CONFINED
FEW-BODY SYSTEMS

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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

- Interactions in ultracold gases.

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- Summary.

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

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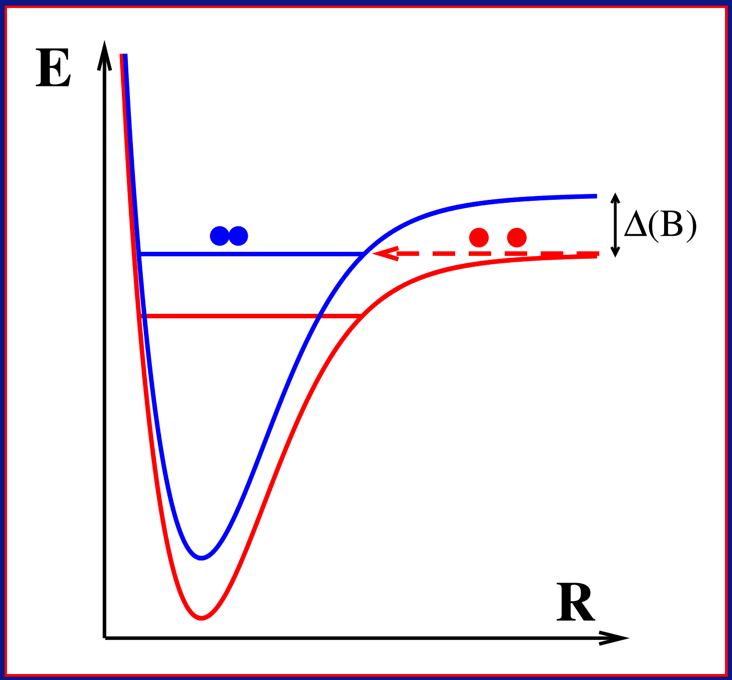
Note: V_{pseudo} is counterintuitive: long-range behaviour described by δ function!!!

Tunable interaction: magnetic Feshbach resonances



Simple picture:

Only **2 channels**:

– open (continuum) channel,

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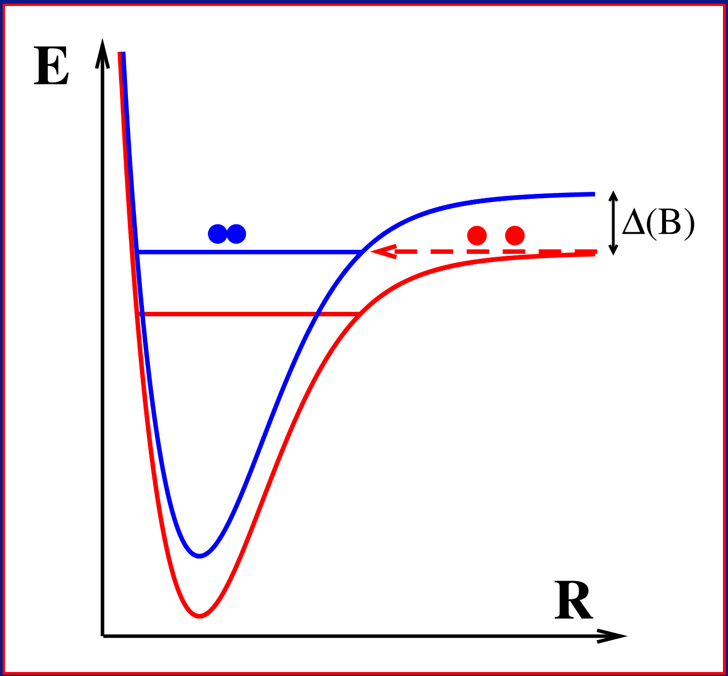

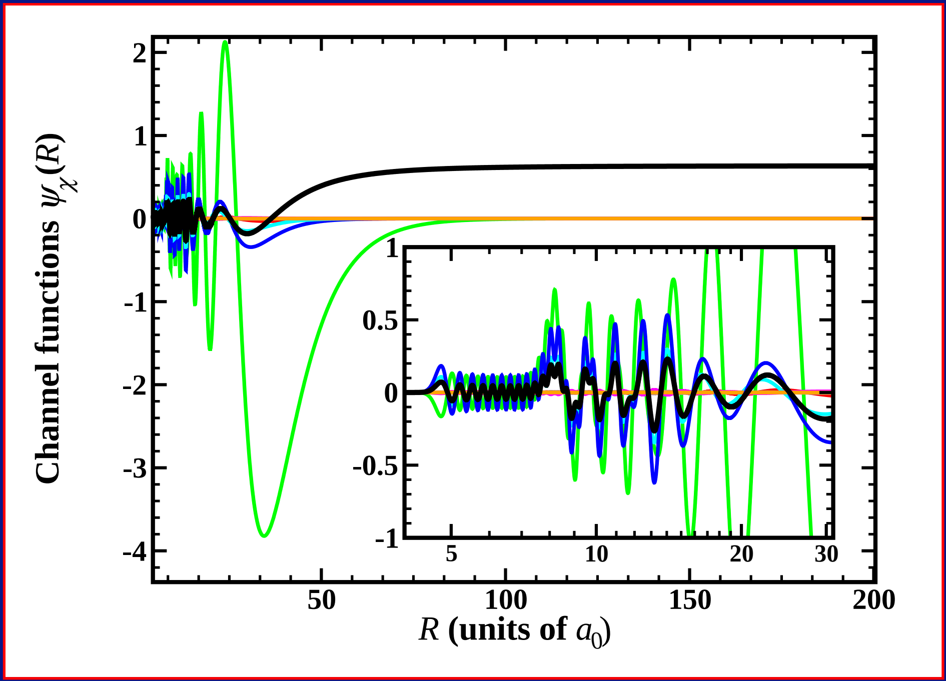

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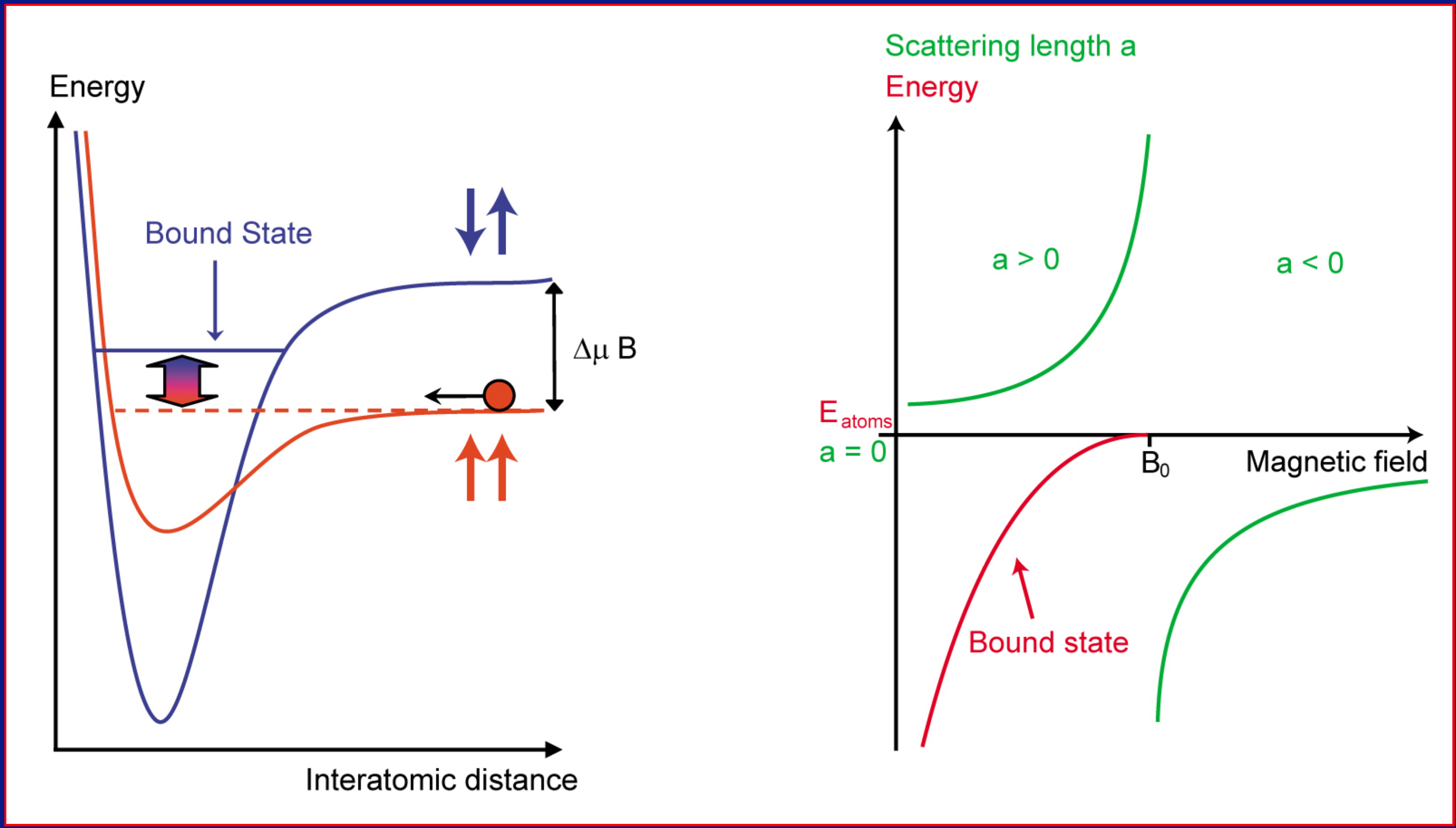
Multichannel reality:

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

– very different length scales involved,

– high quality molecular potential curves required.

Tuning the interparticle interaction



Magnetic Feshbach resonance: magnetic field modifies scattering length a.

Scattering length determines interparticle interaction.

