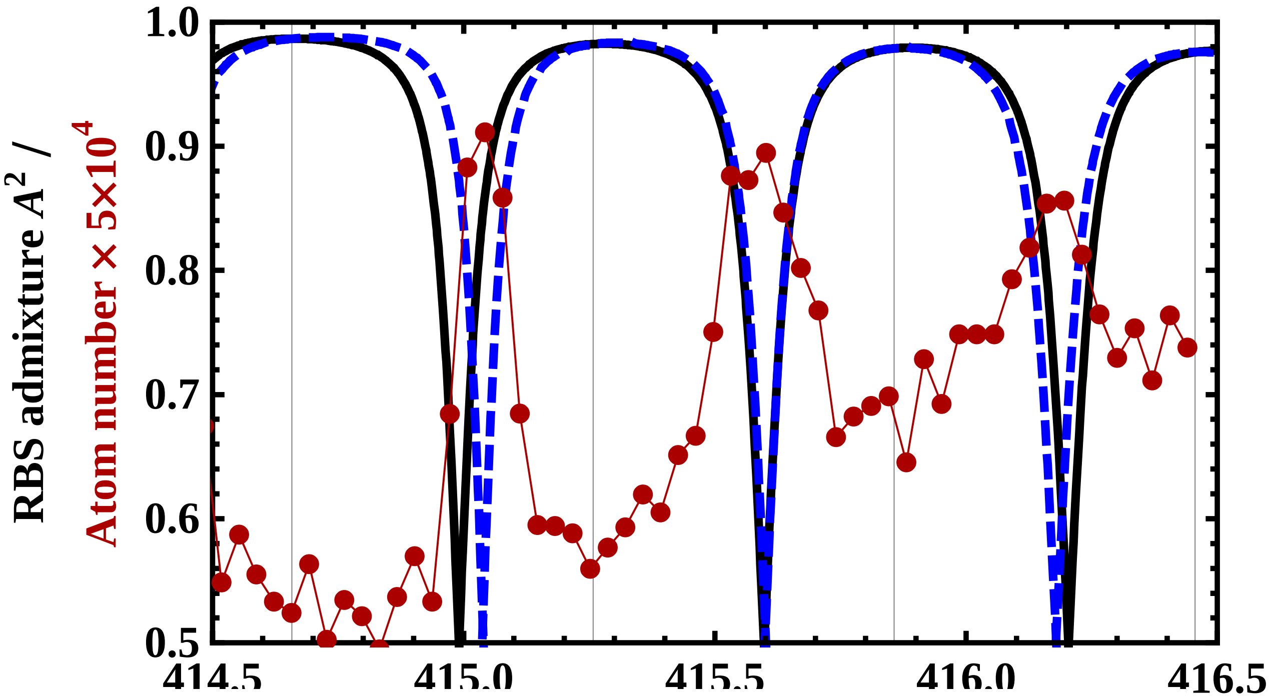

$$a_{\text{bg}}(k)^{-1} = a_0^{-1} - \frac{1}{2}k^2 11400 + \frac{1}{4}k^4 (1770)^3$$

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   - optical lattices (or other tight traps): confined atoms.

   Feshbach resonances in tight (harmonic) traps?

2. Mapping on some model, e.g., the Bose-Hubbard Hamiltonian:

   - even the hamonic approximation fails in principle for atoms in different states, heteronuclear systems, all multi-well potentials (thus for optical lattices!).
   - Problem: coupling of center-of-mass and relative motion!

   Do we simulate what we think we simulate?

Present theoretical approach

Hamiltonian (6D):

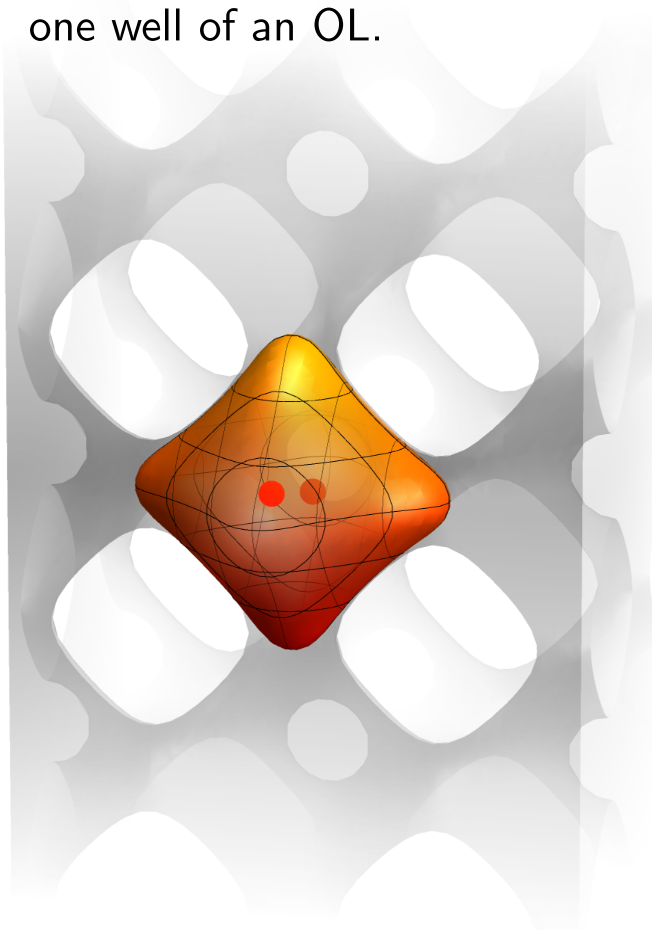
$$\hat{\mathrm{H}}(\vec{R},\vec{r}) \;=\; \hat{\mathrm{h}}_{\mathrm{COM}}(\vec{R}) \;+\; \hat{\mathrm{h}}_{\mathrm{REL}}(\vec{r}) \;+\; \hat{\mathrm{W}}(\vec{R},\vec{r})$$

with $\vec{R}$: center-of-mass (COM) $\vec{r}$: relative motion (REL) coordinate .

- Taylor expansion of the $\sin^2$ lattice potential (to arbitrary order).
- Also $\cos^2$, mixed, and fully anisotropic lattices possible.
- All separable terms included in either $\hat{\mathrm{h}}_{\mathrm{COM}}$ or $\hat{\mathrm{h}}_{\mathrm{REL}}$.
- Full interatomic interaction potential (typically a numerical BO curve).
- Configuration interaction (CI) type full solution using the eigenfunctions (orbitals) of $\hat{\mathrm{h}}_{\mathrm{COM}}$ and $\hat{\mathrm{h}}_{\mathrm{REL}}$.
- Full consideration of lattice symmetry (and possible indistinguishability of atoms).

Two atoms in a single well: anharmonicity and coupling

We obtained **exact solutions** for two interacting atoms in one well of an OL.



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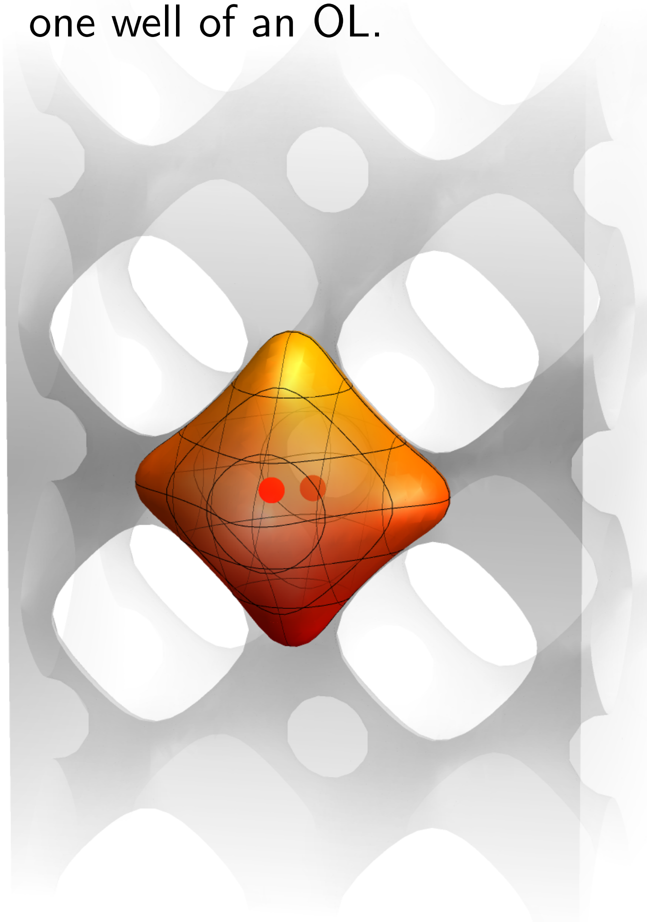
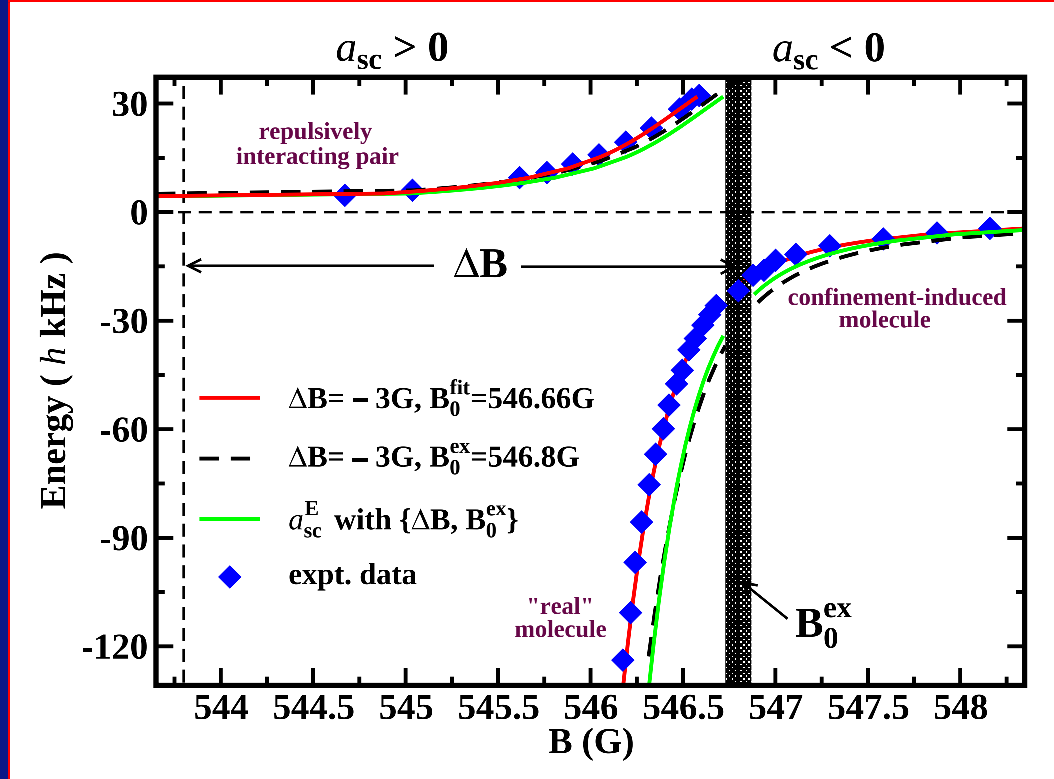


Agreement with experiment on **kHz level**

→ improved resonance parameters by fit?

Fit works only, if **anharmonicity** is considered

→ **coupling of COM and REL motion important!**



[S. Grishkevich *et al.*, Phys. Rev. A **80**, 013403 (2009)]

Bose-Hubbard model of the OL

N-Boson Hamiltonian with additional external confinement $V_{\rm conf}(\mathbf{r})$

$$H_{\rm OL} = \sum_{n=1}^{N} \left(\frac{p_n^2}{2m} + V_{\rm OL}(\mathbf{r}_n) + V_{\rm conf}(\mathbf{r}_n) \right) + \sum_{n<m} \hat{V}_{\rm int}(\mathbf{r}_n - \mathbf{r}_m)$$

is rewritten in basis of Wannier functions $w_i(\mathbf{r})$ (superpositions of Bloch solutions localized at lattice site i) of the first Bloch band as

$$\hat{H}_{BH} = -J \sum_{<i,j>} b_i^\dagger b_j + \sum_i \epsilon_i \hat{n}_i + U \sum_i \frac{\hat{n}_i(\hat{n}_i - 1)}{2}$$

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with $J = -\left\langle w_0 \middle| \frac{\hat{p}}{2m} + \hat{V}_{\text{OL}} \middle| w_1 \right\rangle$, $\epsilon_i = \left\langle w_i \middle| \frac{\hat{p}}{2m} + \hat{V}_{\text{OL}} + \hat{V}_{\text{conf}} \middle| w_i \right\rangle$

and $U = \langle w_0 | \langle w_0 | \hat{V}_{\text{Int}} | w_0 \rangle | w_0 \rangle$

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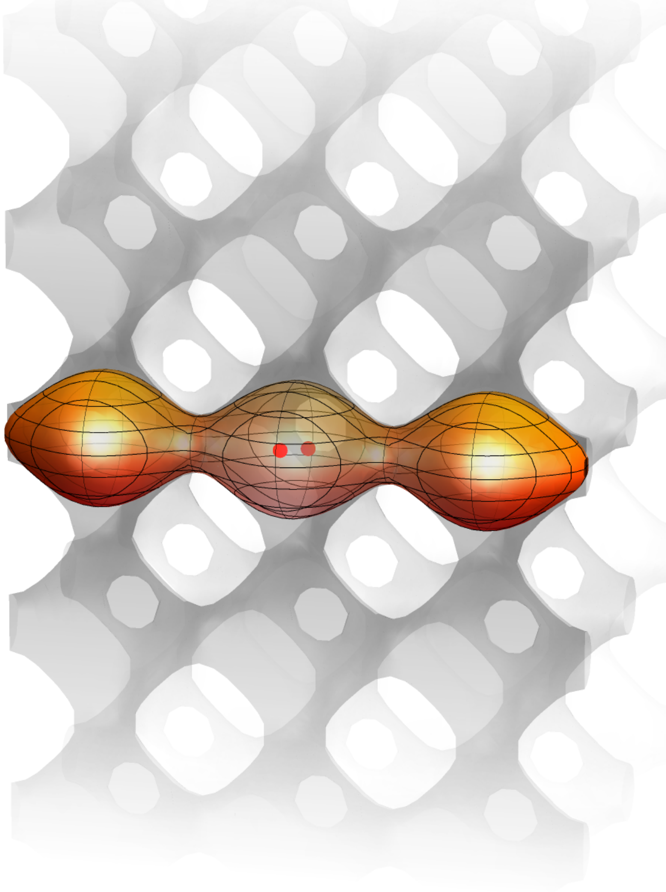