$\longrightarrow$ **Tuning the interparticle interaction with a magnetic field!**

Intermezzo: SFA (KFR) approximation

$$S_{fi} = \lim_{t\to\infty} \langle \Phi_f | \Psi_i^{(+)} \rangle = \lim_{t\to -\infty} \langle \Psi_f^{(-)} | \Phi_i \rangle$$

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- Final state: ignore influence of remaining ion on ionized electron.
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- **Keldysh:** length gauge (L), reversed-time S matrix.
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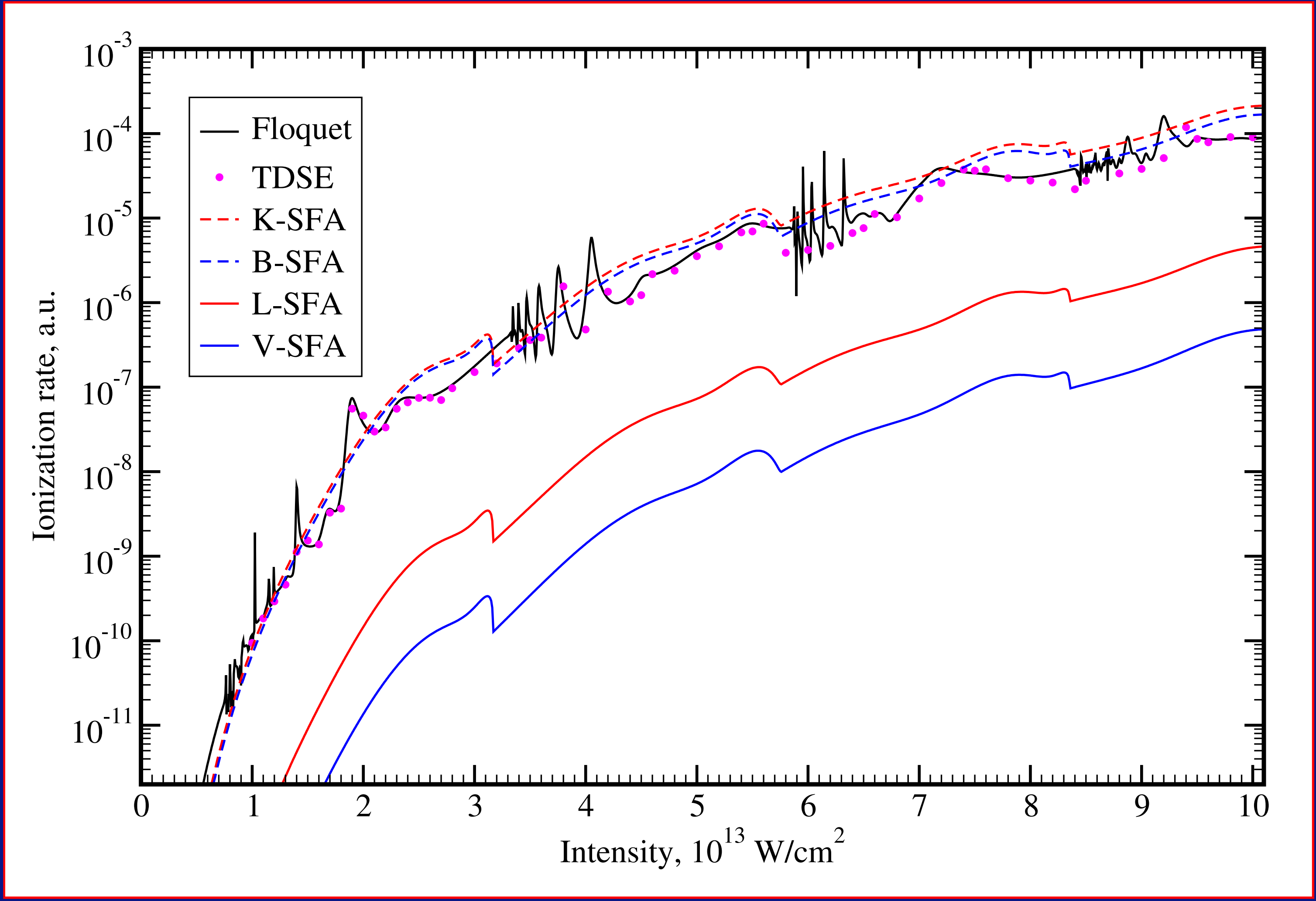
- **Reiss:** velocity gauge (V), reversed-time S matrix.
- **W. Becker:** dressing of initial state required.
- **Mishima** *et al.*, **Chao**: "exact" Keldysh theory:
  use residue theorem instead of saddle-point approximation.

Validity of the strong-field approximation (SFA): 800 nm



Ionization rates of H atoms (λ=800 nm)

L - length gauge, V - velocity gauge, K - Krainov corrected L-SFA, B - Becker corrected V-SFA.

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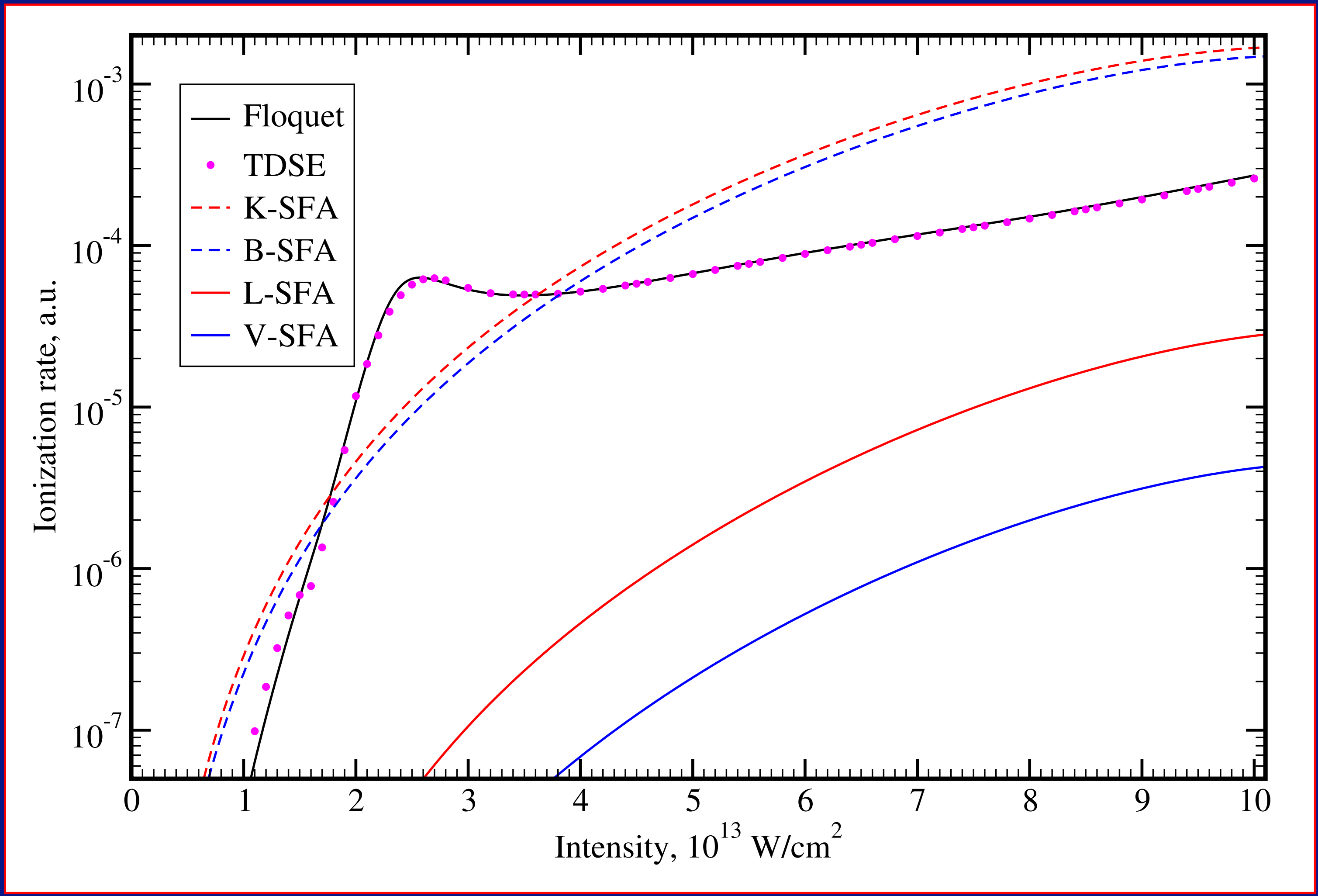