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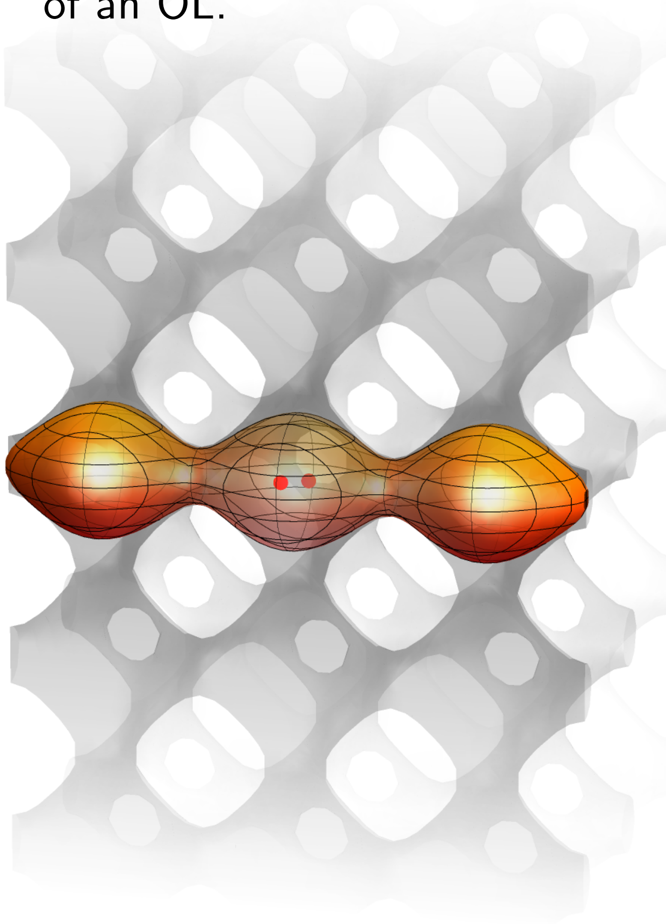
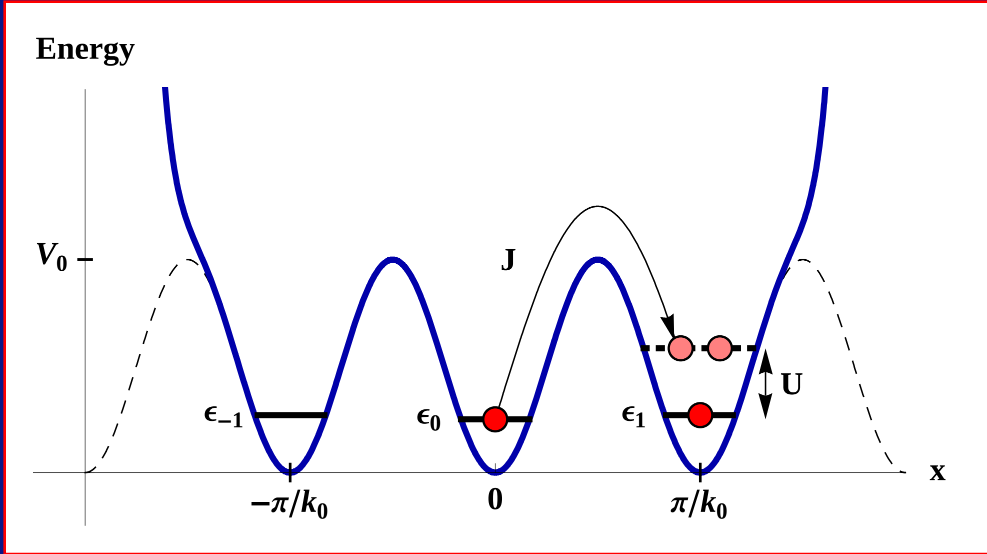


- Comparison with **BH model** with Hamiltonian

$$\hat{H}_{\rm BH} = J \sum_{<i,j>} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) + \sum_i \epsilon_i \hat{b}_i^\dagger \hat{b}_i$$

yields **optimal BH parameters** $J^{\rm opt}, U^{\rm opt}, \epsilon_i^{\rm opt}$ and **validity range of BH model**.



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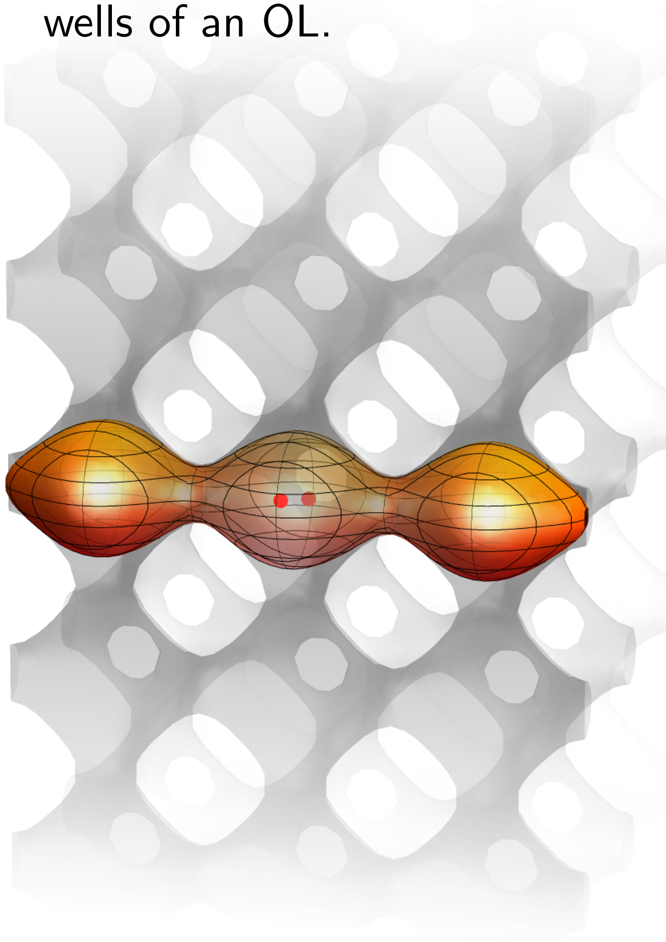

- Introduction of **improved U parameter** by correction of harmonic interaction energy: $U^{\mathrm{corr}} = \mathcal{A} U^{\mathrm{harm}}$ with

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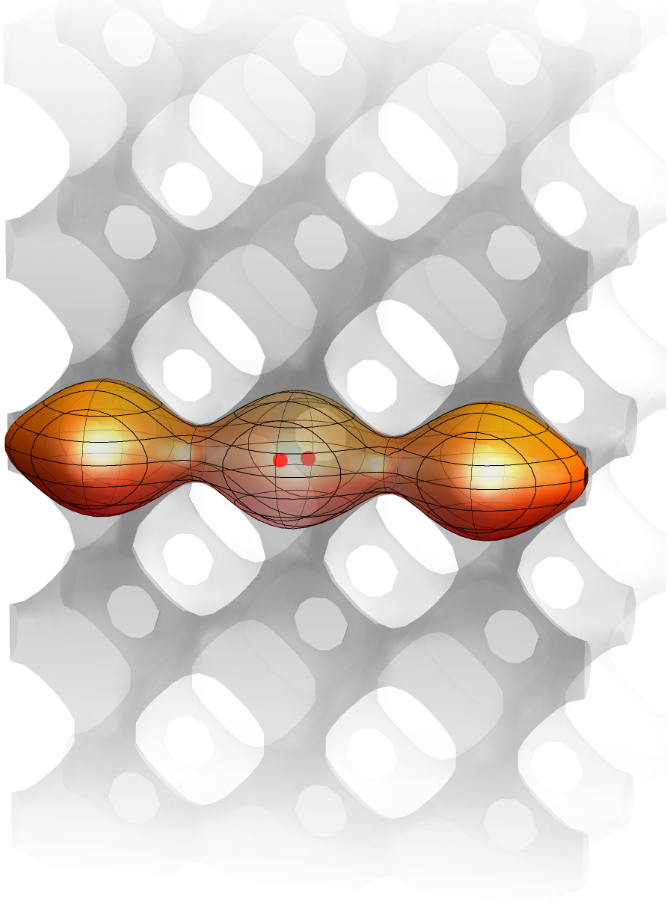

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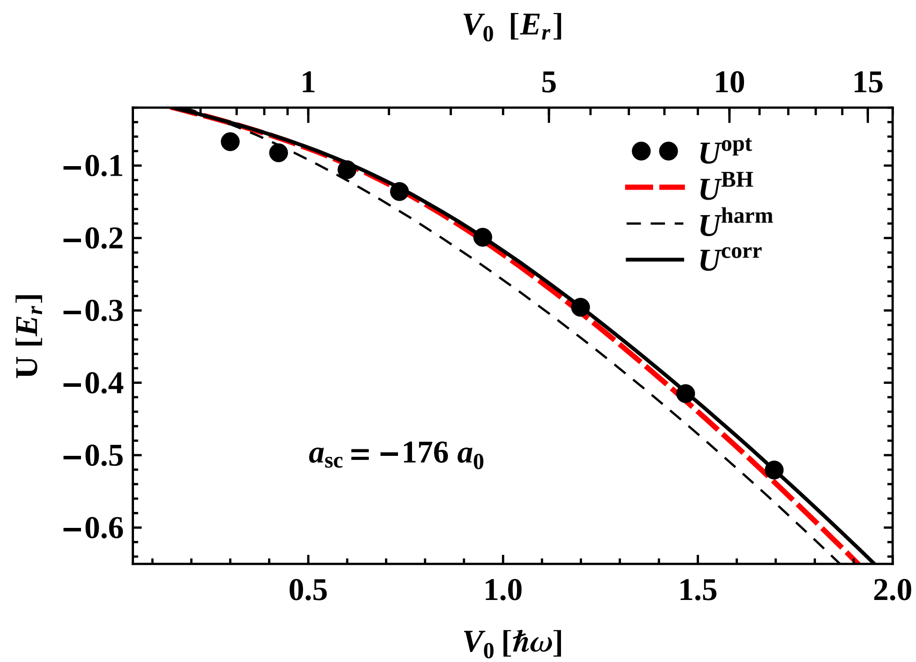

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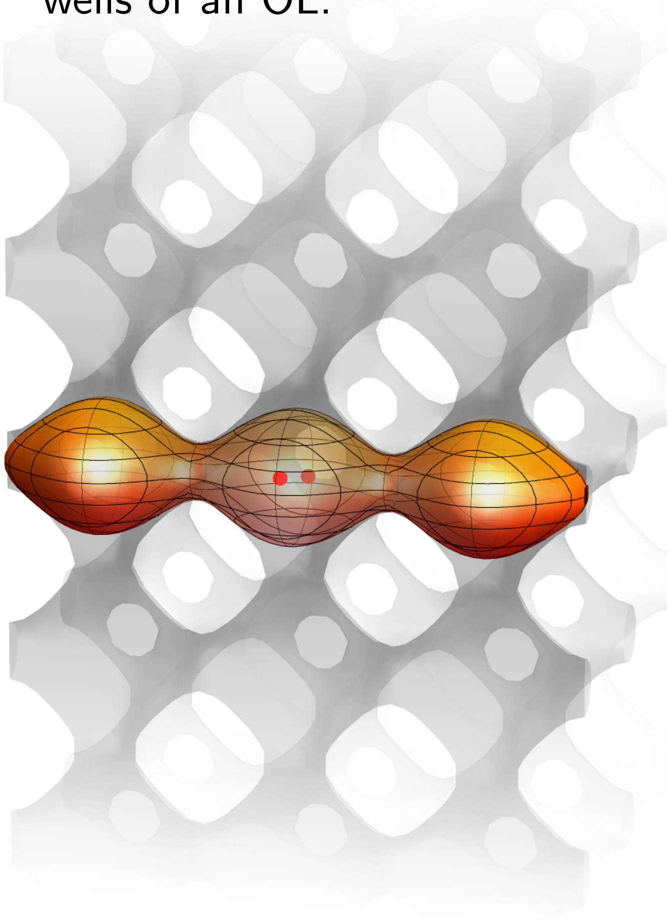

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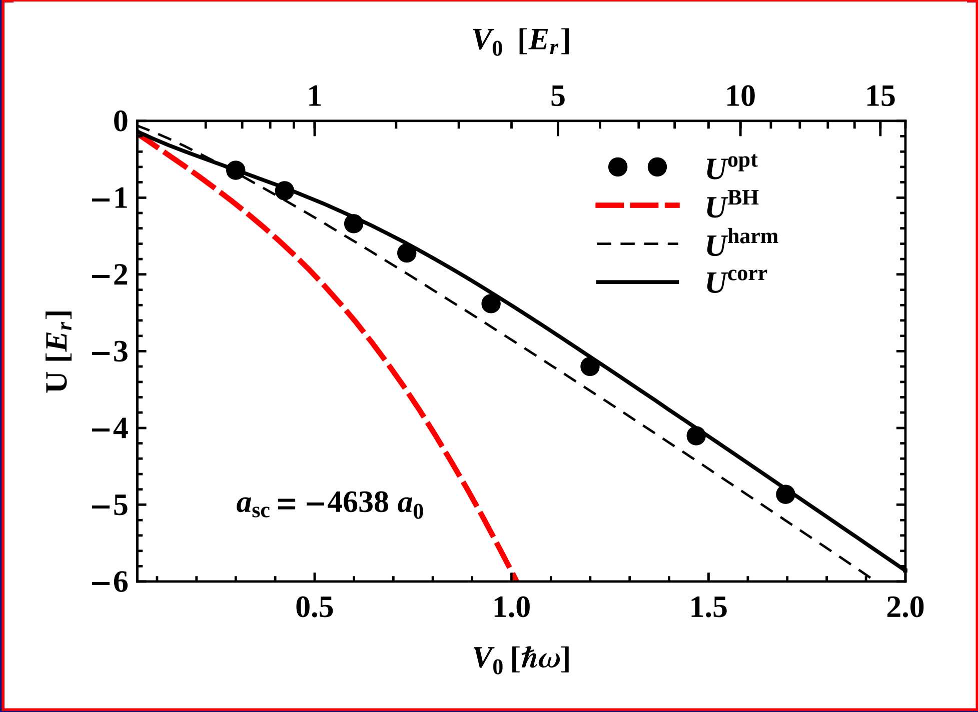

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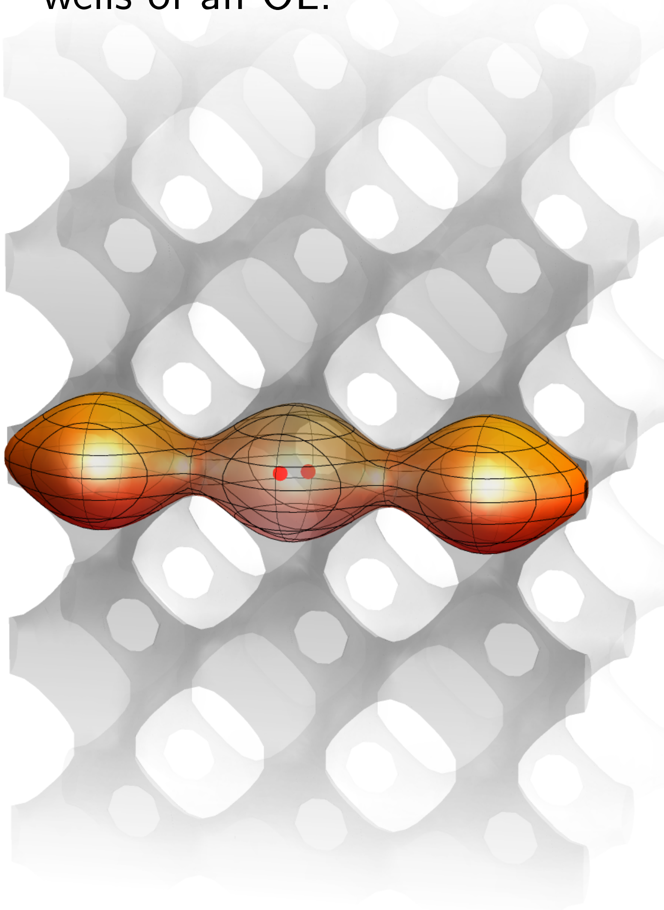

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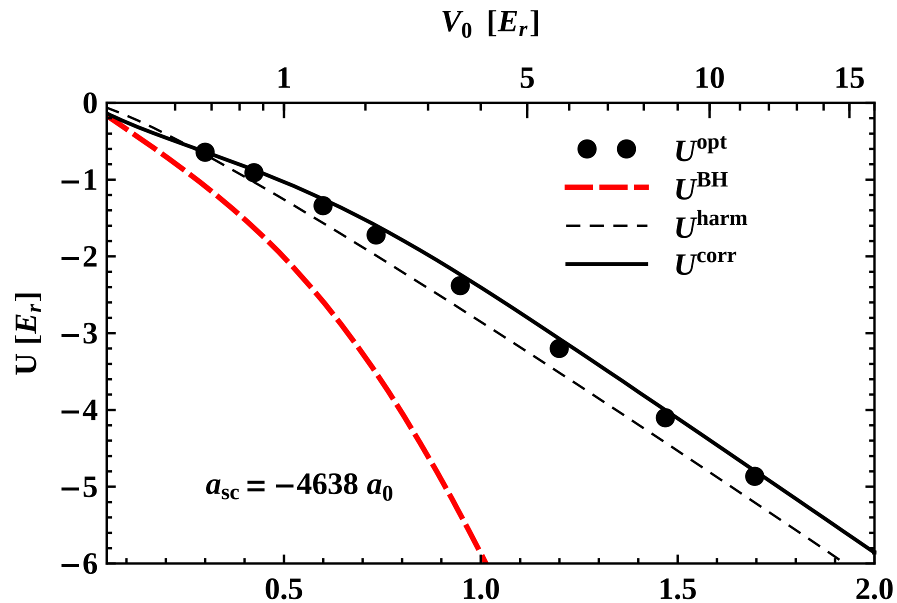
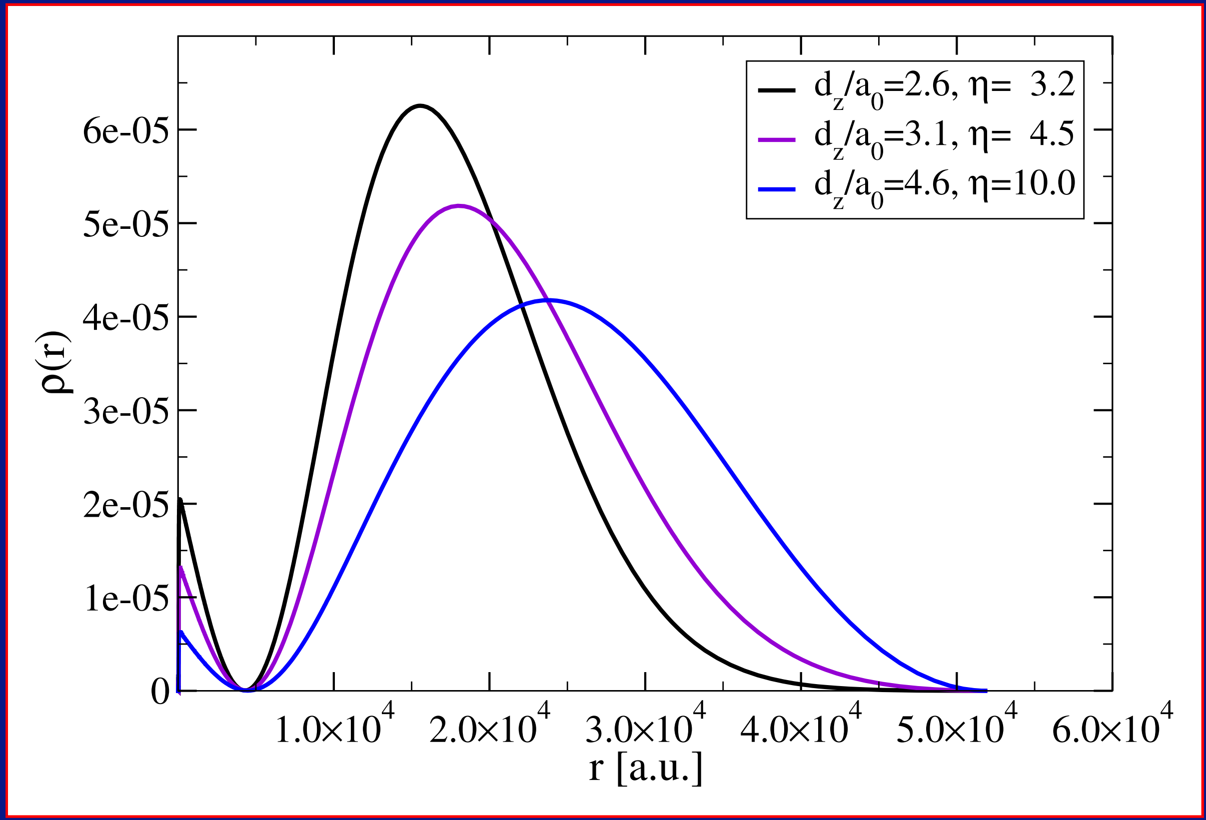


more in Phys. Rev. A **80** 013404 (2009)

Reduced dimension: fermionization of bosons (1D vs. quasi 1D)



Radial density of two atoms in a quasi-1D (cigar-shaped) confinement:

– scattering length $a_0 = 5624$ a.u.

– **anisotropy** $\eta = (d_z/d_\perp)^2$

– transversal trap length $d_\perp = 1.46\, a_0$

– full Born-Oppenheimer potential.

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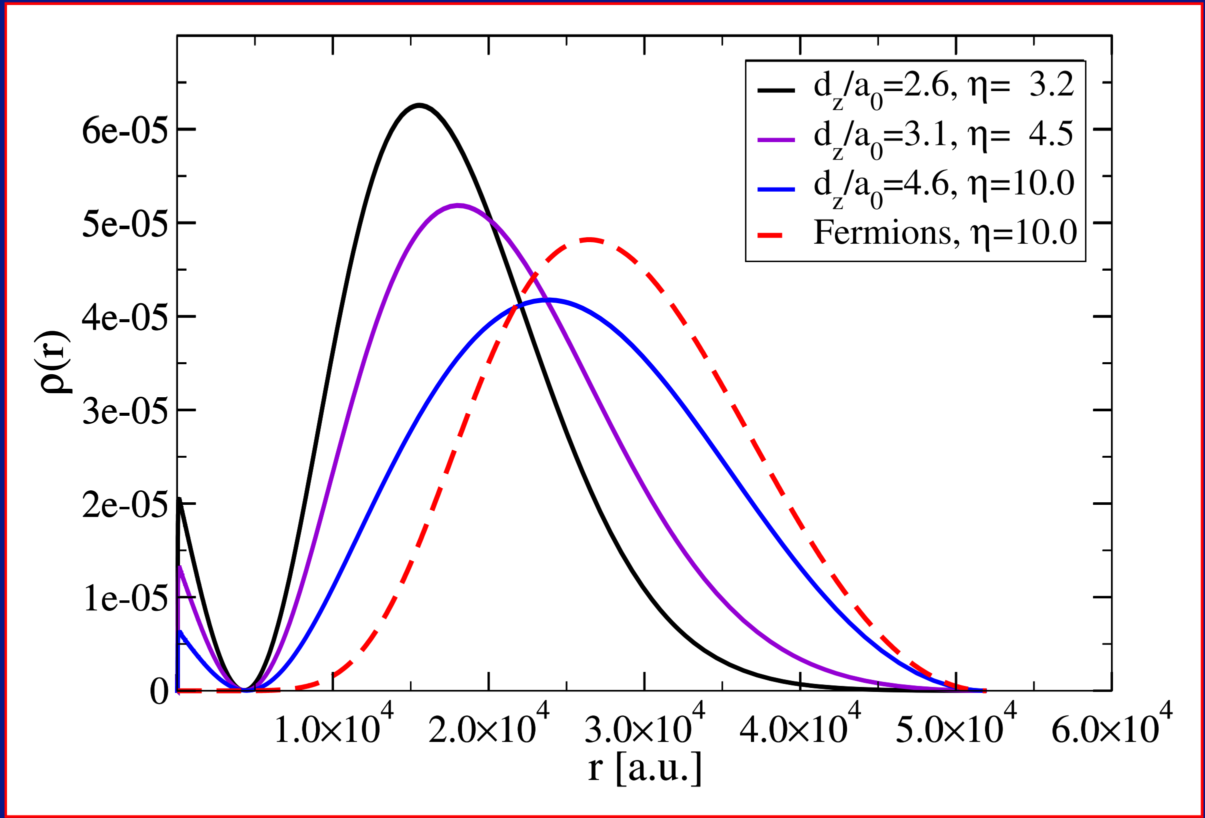

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Confinement-induced resonances (CIR)

Relative-motion s-wave scattering theory for two ultracold atoms in an harmonic quasi 1D confinement: mapping of quasi-1D system onto pure 1D system.

Renormalized 1D interaction strength [M. Olshanii, PRL 81, 938 (1998)]:

$$g_{1D} = \frac{2a\hbar^2}{\mu d_\perp^2} \frac{1}{1 + \zeta(\frac{1}{2}) \frac{a}{d_\perp}}$$

$a :=$ s-wave scattering length

$\mu :=$ reduced mass

$d_\perp = \sqrt{\frac{\hbar}{\mu\omega_\perp}}$: transversal confinement

$\zeta(x) = \sum_{k=1}^{\infty} k^{-x}$

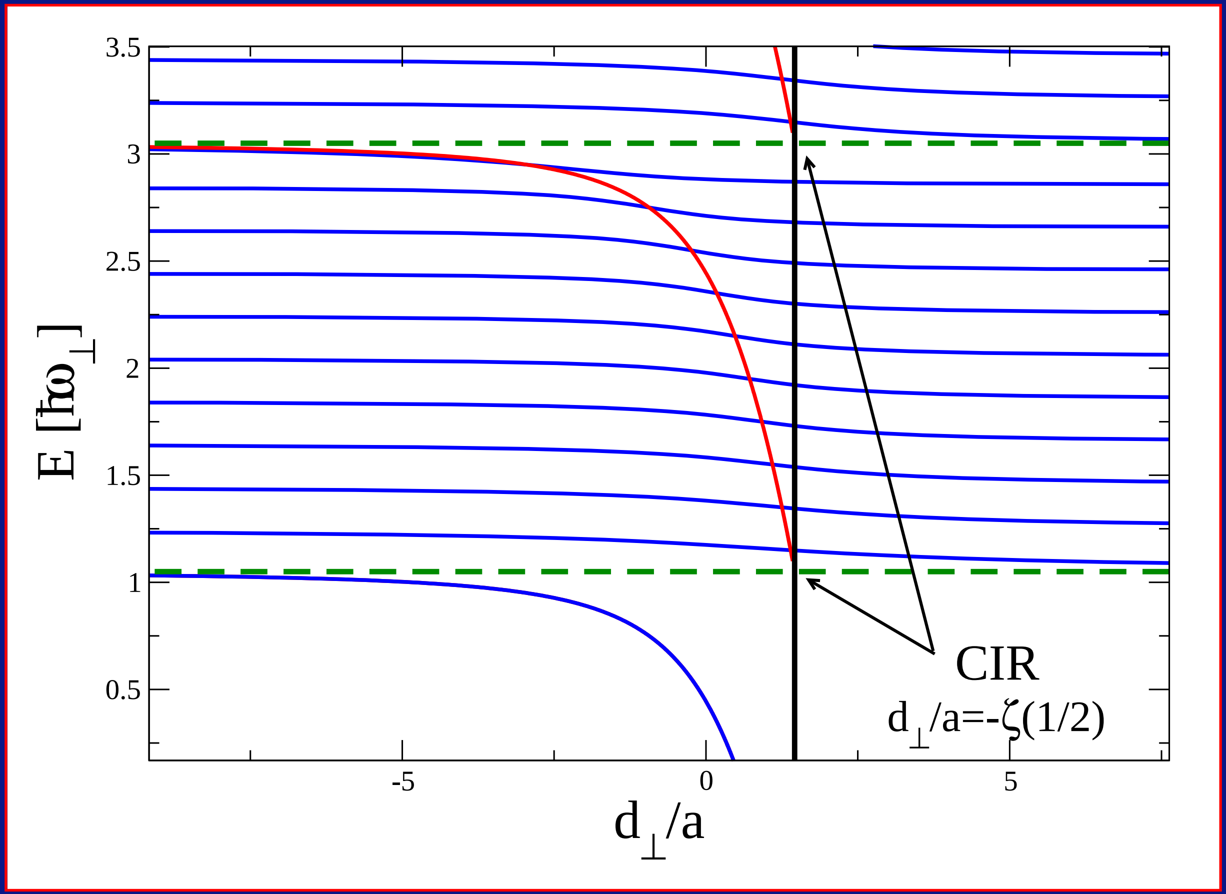
Resonance: $g_{1D} \to \infty$ for $\frac{d_\perp}{a} = -\zeta(\frac{1}{2}) \approx 1.46\ldots$

Analogously: confinement-inuced resonance occurs also in (quasi) 2D

[Petrov, Holzmann, Shlyapnikov, PRL **84**, 2551 (2000)].