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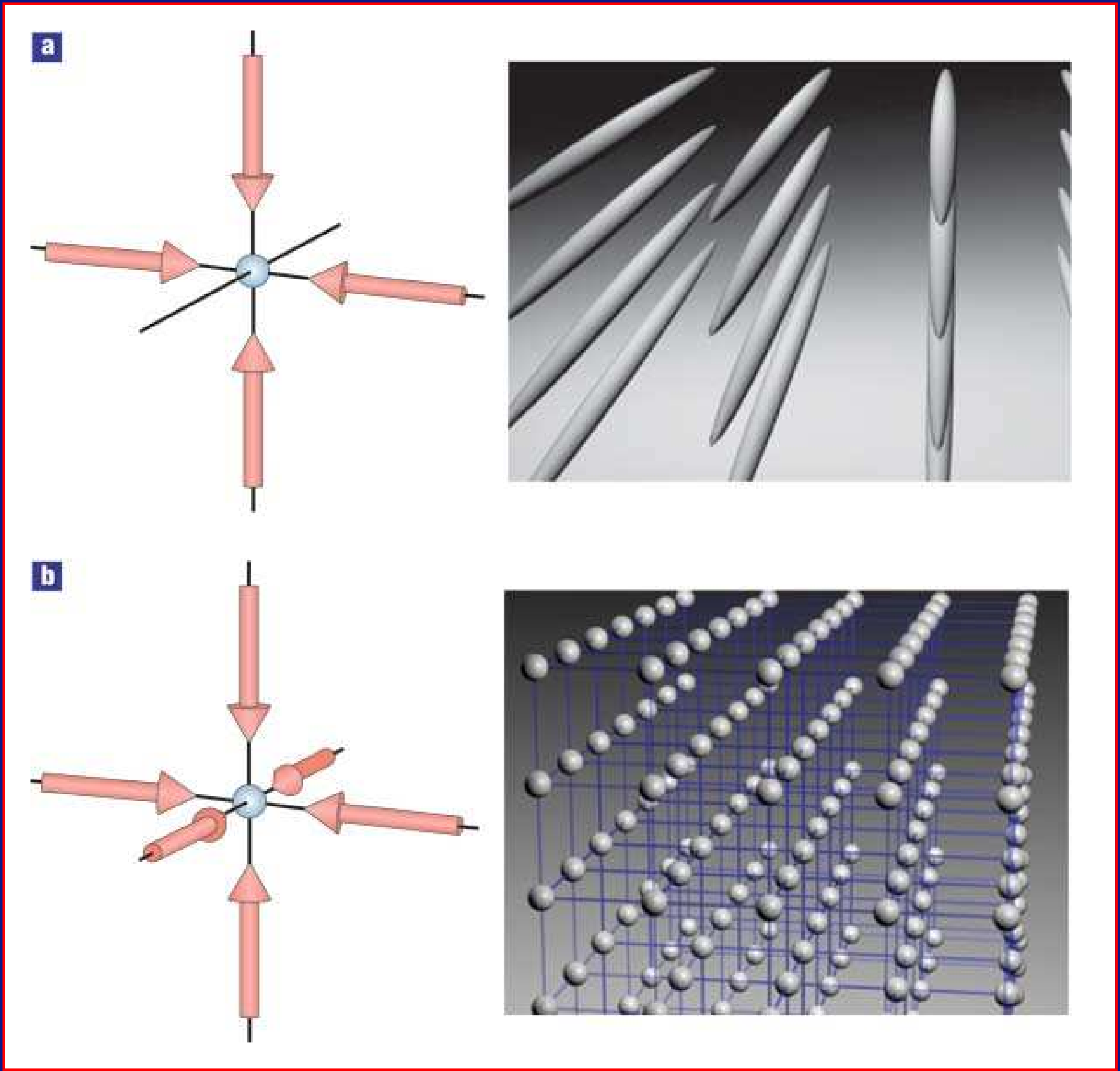
Optical lattices: shaped (tight) confinement



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

Counterpropagating lasers:

$\longrightarrow$ standing light field.

Trap potential varies as

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

with

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

λ: laser wavelength.

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

with

laser intensity I and

atomic polarizability α.

Why is few-body physics of interest?

Mott state with 1 or 2 atoms/molecules:

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

Pseudopotential approximation in traps

Atom-atom interaction: $V_{\rm mol}(R) \;\rightarrow\; V_{\rm pseudo}(R) \;=\; \frac{4\pi\,\hbar^2}{\mu\,R^2}\,a_{\rm sc}\,\delta(R)$

- This relation was derived for $k \rightarrow 0$ (limit of zero-collision energy).
- In a (tight) trap energy is quantized: zero-point motion.
- Intercept of Ψ on R axis does not agree with $a_{\rm sc}$.

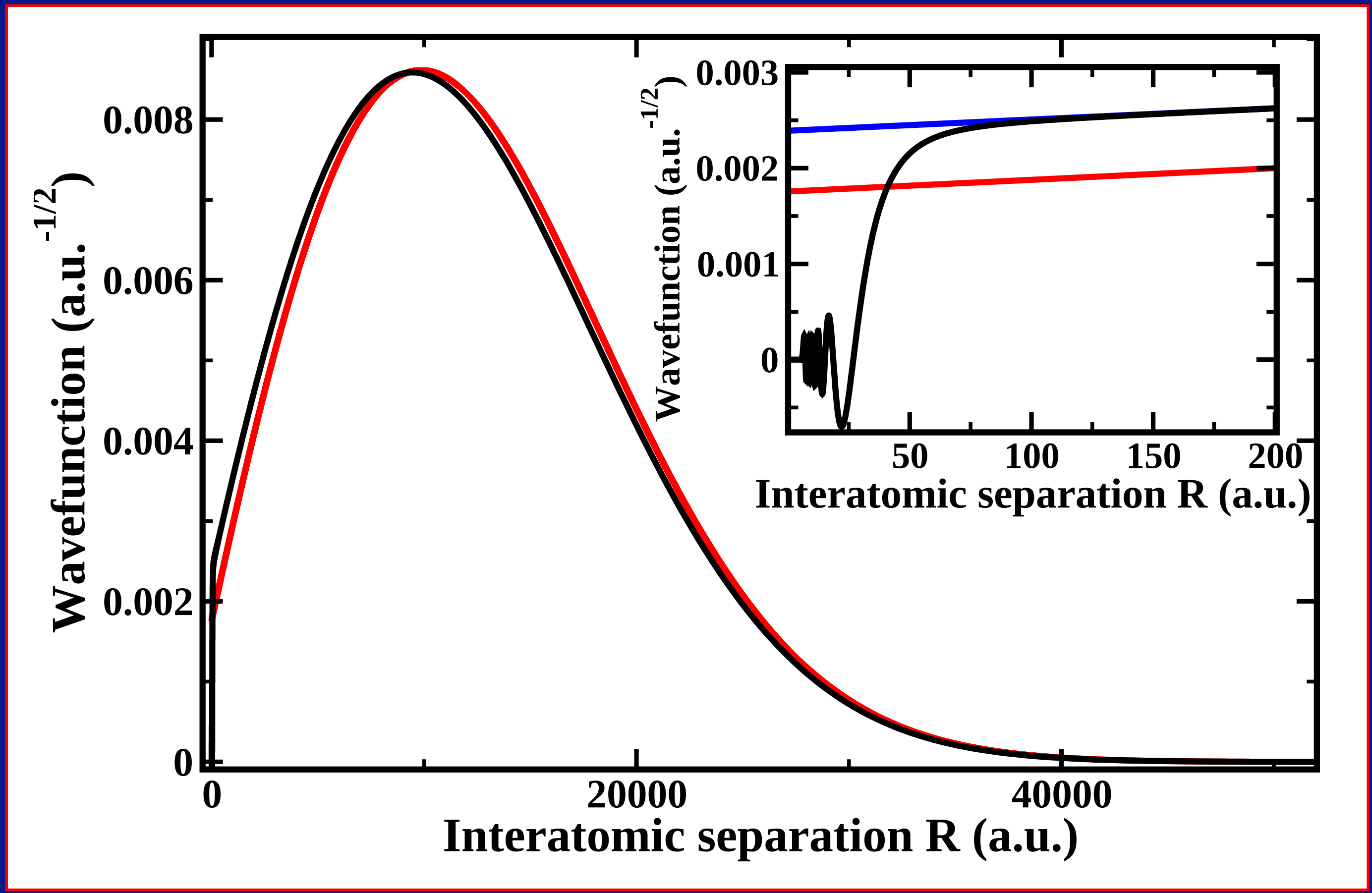
  Deviation for Ψ small, e. g., 10 kHz trap yields intercept on -2023 for $a_{\rm sc} = -2030\,a_0$.

  This is not true for $\Psi_{\rm pseudo}$: intercept on -1447 for $a_{\rm sc} = -2030\,a_0$.

  $\longrightarrow$ Wrong prediction of photoassociation window (for $a_{\rm sc} \gg 0$).
- Introduce an energy-dependent $a_{\rm sc}(E)$ that inserted in $V_{\rm pseudo}(R)$ matches (for $E = \frac{3}{2}\,\hbar\omega_{\rm trap}$) the correct Ψ (at $R \rightarrow \infty$).

Note: In contrast to the physical $a_{\rm sc}$ the empirical parameter $a_{\rm sc}(E)$ follows only from the correct Ψ obtained with $V_{\rm mol}(R)$!

Validity of the pseudopotential approximation



Spin-polarized ^{6}Li atoms (a $^3\Sigma_u$) in a 10 kHz trap:

"correct" wavefunction (black, $a_{\rm sc} = -2030\,a_0$) vs. energy independent (red, $a_{\rm sc} = -2030\,a_0$) and dependent (blue, $a_{\rm sc} = -2872\,a_0$) pseudopotential results.

Theoretical challenges:

- Non-trivial, **non-analytic atom-atom interaction** (unlike Coulomb interaction).
- Magnetic Feshbach resonances: **multi-scale, multi-channel problem**.

  Multi-channel R-matrix approach (incl. combined exp. and theor. determination of ^{7}Li^{87}Rb resonances) [Phys. Rev. A **79**, 012717 (2009)].