Olshanii's model (I)

Resonance occurs where artificially excited bound state crosses the free ground-state threshold:

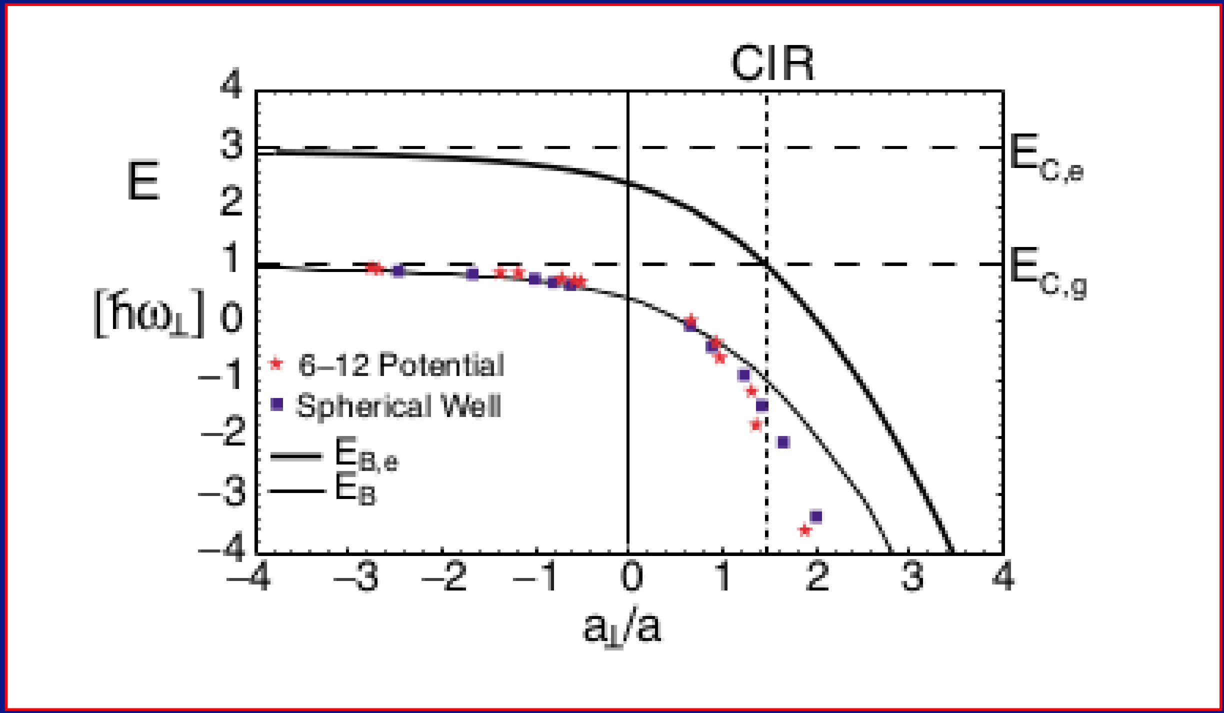


Blue: quasi 1D spectrum

Red: artificially(!) excited bound state

Green: quasi continuum threshold

Olshanii's model (II)



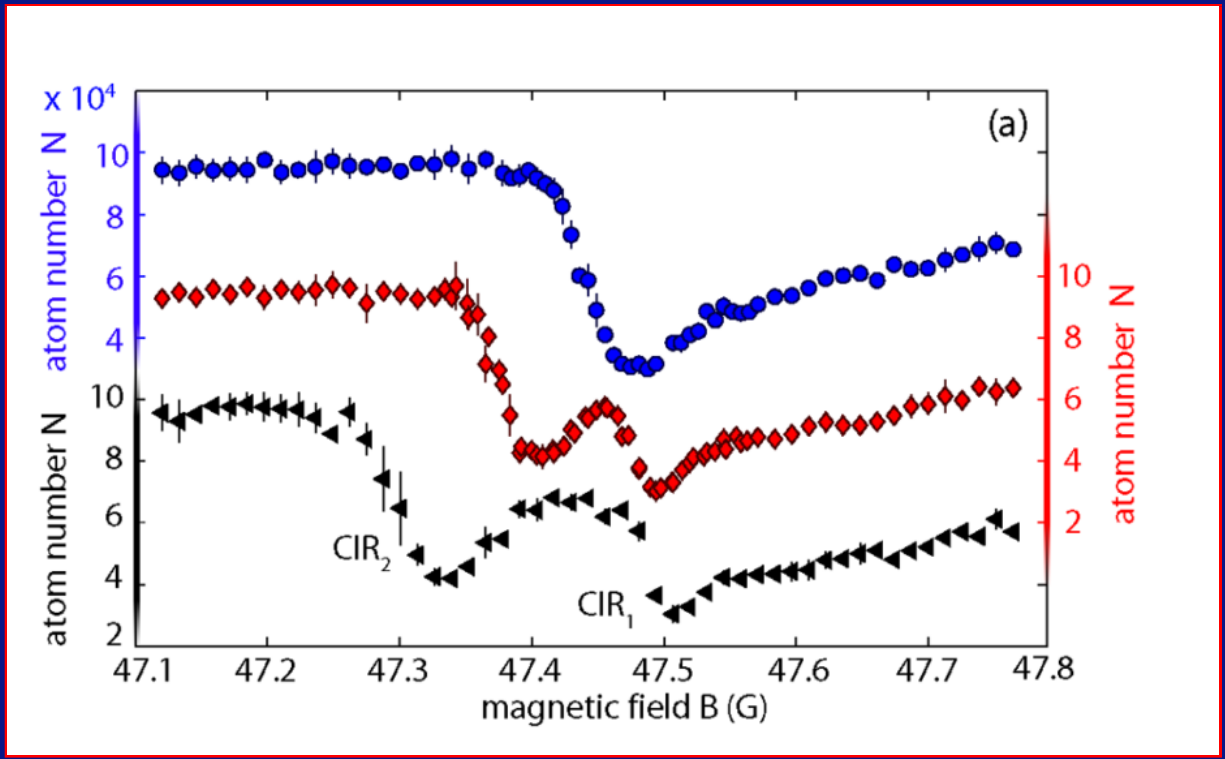
T. Bergeman et al., PRL **91**, 163201 (2003)

Result:

Confinement-induced resonances (CIR) are not an artefact of the δ potential.

Note: No data points on shifted state!

Innsbruck experiment (Cs atoms)

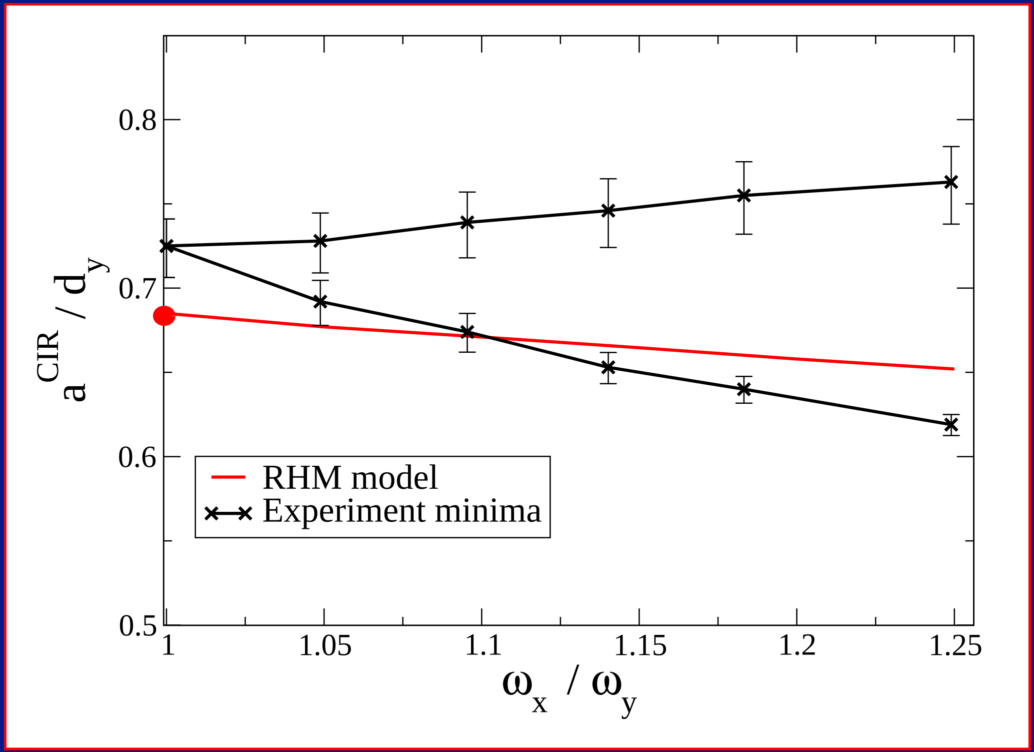


Blue curve: Atom losses for $\omega_x = \omega_y \gg \omega_z$ (anisotropy fixed, a varied).

Red and blue curves: Atom losses for $\omega_x \neq \omega_y \gg \omega_z$

E. Haller et al., PRL **104**, 153203 (2010)

Problem: agreement and conflict with theory



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⇒ Good agreement with Olshanii prediction for single anisotropy ($\omega_x = \omega_y$)

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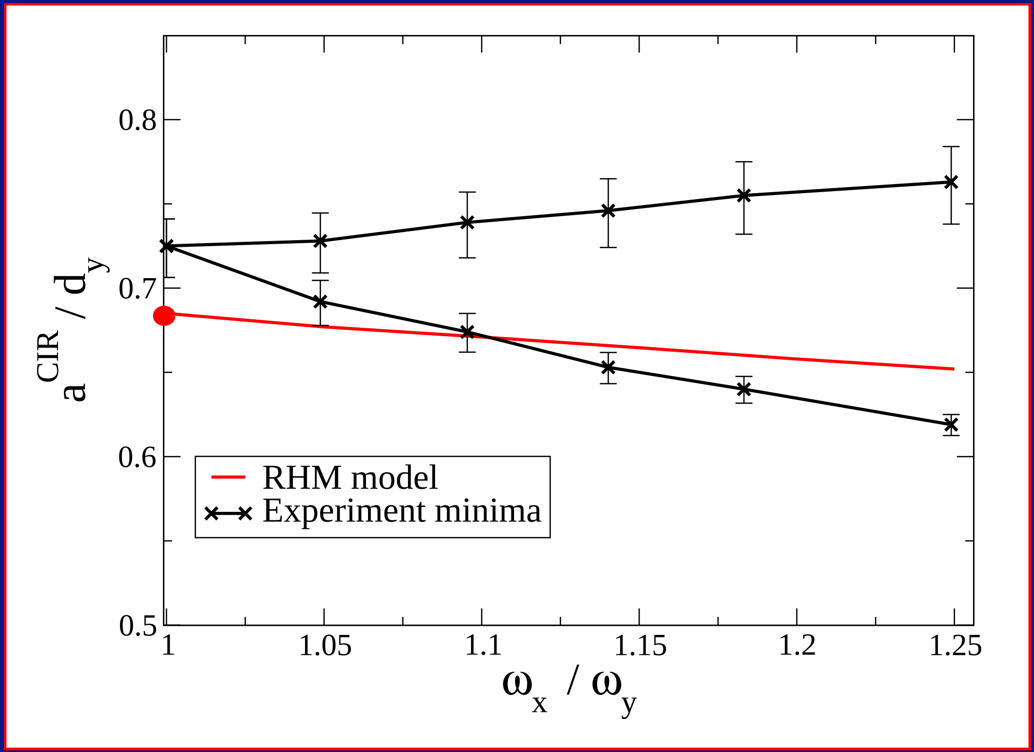

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⇒ Good agreement with Olshanii prediction for single anisotropy ($\omega_x = \omega_y$)

⇒ **Olshanii theory: no splitting ($\omega_x \neq \omega_y$)!!!** Peng et al., PRA **82**, 063633 (2010)

Complete confusion:

Innsbruck loss experiment (Haller et al.):

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Cambridge radio-frequency experiment (Froehlich et al.):

- **Quasi-2D:** CIR appears at "correct" value of a (also seen by Chris Vale).
- Note: direct measurement of the binding energies.

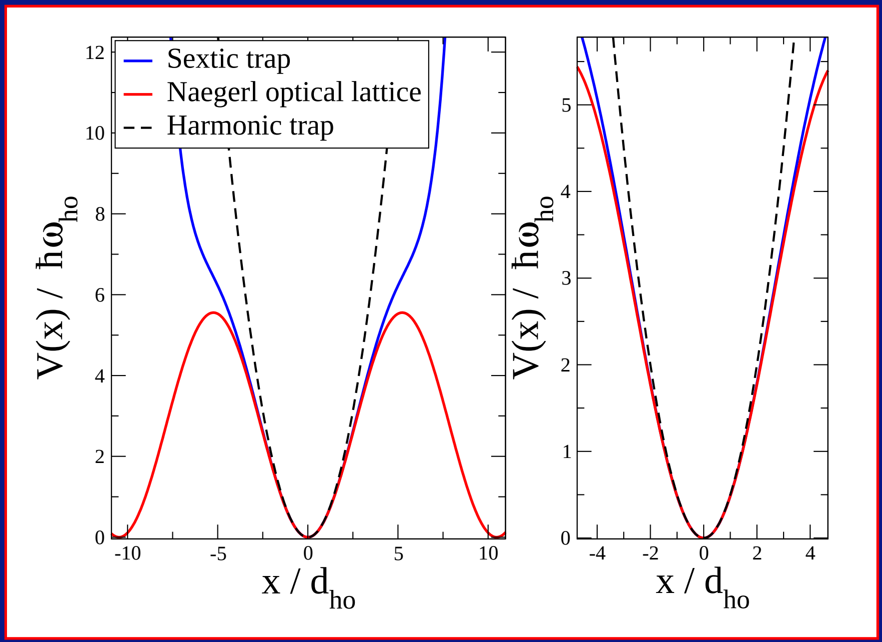
Full treatment of two atoms in quasi-1D trap:

Full Hamiltonian: center-of-mass (COM) and relative motion (REL) motion:

$$H(\mathbf{r},\mathbf{R}) = T_{\rm REL}(\mathbf{r}) + T_{\rm COM}(\mathbf{R}) + V_{\rm REL}(\mathbf{r}) + V_{\rm COM}(\mathbf{R}) + U_{\rm int}(r) + W(\mathbf{r},\mathbf{R})$$

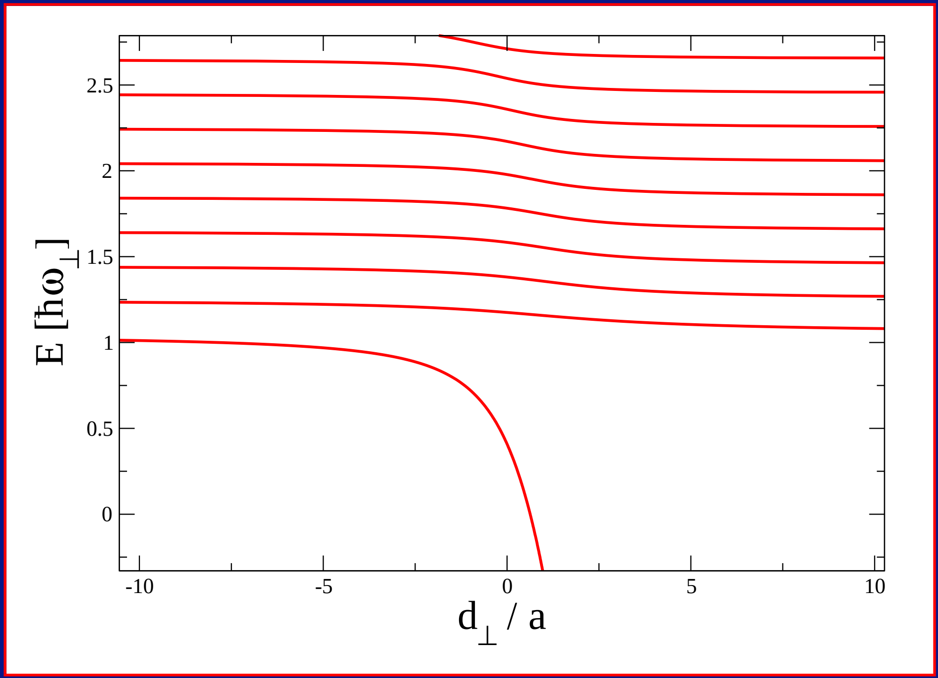
Note:

Anharmonic optical-lattice potential $\Rightarrow$ COM and REL coupling $(W(\mathbf{r},\mathbf{R}) \neq 0)$!

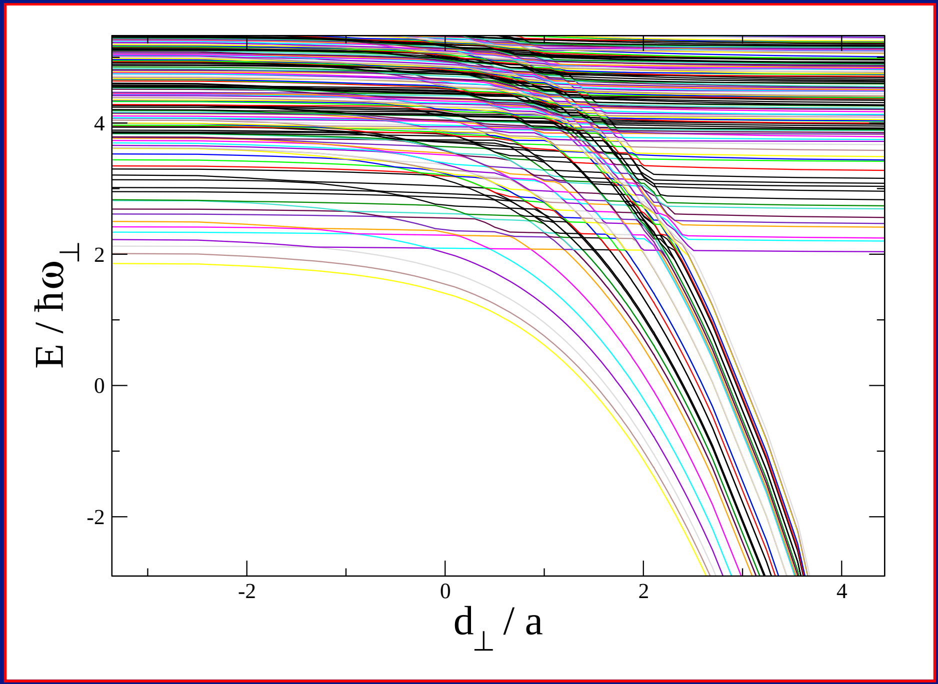


Spectra

Relative motion spectrum in harmonic trap vs. coupled spectrum in sextic trap



REL



REL + COM + COUPLING

Many crossings are found in the coupled model,

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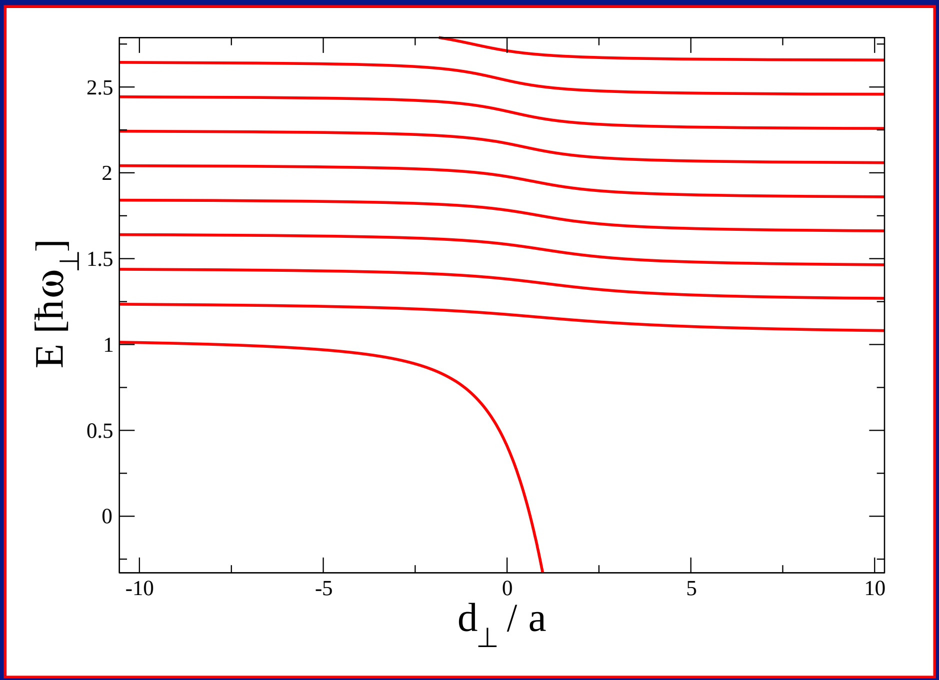
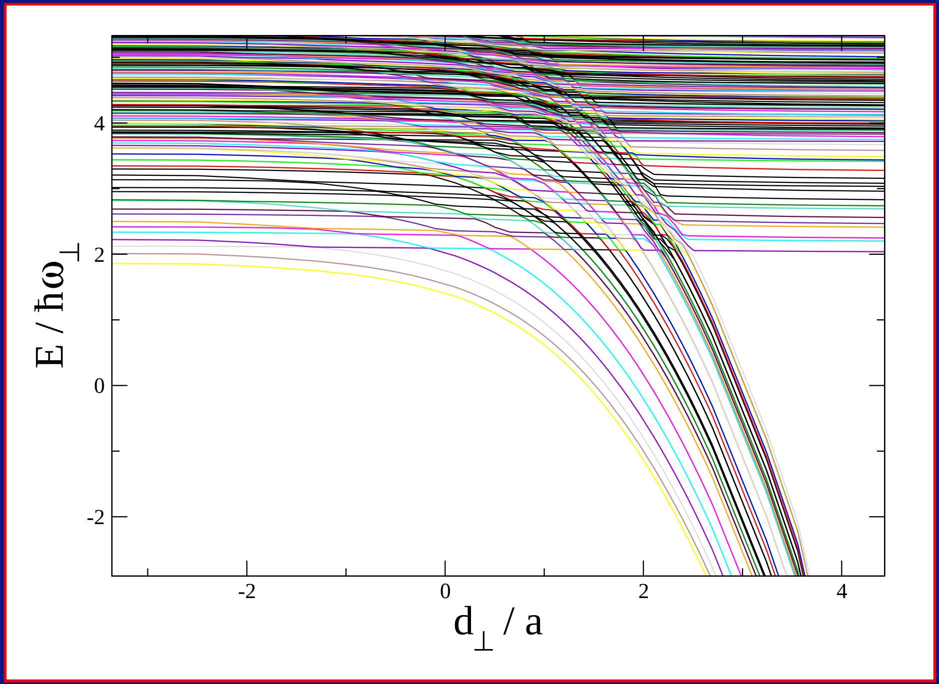


REL



REL + COM + COUPLING

Many crossings are found in the coupled model,

but which of them lead to resonances?

Approximate selection rules

Coupling matrix element:

$$W_{(n,m,k)} = \langle\, \phi_n(\mathbf{R})\, \psi_b(\mathbf{r}) \,|\, W(\mathbf{r},\mathbf{R}) \,|\, \phi_m(\mathbf{R})\, \psi_k(\mathbf{r}) \,\rangle$$

$$W(\mathbf{r},\mathbf{R}) = \sum_{j=x,y,z} W_j(r_j, R_j)$$

$$W_{(n,m,k)} \approx \delta_{n_z,m_z}\, F_{(n,m,k)}(W)$$

$$F_{(n,m,k)}(W) = \Big[\delta_{n_y,m_y} \langle\phi_{n_x}(X)|W_x(X)|\phi_{m_x}(X)\rangle \langle\psi_b(\mathbf{r})|W_x(x)|\psi_k(\mathbf{r})\rangle$$
$$+\delta_{n_x,m_x} \langle\phi_{n_y}(Y)|W_y(Y)|\phi_{m_y}(Y)\rangle \langle\psi_b(\mathbf{r})|W_y(y)|\psi_k(\mathbf{r})\rangle\Big]$$

REL bound state: $|\psi_b(\mathbf{r})\rangle$

REL trap state: $\psi_k(\mathbf{r})$

COM states: $\phi_n(\mathbf{R}) = \phi_{n_x}(X)\, \phi_{n_y}(Y)\, \phi_{n_z}(Z)$

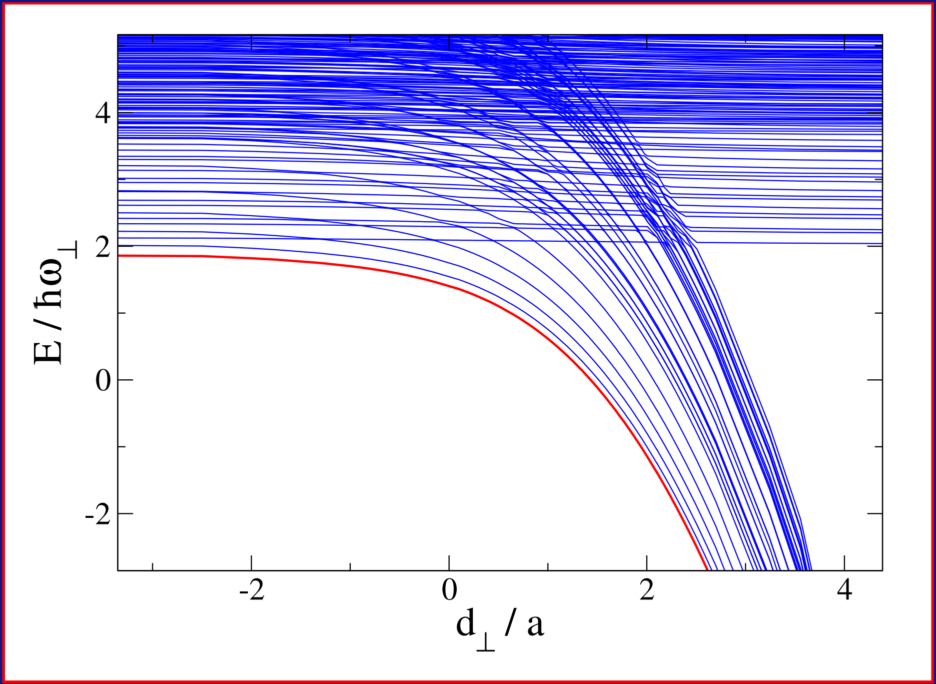
Ultracold: only ground trap state populated $\Longrightarrow m = k = 0$.

Resonances:

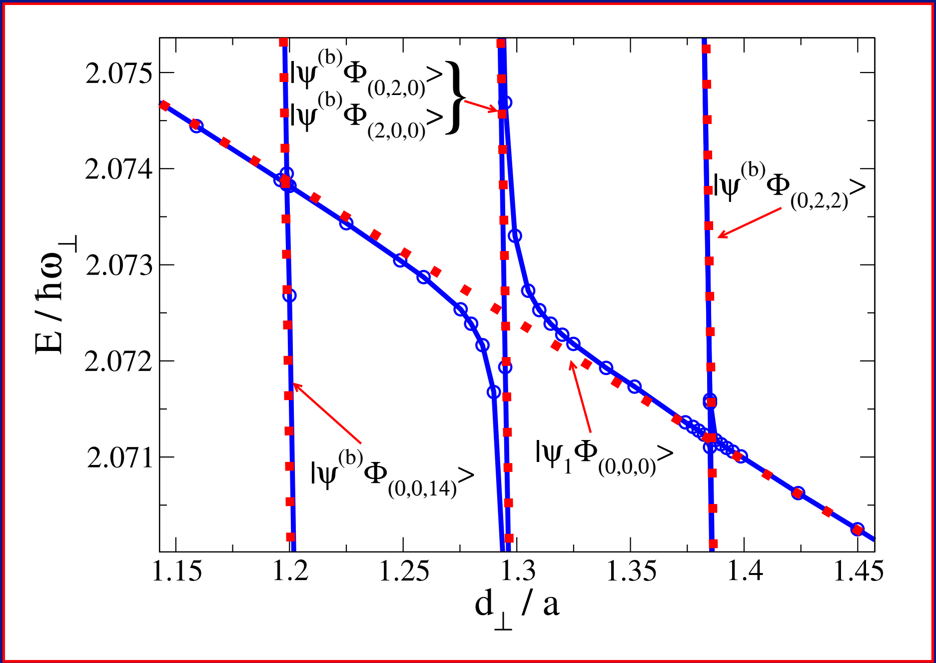
Crossing of transversally COM excited REL bound state with ground (COM and REL) trap state.

Avoided Crossings (I)

Only few crossings are **avoided** (approx. selection rules):



Large part of spectrum



Zoom-in in spectrum.