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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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$$\frac{a}{a_{\mathrm{ho}}} = f(E) \equiv \frac{\Gamma\left(1/4 - E/2\hbar\omega\right)}{\Gamma\left(3/4 - E/2\hbar\omega\right)}$$

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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

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

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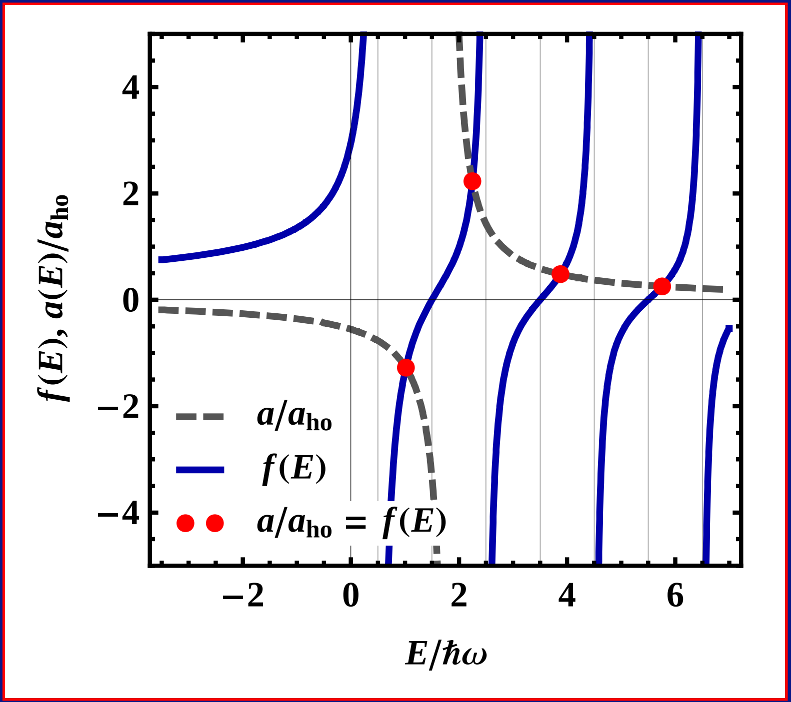

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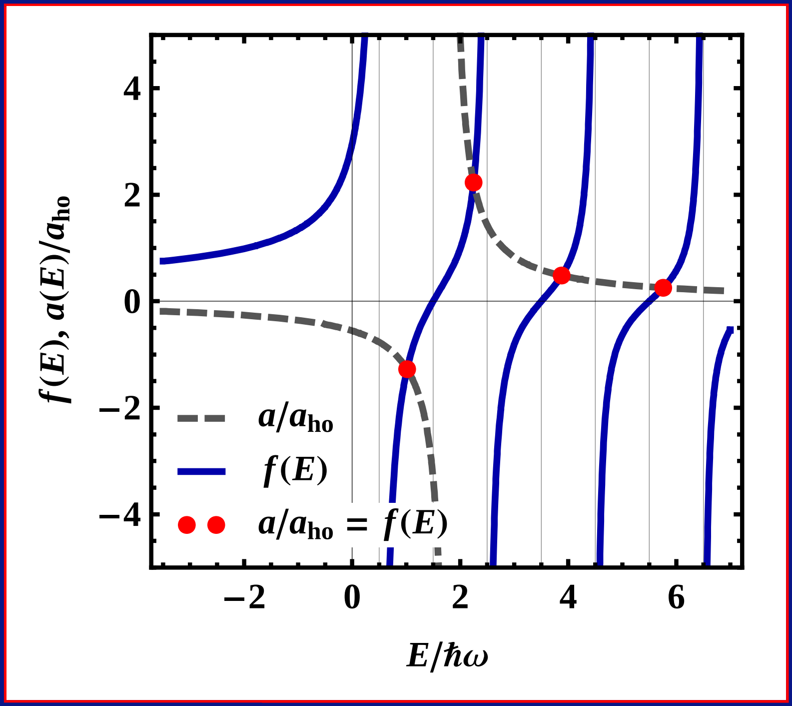

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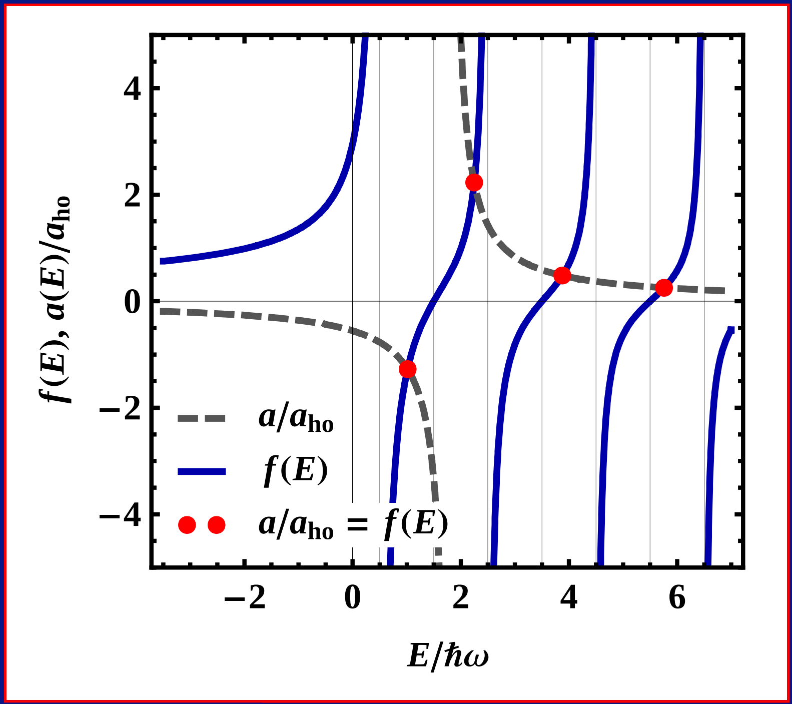
3. derive the admixture of the closed channel

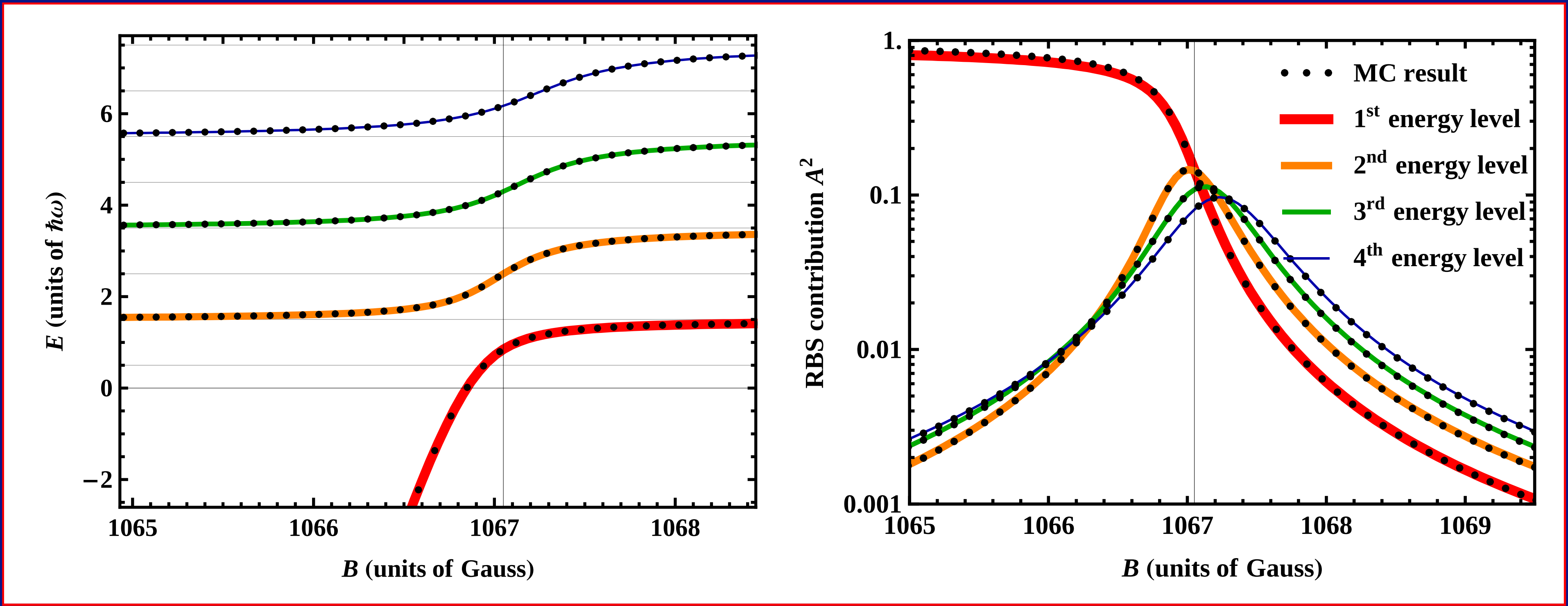
$$\frac{A}{C} \propto \frac{f(E) - a_{\mathrm{bg}}/a_{\mathrm{ho}}}{\sqrt{f'(E)}}$$



(Shift δB and slope $\mu = E_{\mathrm{RBS}}(B)/(B - B_0)$ exp. predictable.)

How good is the model?

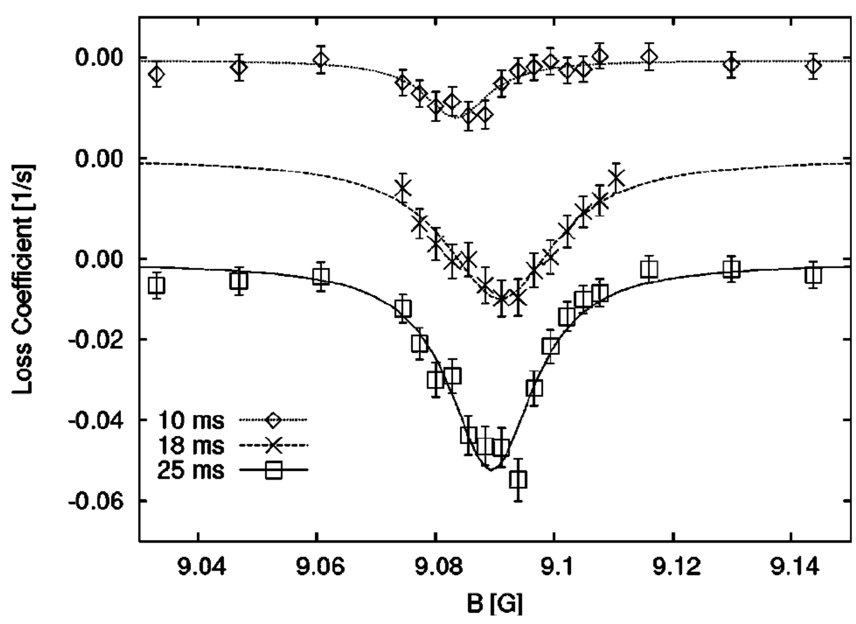
Comparison with full coupled-channel calculations for ^{6}Li-^{87}Rb in a 200 kHz trap:

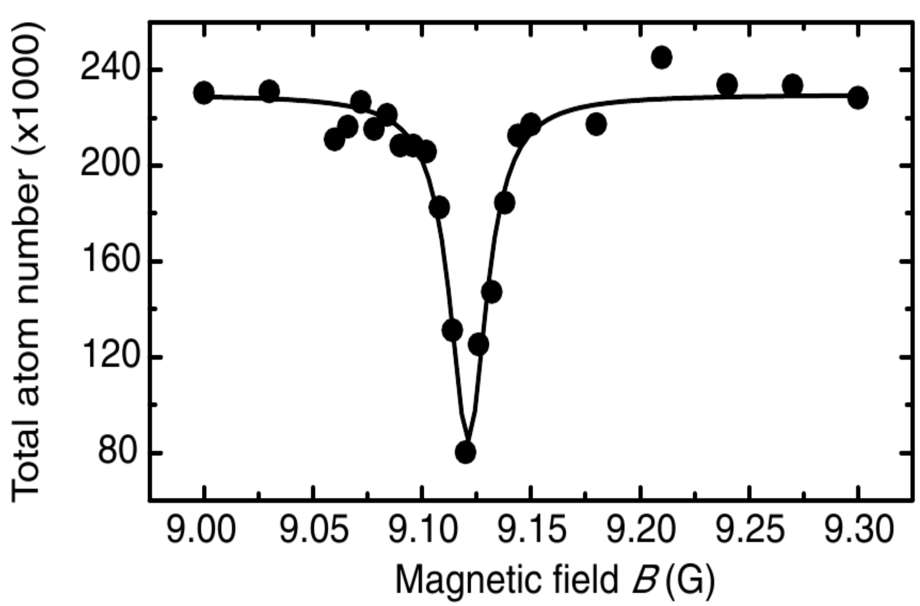


- **Energy deviation** $< 0.003\,\hbar\omega$.
- **Closed-channel admixture deviation** $< 0.1\%$.

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).

Harmonic vs. anharmonic confinement (optical lattice)

Analytical separable solution exists for the atom pair, if

- the interatomic interaction is described by a pseudo potential ($V_{\mathrm{atom-atom}} \propto a_{\mathrm{sc}}\, \delta(\vec{r})$ with s-wave scattering length a_{sc}),
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However, coupling of center-of-mass (COM) and relative (REL) motion

- for the (correct) $\sin^2$ potential (or any physical trap),
- even in harmonic traps, if the two atoms experience different trap potentials
  - ⋆ heteronuclear atom pairs or
  - ⋆ atoms in different electronic states.

Present theoretical approach

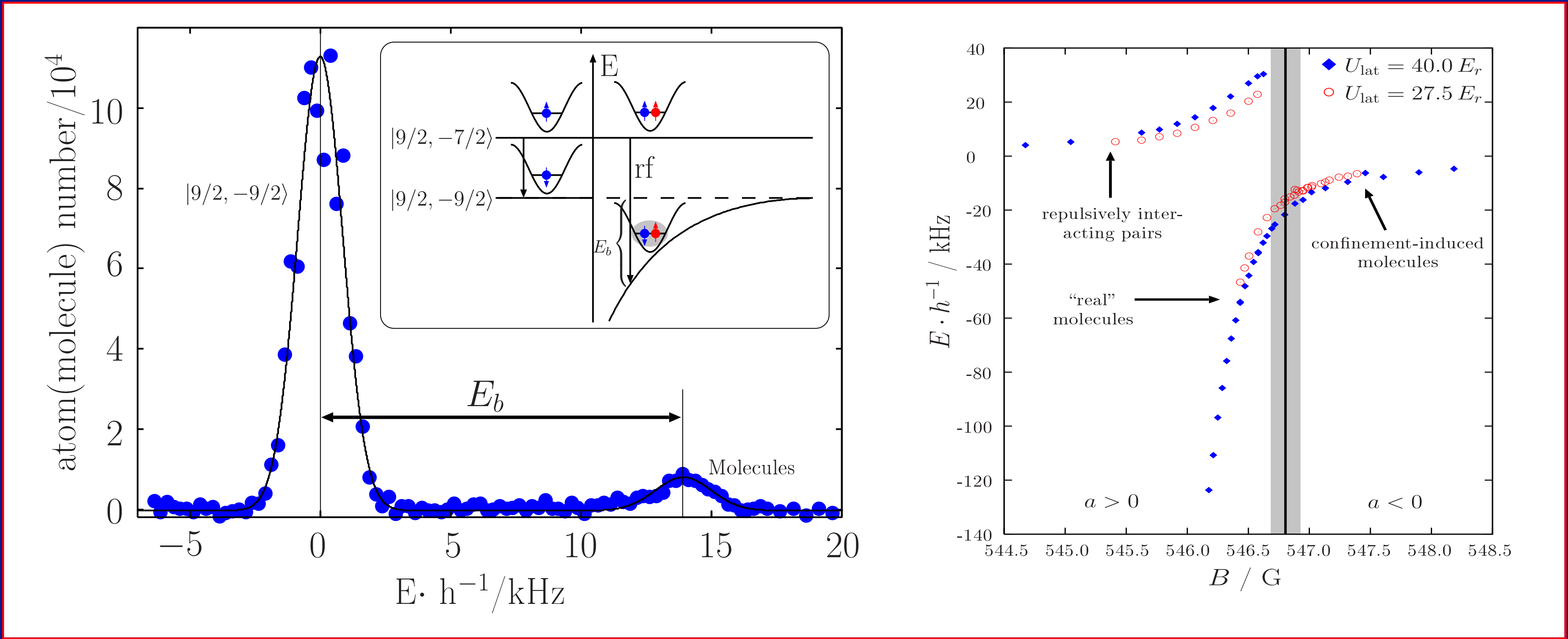
Hamiltonian (6D):

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

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).
- Arbitrary isotropic (or additional anisotropic dipole-dipole) interaction.

Heteronuclear-molecule formation in optical lattices



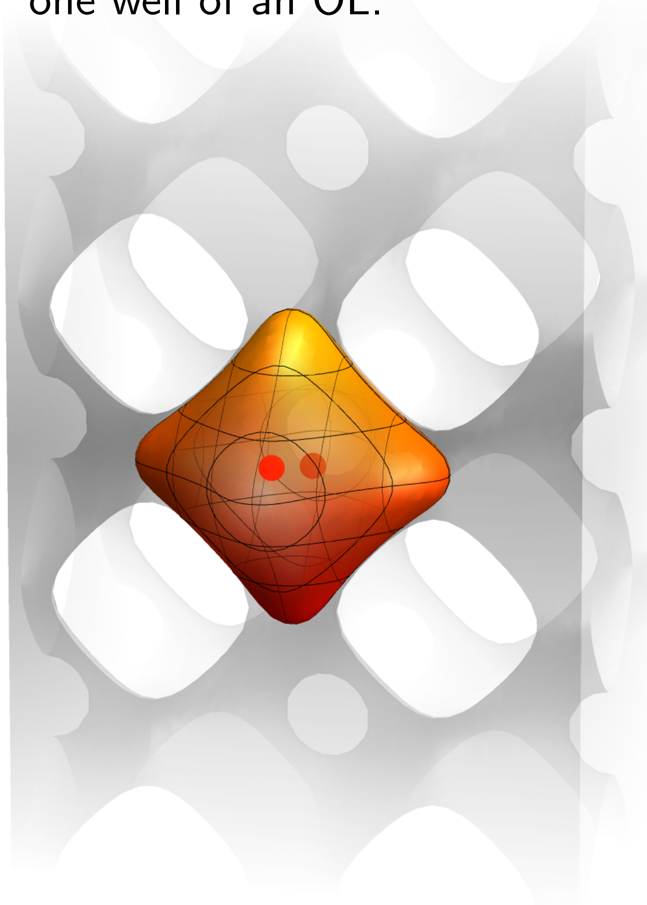
C. Ospelkaus et al. [*Phys. Rev. Lett.* **97** 120402 (2006)]:

- Formation of ^{87}Rb-^{40}K by radio frequency (rf) association.
- Measurement of the binding energy (on absolute scale).

Claim: Deviations from separable harmonic approximation are seen!