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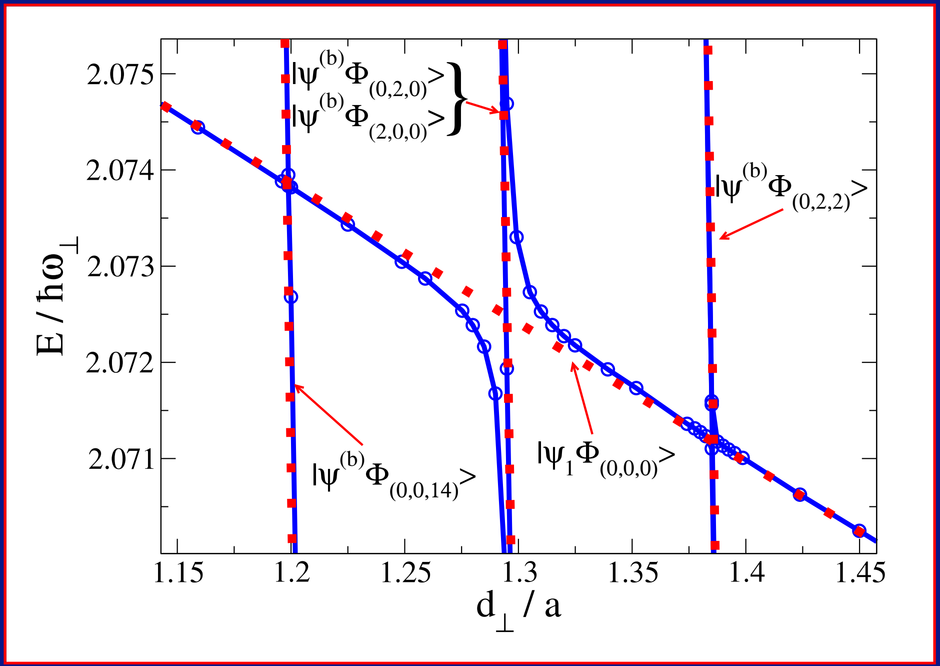
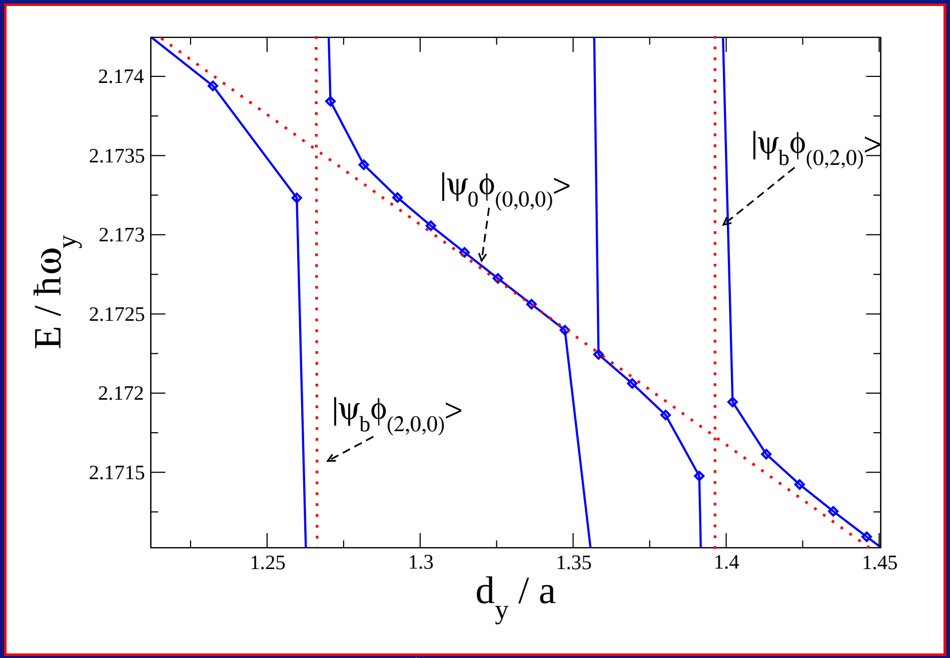


$\omega_x = \omega_y \gg \omega_z$



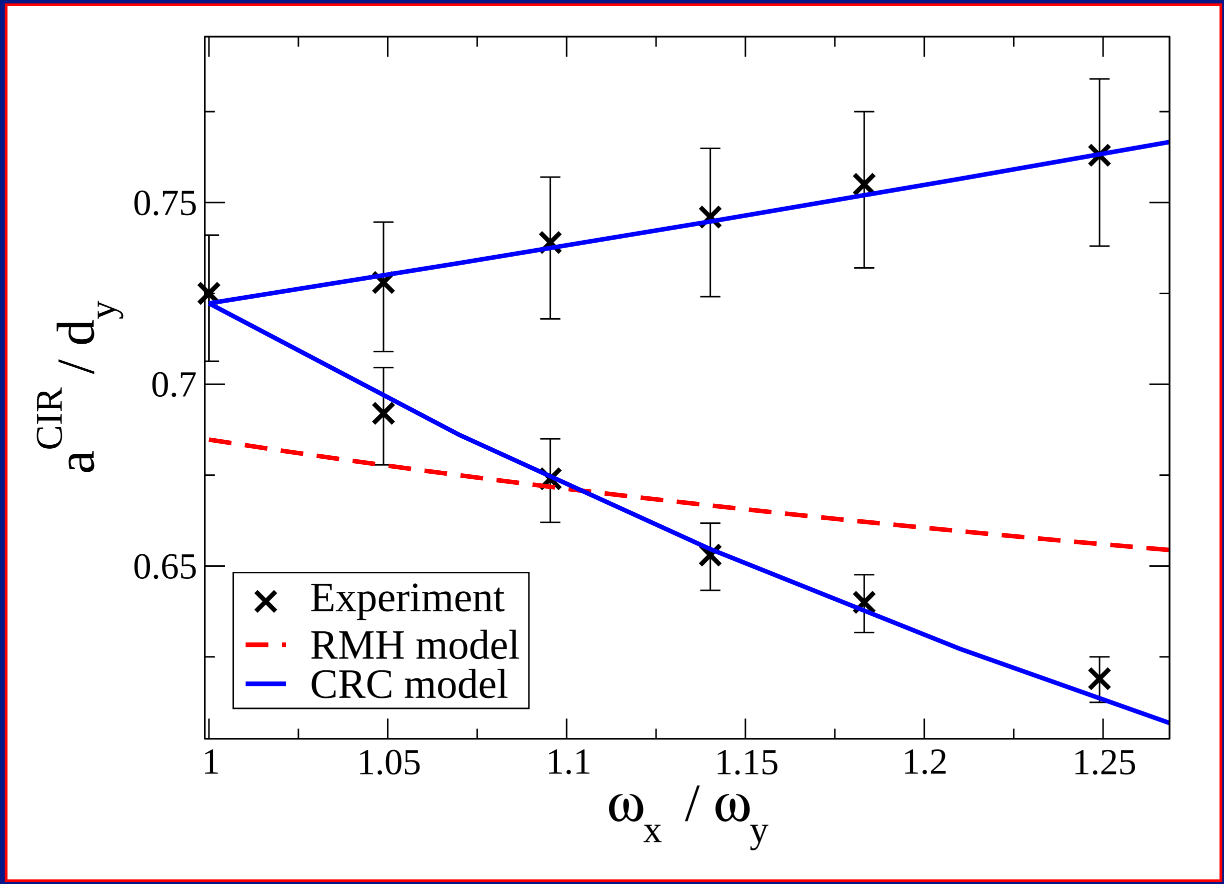
$\omega_x \neq \omega_y \gg \omega_z$

⇒ single anisotropy ($\omega_x = \omega_y \gg \omega_z$): degeneracy

⇒ totally anisotropic case $\omega_x \neq \omega_y \gg \omega_z$: splitting

[S. Sala, P.-I. Schneider, A.S., *Phys. Rev. Lett.* **109**, 073201 (2012)]

Comparison with Innsbruck Experiment



Agreement not only for positions, but also for **width**.

Quantitative agreement also for **quasi-2D resonance:** $a = 0.593\, d_y$ (exp.) vs. $a = 0.595\, d_y$ (th.) [S. Sala, P.-I. Schneider, A.S., *Phys. Rev. Lett.* **109**, 073201 (2012)]

Preliminary summary

Our conclusion:

- **Two types of resonances:** elastic (Olshanii, Petrov et al.) and inelastic ones.
- **Elastic CIR:** no molecule formation, (almost) no losses (invisible in Innsbruck experiment).
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Note: The possibility to create molecules due to anharmonicity had earlier been suggested: Bolda, Tiesinga, Julienne [PRA **71**, 033404 (2005)]; Schneider, Grishkevich, A.S, [*Phys. Rev. A* **80**, 013404 (2009)]; Kestner, Duan [*N. J. Phys.* **12**, 053016 (2010)].

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However, not everyone (e.g. 2 out of 3 referees) is convinced!

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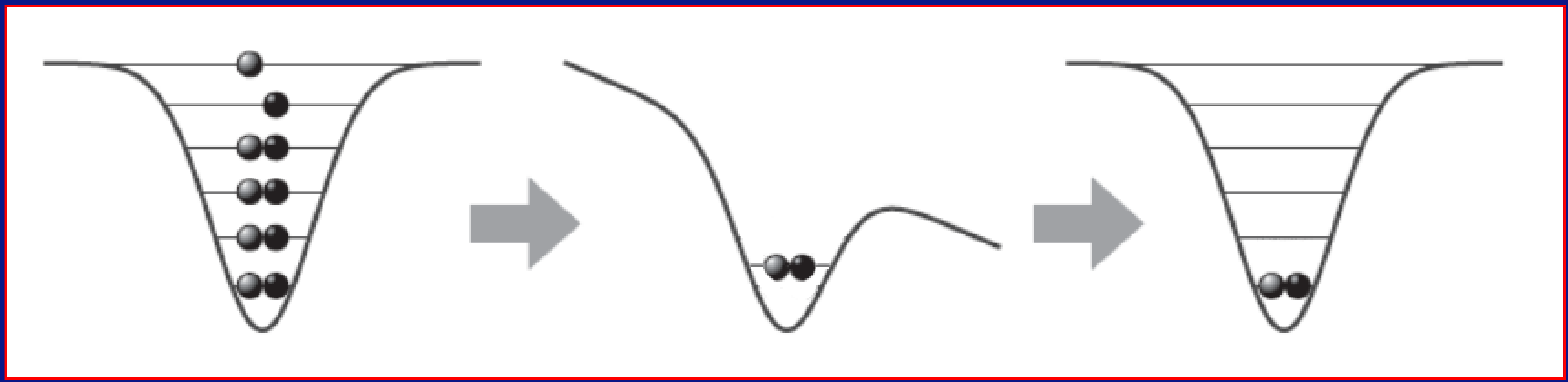
- Multichannel CIR effect.[Melezhik, Schmelcher *Phys. Rev. A* **84**, 042712 (2011)]
- Losses in a many-body system (Innsbruck experiment) are very unspecific, in contrast to Cambridge rf experiment.

Experimental test (with group of S. Jochim

Exclusion of many-body and multi-channel effects:

Experiment with exactly two Li atoms in high-fidelity ground state

cf. [Serwane *et al.*, *Science* **332**, 336 (2011)]



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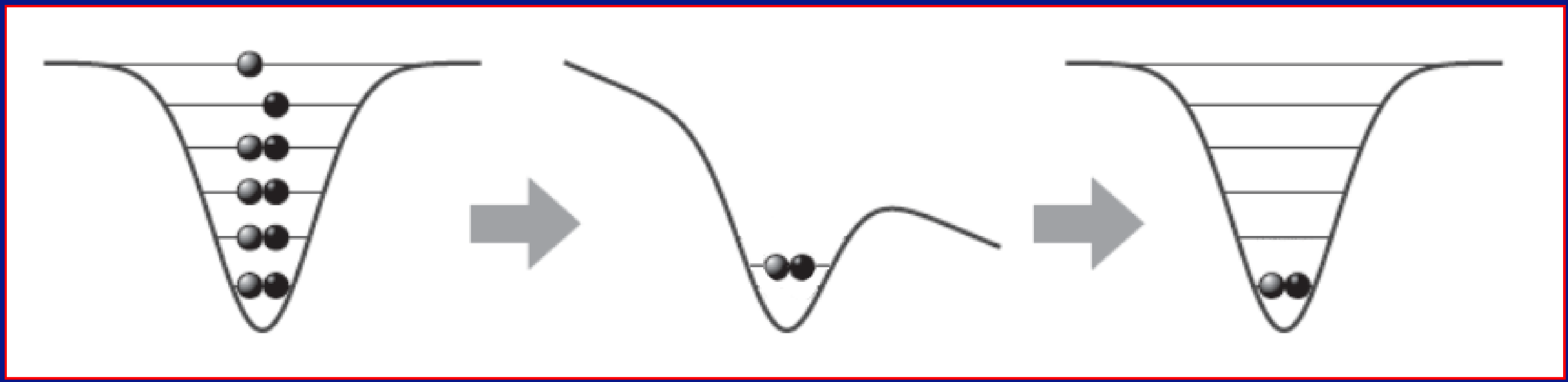

1. Confirmation of the elastic CIR by measuring the tunnel rate:

Interaction energy shifts two-atom ground state ⇒ modified **atomic** tunnel rate.

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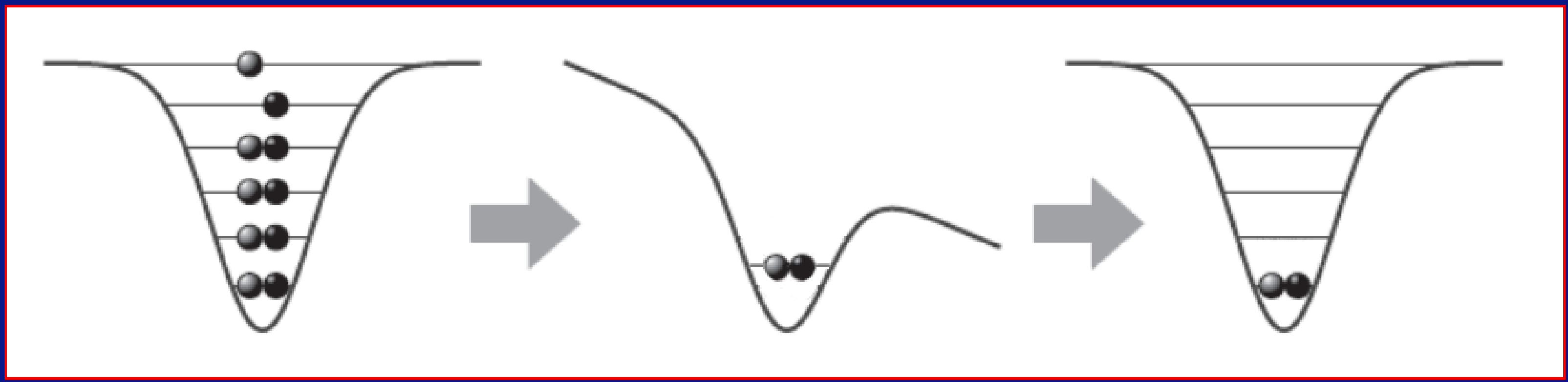

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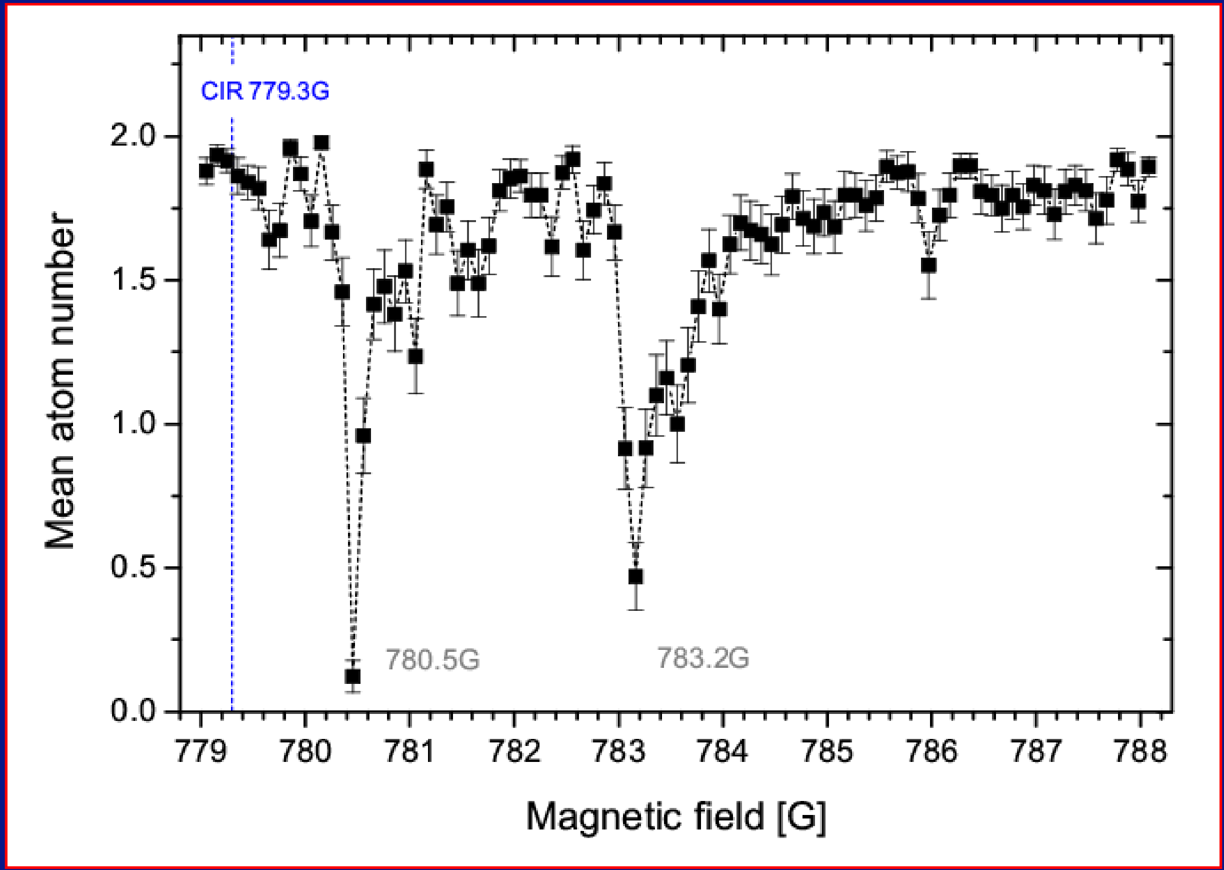
Interaction energy shifts two-atom ground state ⇒ modified **atomic** tunnel rate.

2. Detection of molecules: measurement of tunneling atoms at a B field where deeply bound molecules do not tunnel.

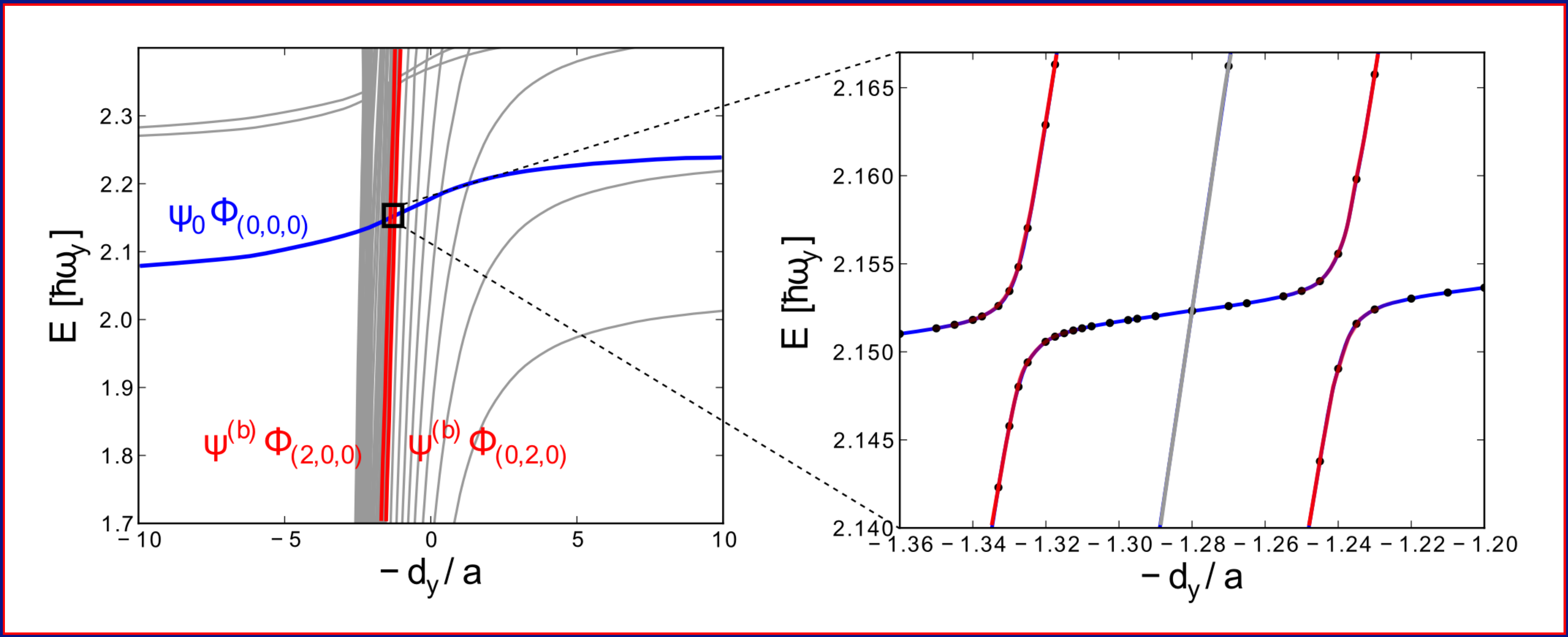
Measurement of the mean atom number



Positions for molecule formation: 776.01 G & 779.02 G

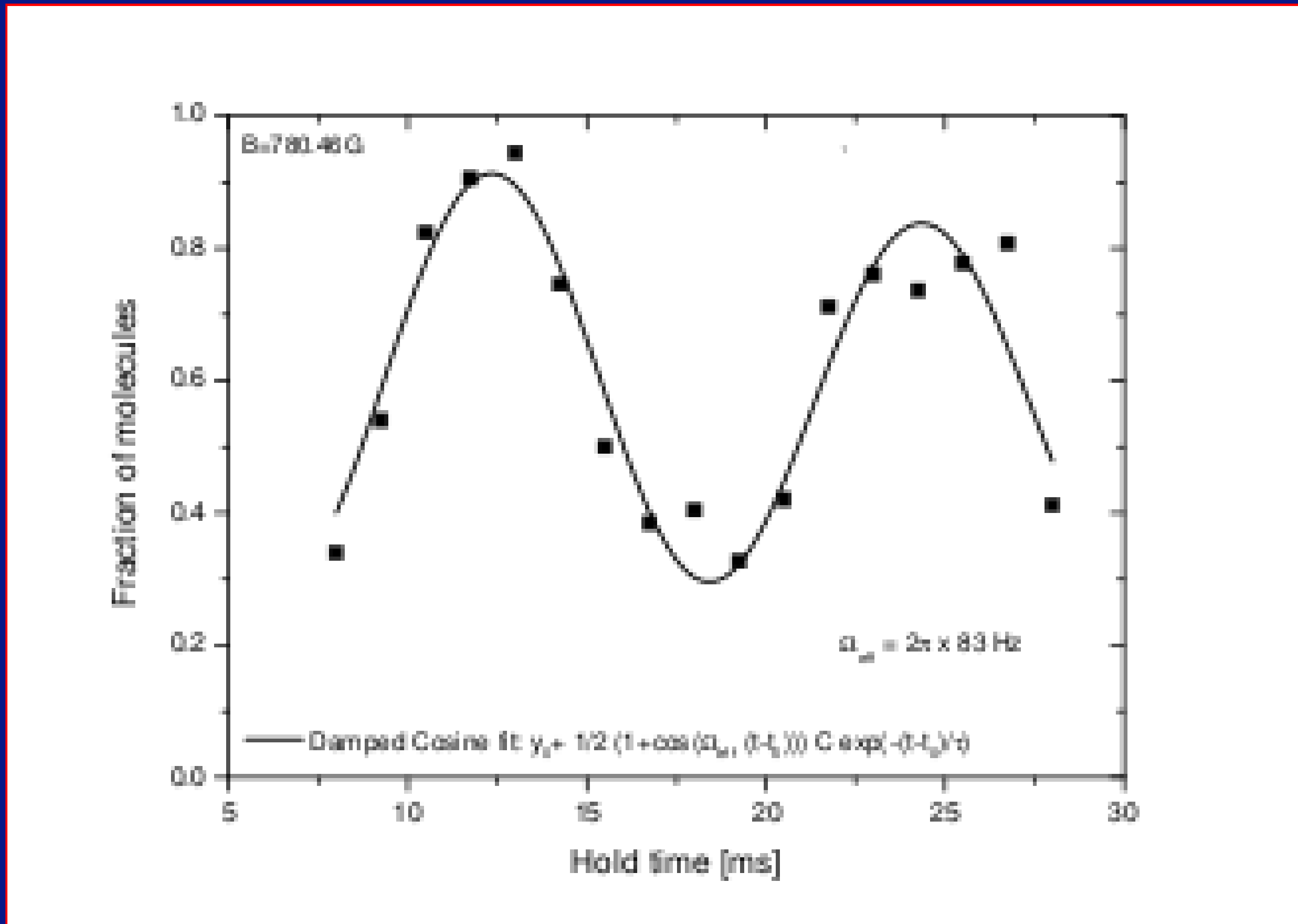
Ab initio calculation

Exact diagonalization (full 6D) of Li_2 Hamiltonian in a trap with experimental parameters (varying scattering length with inner-wall shift).



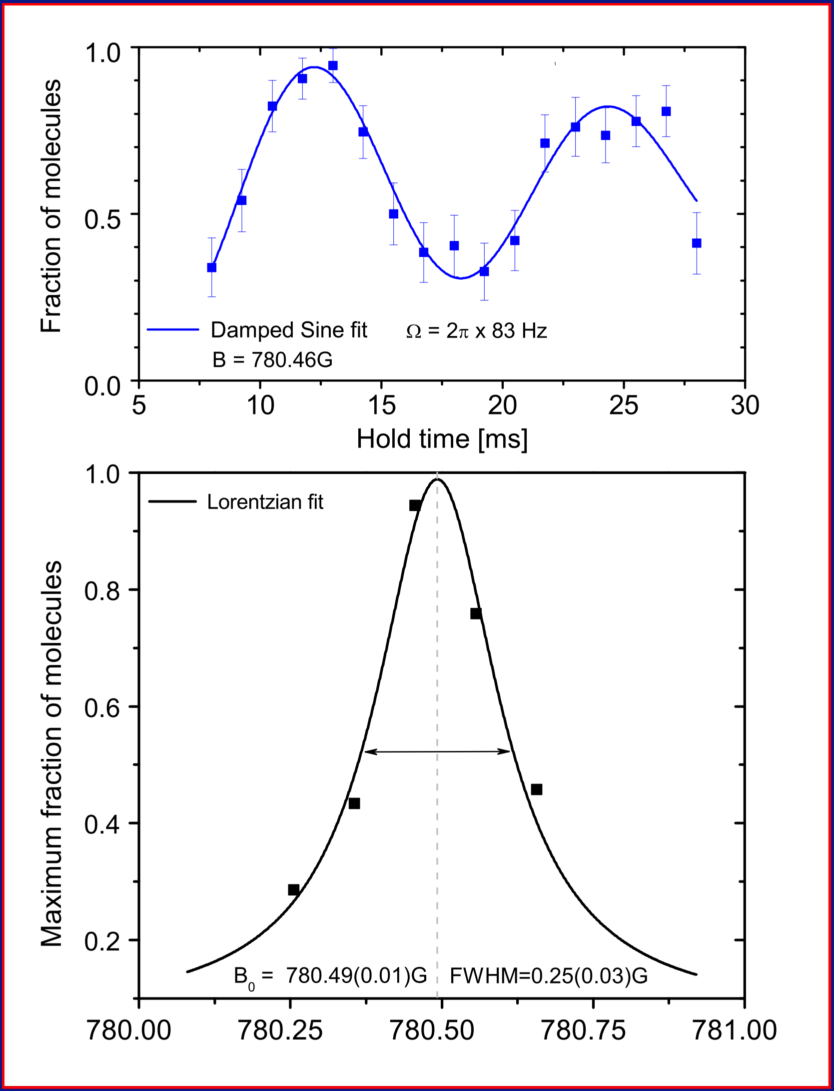
Due to anisotropy ($\omega_x \neq \omega_y \gg \omega_z$) two inelastic CIR (avoided crossings) expected.

More precise CIR detection (I)



Ramp B field non-adiabaticlly into region of avoided crossing:
coherent superposition of molecules and repulsive trap state (Rabi oscillation).

More precise CIR detection (II)



Rabi frequency:

$$\Omega = \frac{1}{\hbar}\sqrt{W_{\mathbf{n}}^2 + \delta^2}$$

$$W_{\mathbf{n}} = \langle \psi^{(b)}\,\Phi_{\mathbf{n}} | W | \psi_0\,\Phi_{(0,0,0)} \rangle$$

Variation of B:

allows fit of position and width.