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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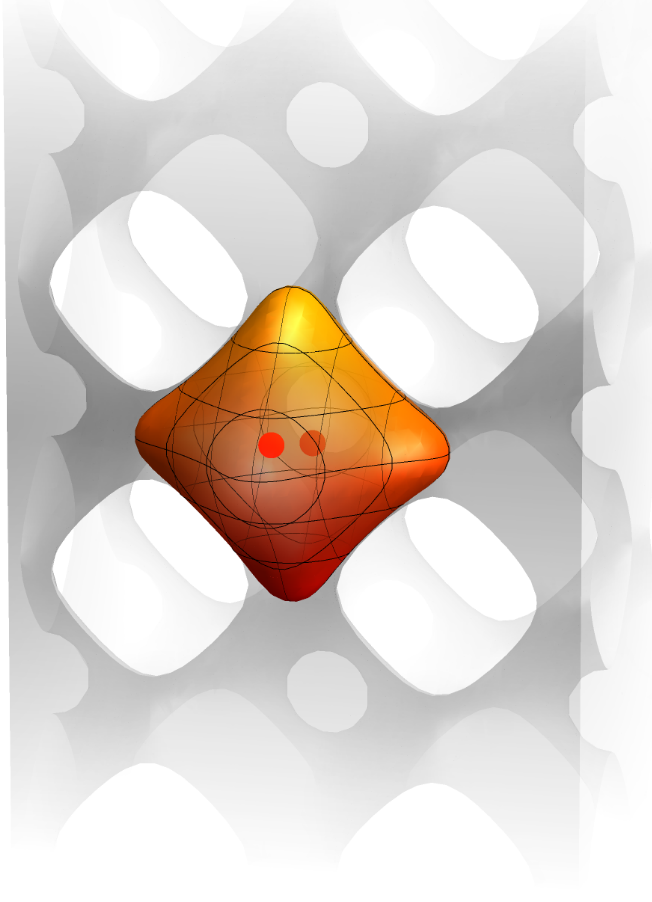
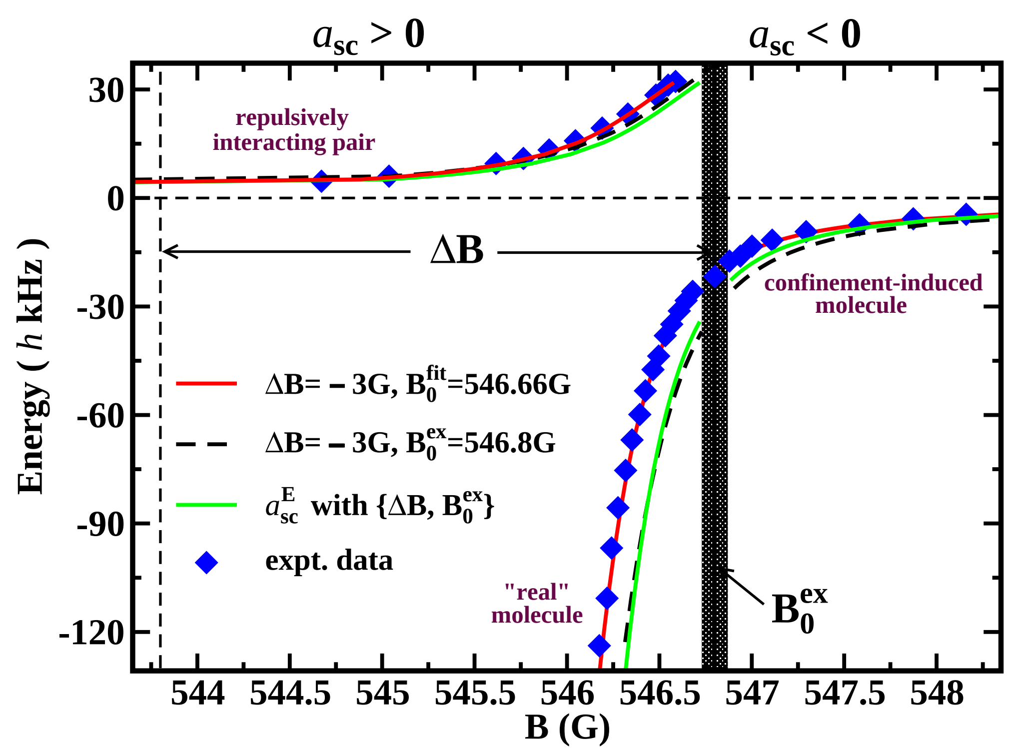


Agreement with experiment on **kHz level**

→ improved resonance parameters by fit?

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

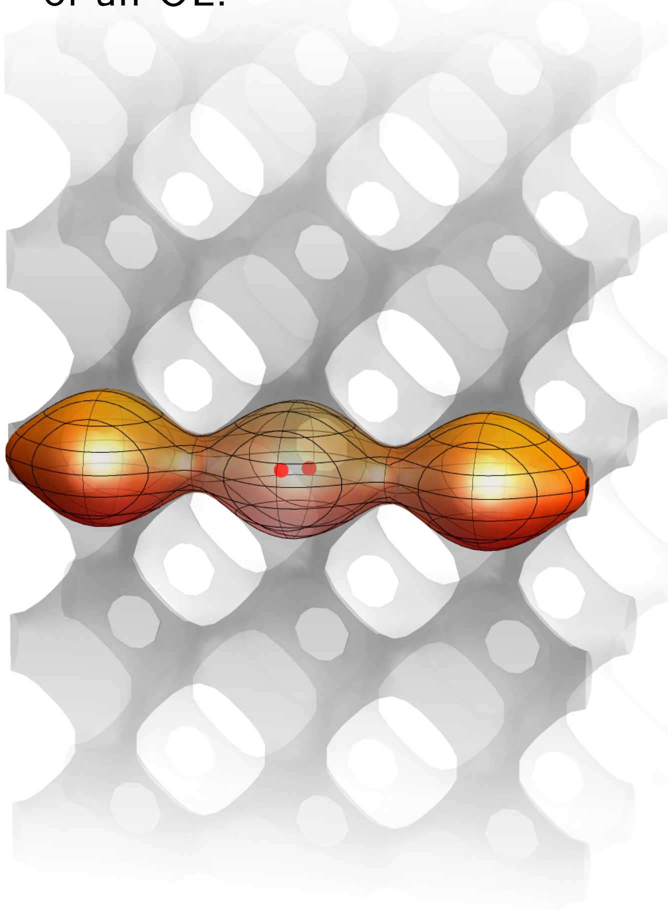
→ **coupling of COM and REL motion important!**



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

Few-body physics for improving many-body models

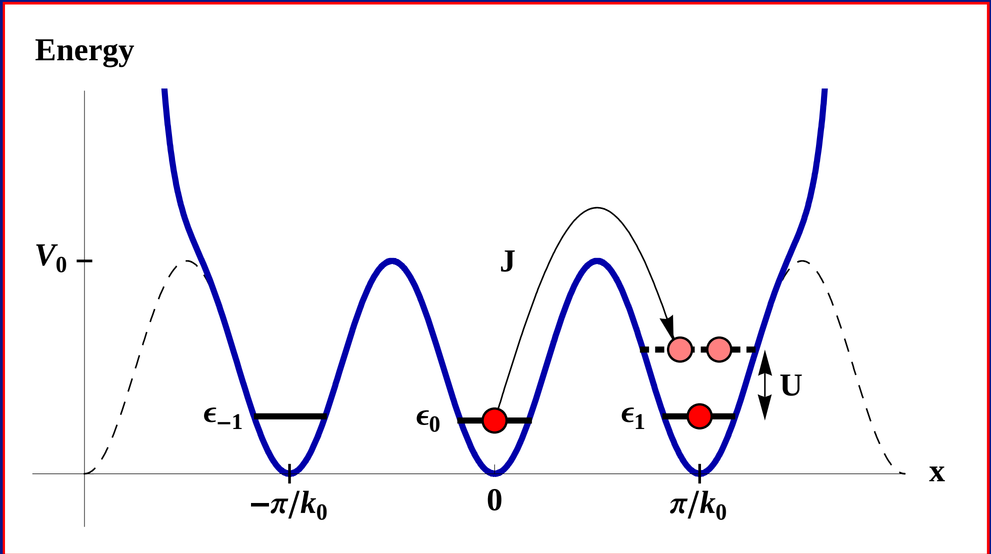
We obtain **exact solutions** for two interacting atoms in 3 wells of an OL.



- 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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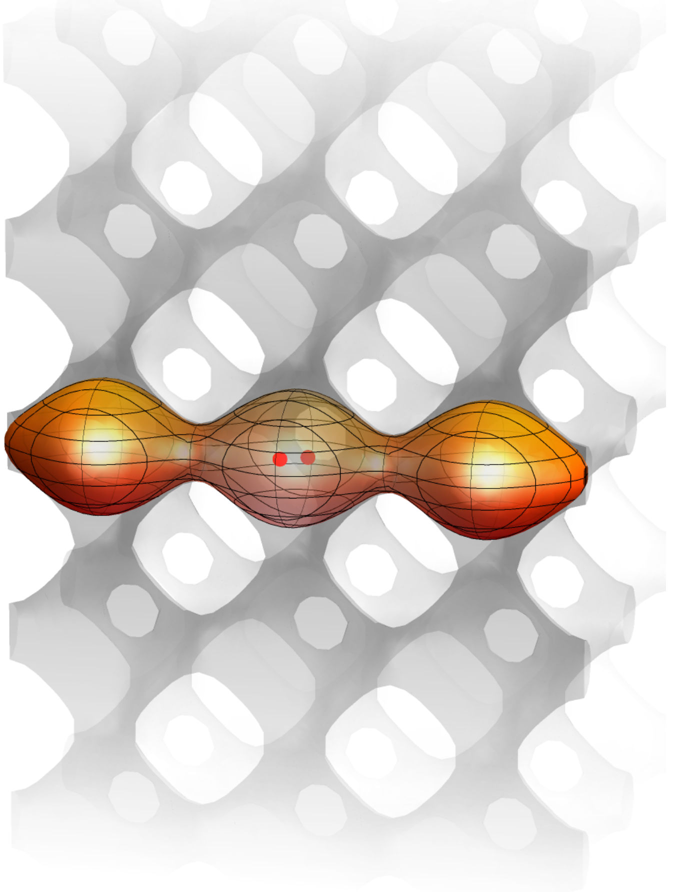
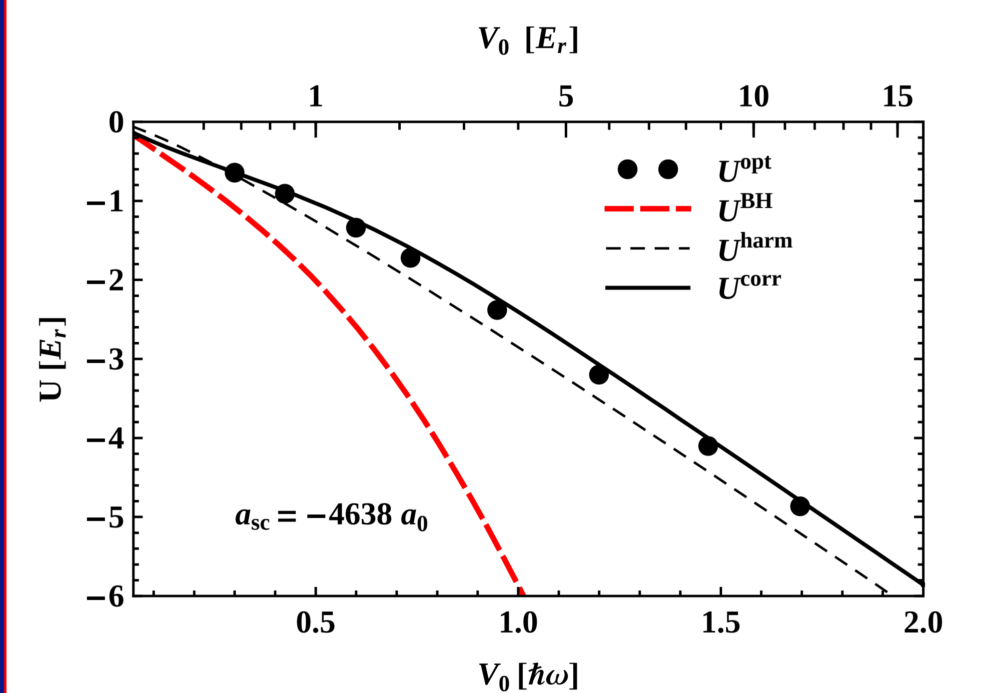


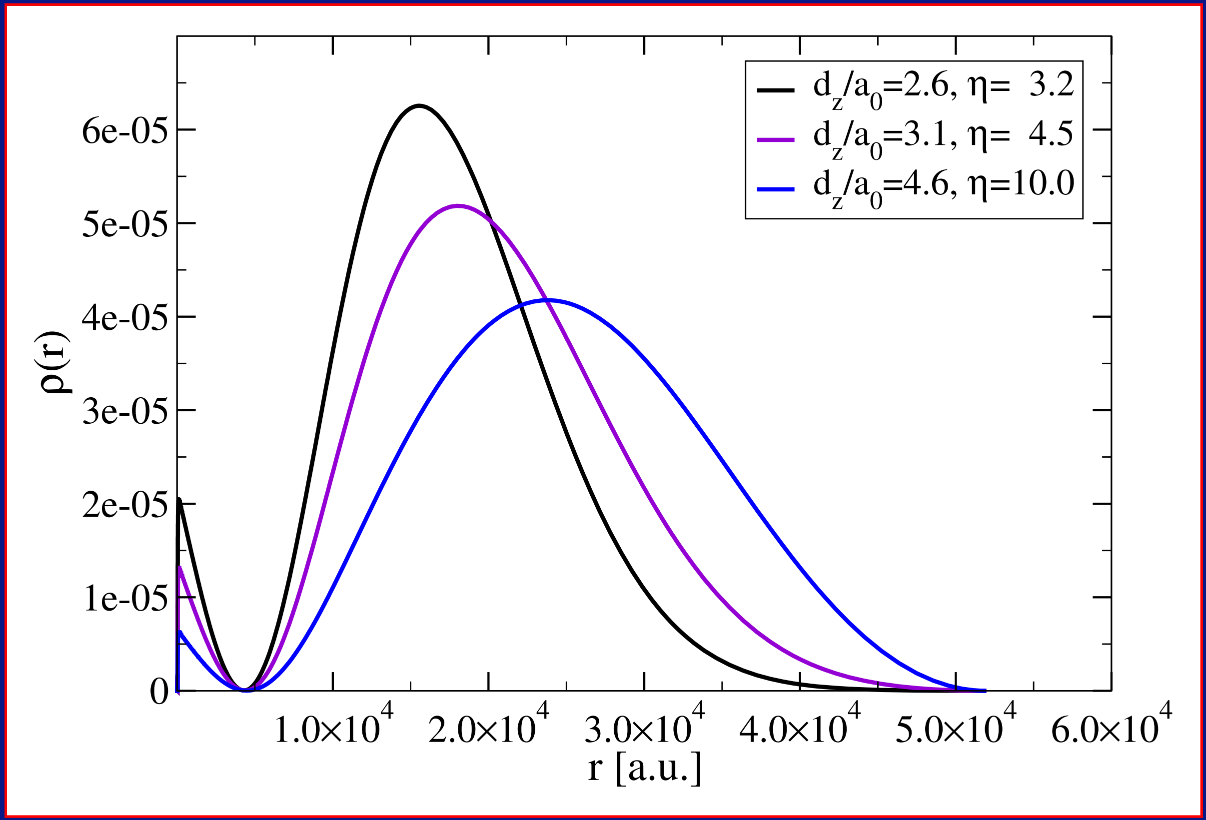
- Introduction of **improved U parameter** by correction of harmonic interaction energy: $U^{\mathrm{corr}} = \mathcal{A} U^{\mathrm{harm}}$ with

$$\mathcal{A} = 2\left(\frac{\pi\hbar}{m\omega}\right)^{\frac{3}{2}} \int d^3\vec{r}\,|w_0(\vec{r})|^4$$



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

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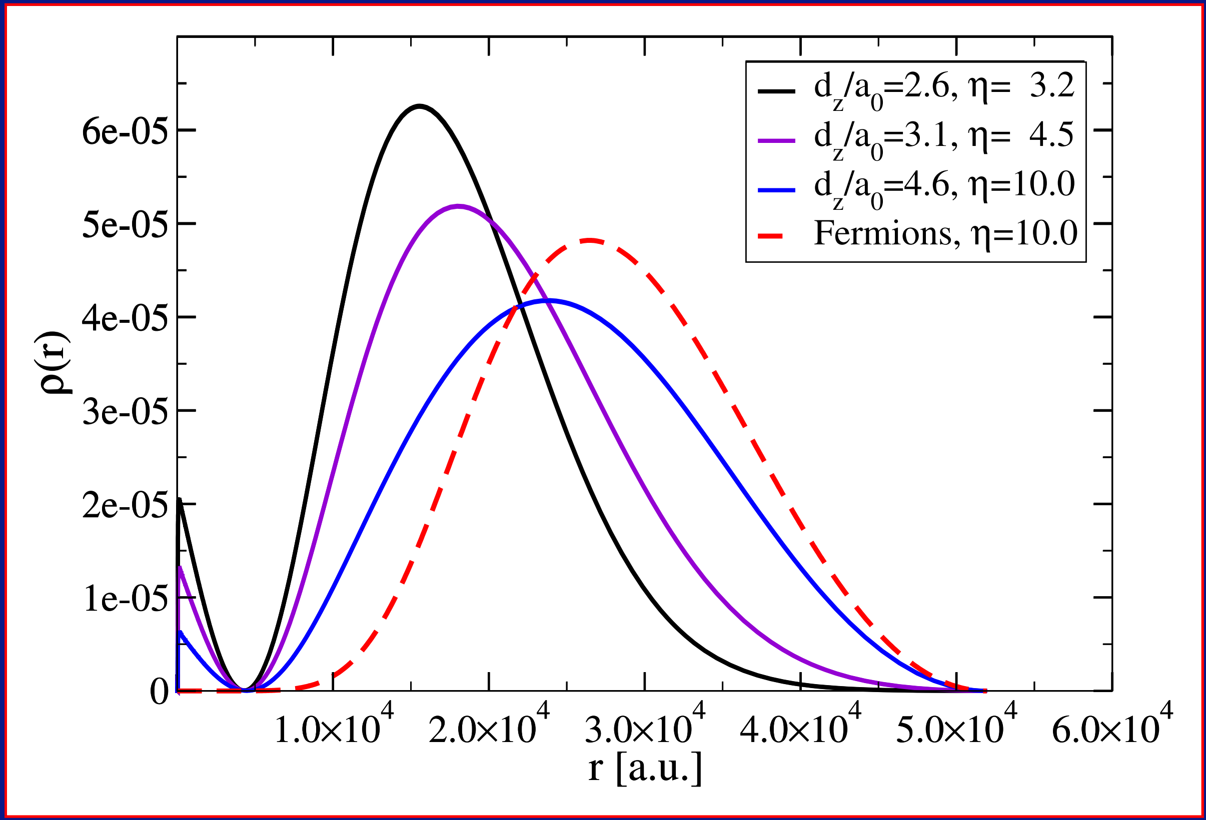

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Confinement-induced resonances (CIR)

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

μ := reduced mass

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

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

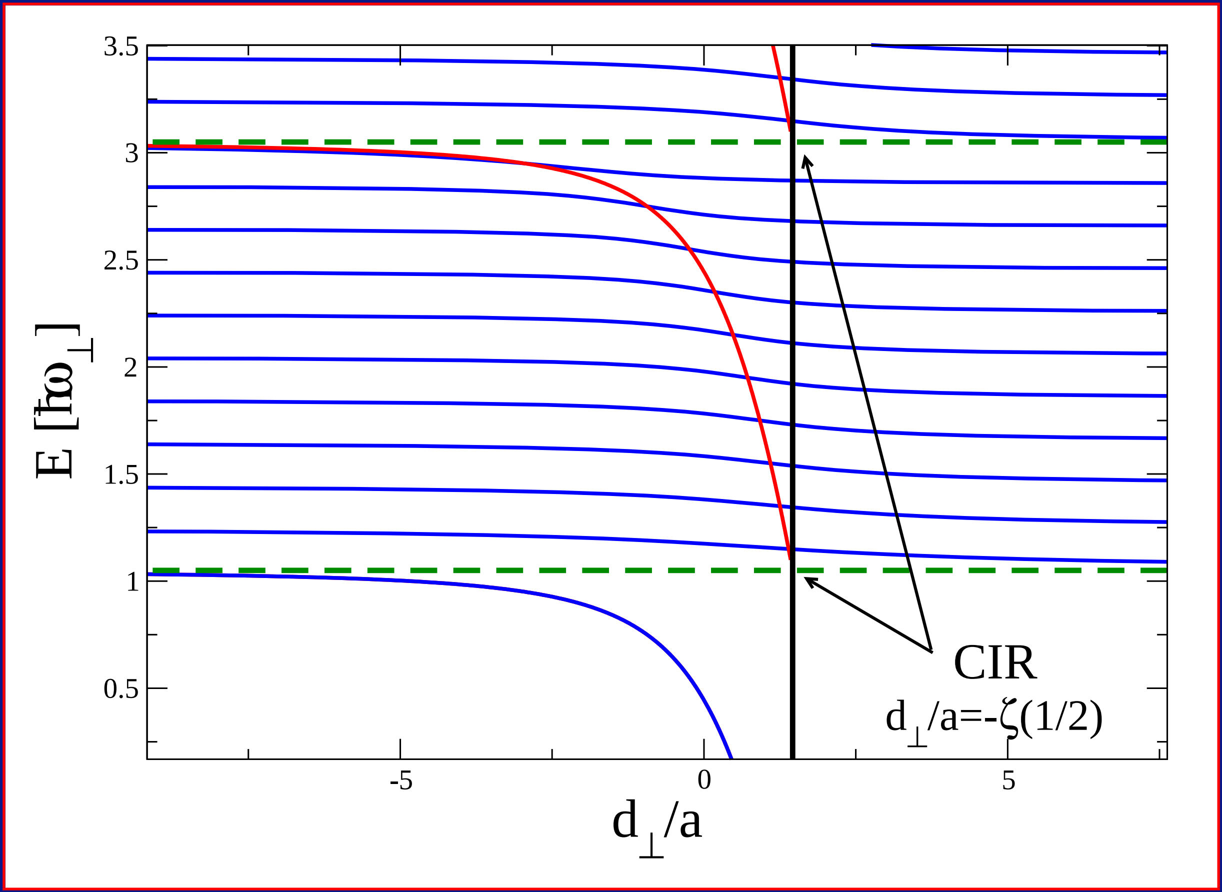
Resonance: $g_{1D} \to \infty$ for $\frac{d_\perp}{a} = -\zeta(\frac{1}{2}) \approx 1.46\ldots$

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

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

Olshanii's model (I)

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

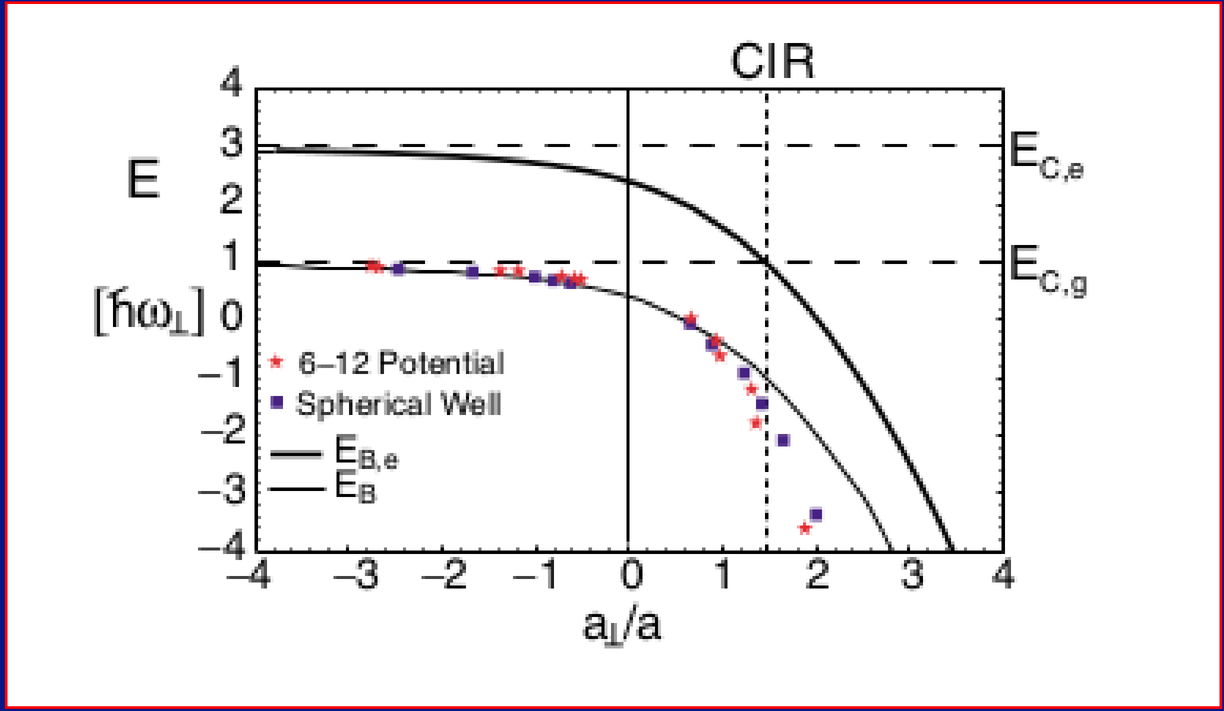


Blue: quasi 1D spectrum

Red: artificially(!) excited bound state

Green: quasi continuum threshold

Olshanii's model (II)



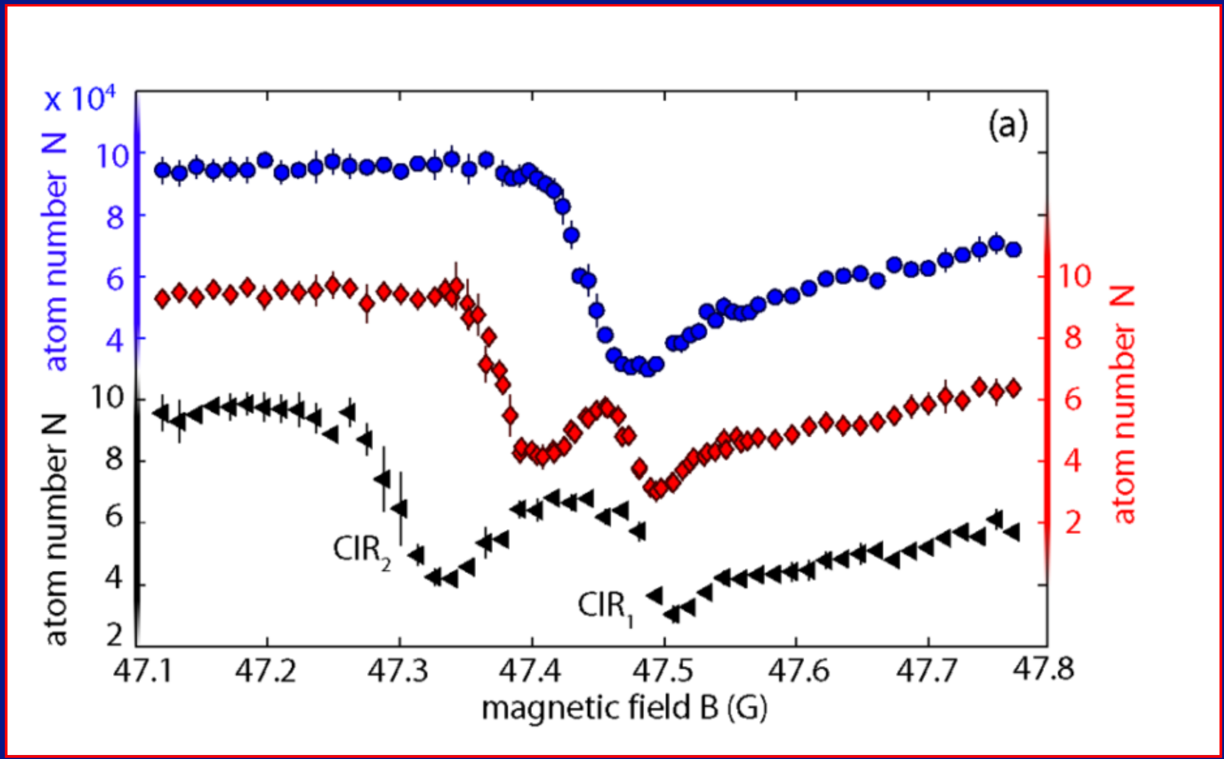
T. Bergeman et al., PRL **91**, 163201 (2003)

Result:

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

Note: No data points on shifted state!

Innsbruck experiment (Cs atoms)

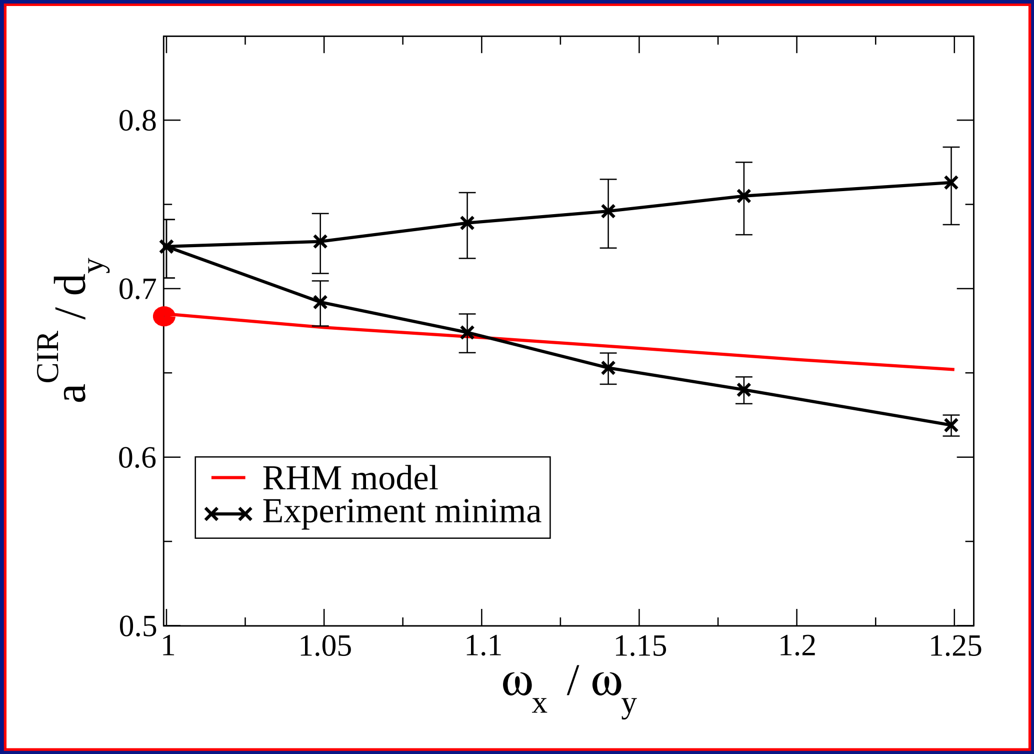


Blue curve: Atom losses for $\omega_x = \omega_y \gg \omega_z$ (anisotropy fixed, a varied).

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

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