Comparison ab initio result to experiment

COM excitation	Position [G]		FWHM[G]		Ω_0[Hz]/ 2π	
	exp.	num.	exp.	num.	exp.	num.
$(2,0,0)$	780.5	776.01	0.25(0.03)	0.35	83	64
$(0,2,0)$	783.2	779.02	0.42(0.06)$^{(*)}$	0.35	75 $^{(*)}$	69

$^{(*)}$ Magnetic field gradient $B' = 18.92$ G/cm applied.

More details:

Sala, Zürn, Lompe, Wenz, Murmann, Serwane, Jochim, A.S., *arXiv:1303.1844*.

Recent extensions:

- Solution of the time-dependent Schrödinger equation.
  Full 6D plus time for time varying (optical-lattice) potential.
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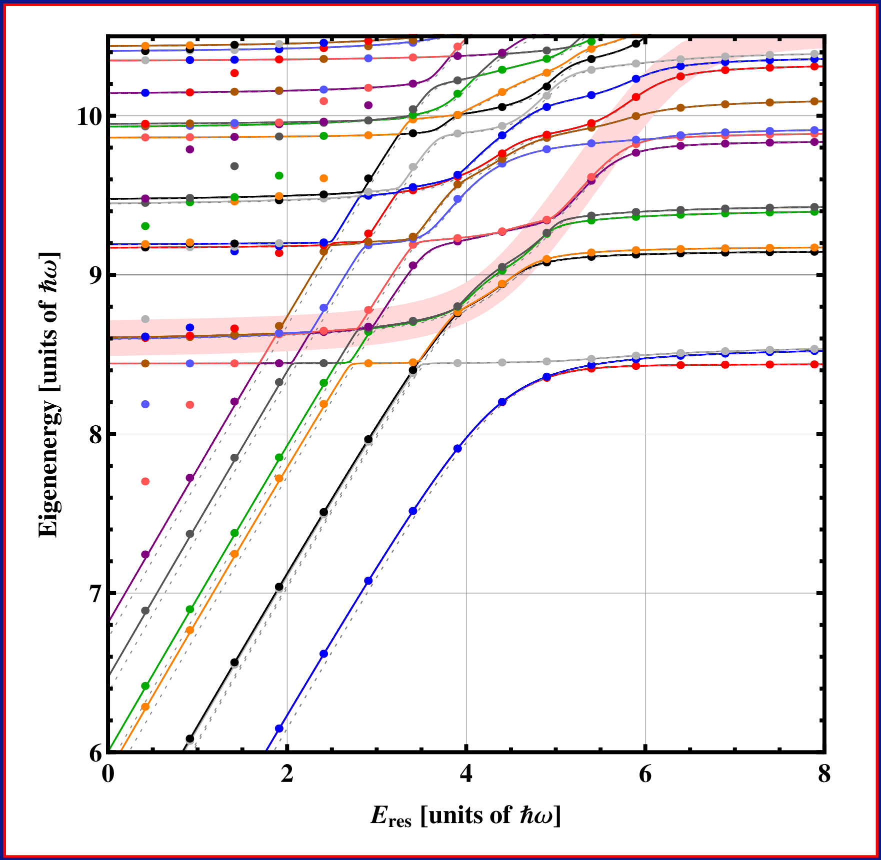
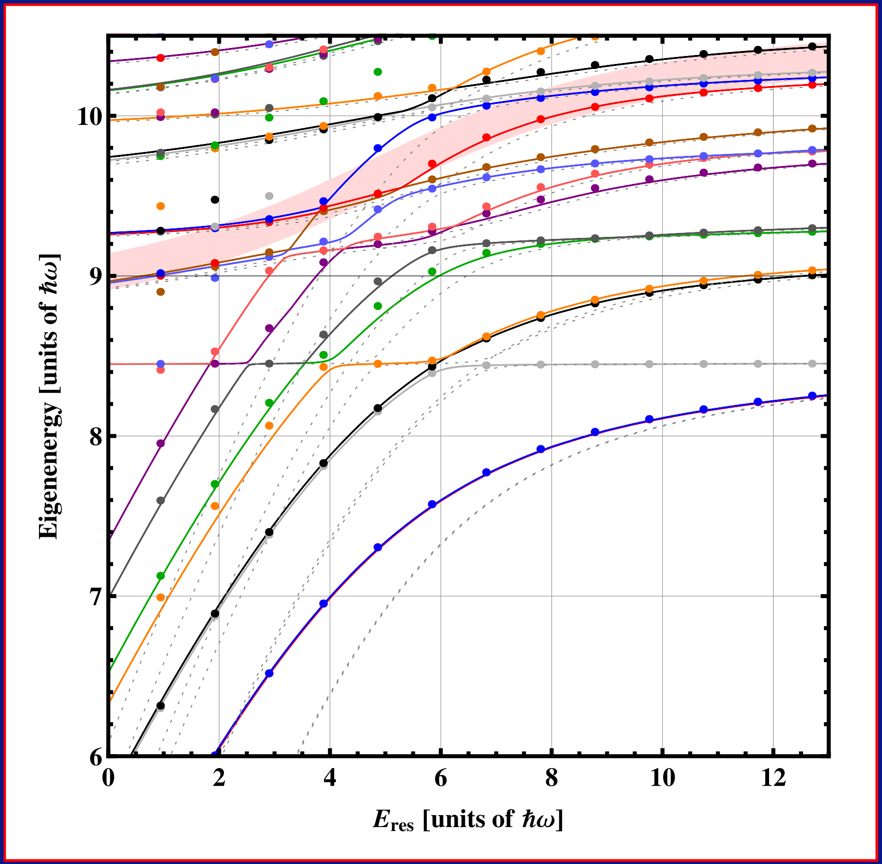
Example result: two-channel model (I)



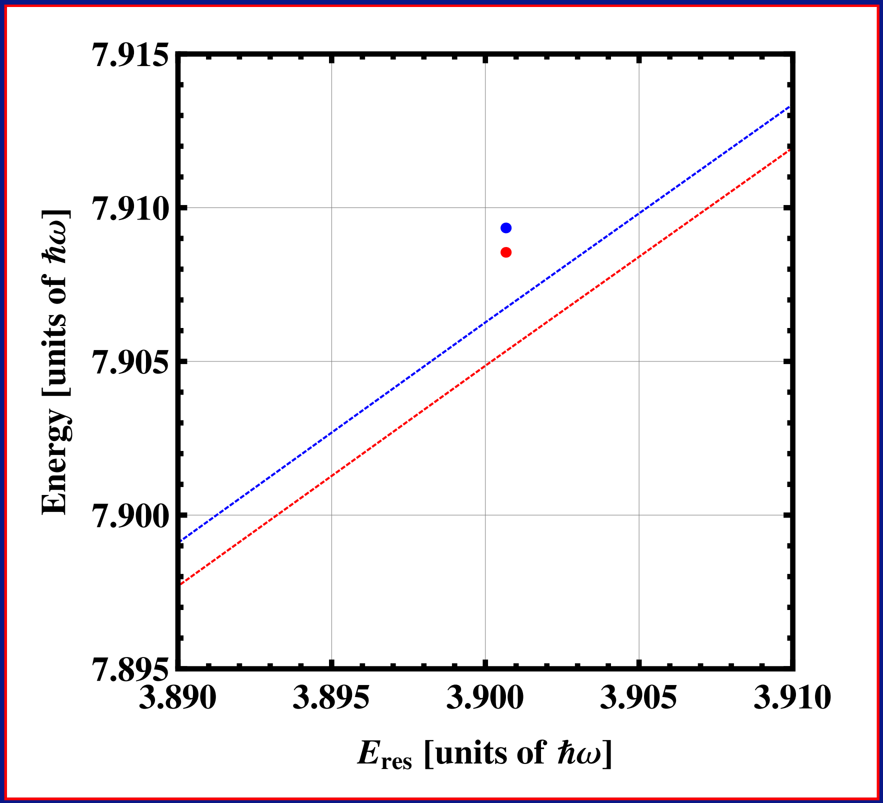


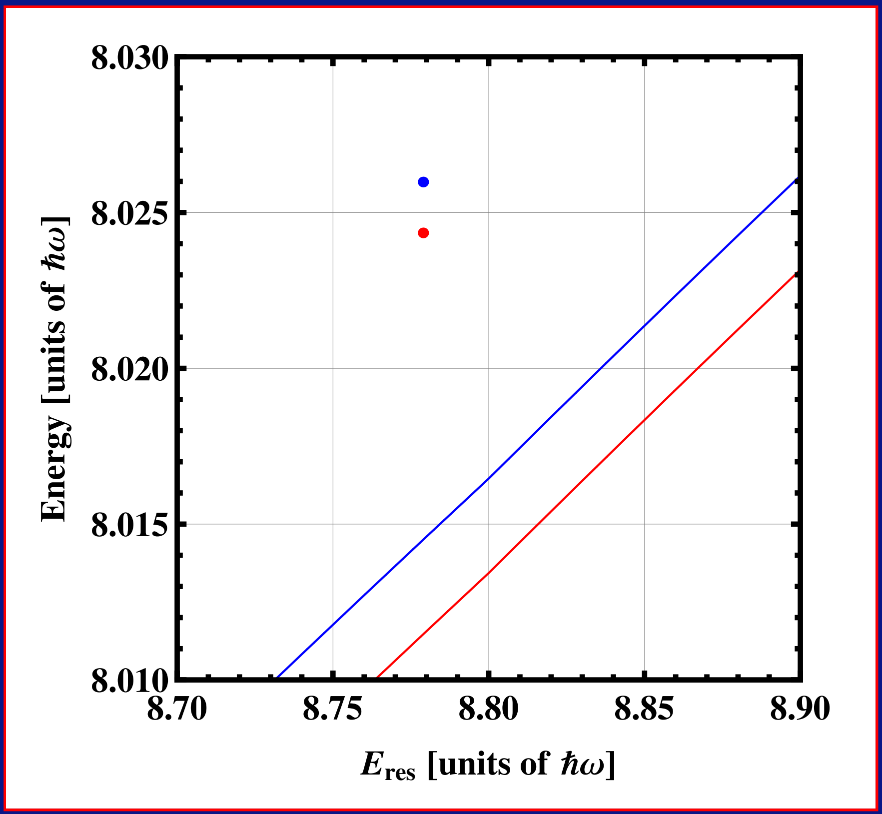
Left: narrower resonance

Right: broader resonance.

[Schneider, A.S., *arXiv:1303.4570*]

Example result: two-channel model (II)





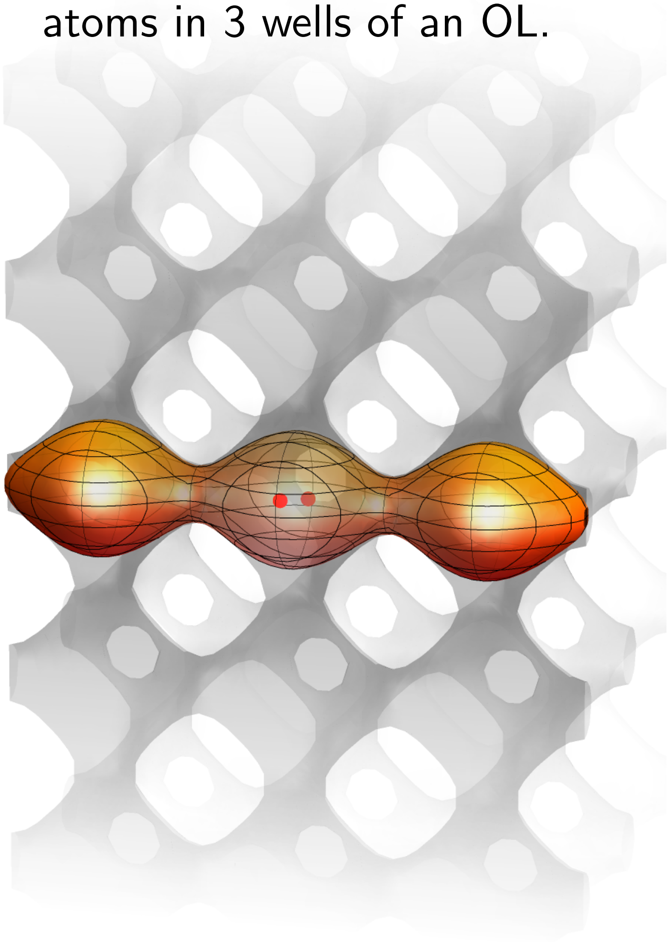
Left: narrower resonance **Right:** broader resonance.

Tunnel splitting ("hopping") increases for broader resonance.

cf. M. Wall and L. Carr

Work in progress: dynamics and transport

Time propagation with **exact solutions** for two interacting atoms in 3 wells of an OL.



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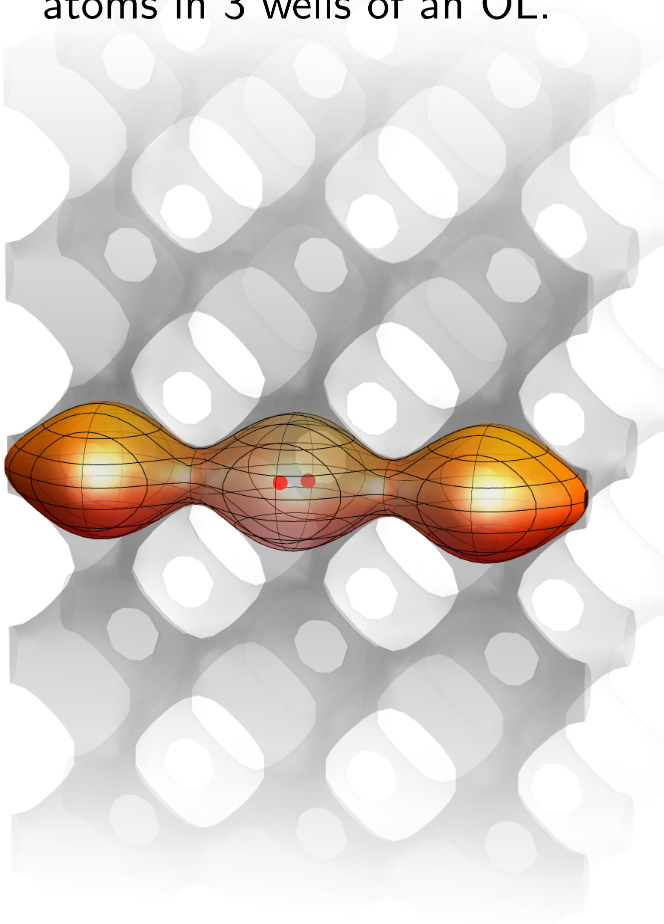

Quantum dynamics/transport in triple well: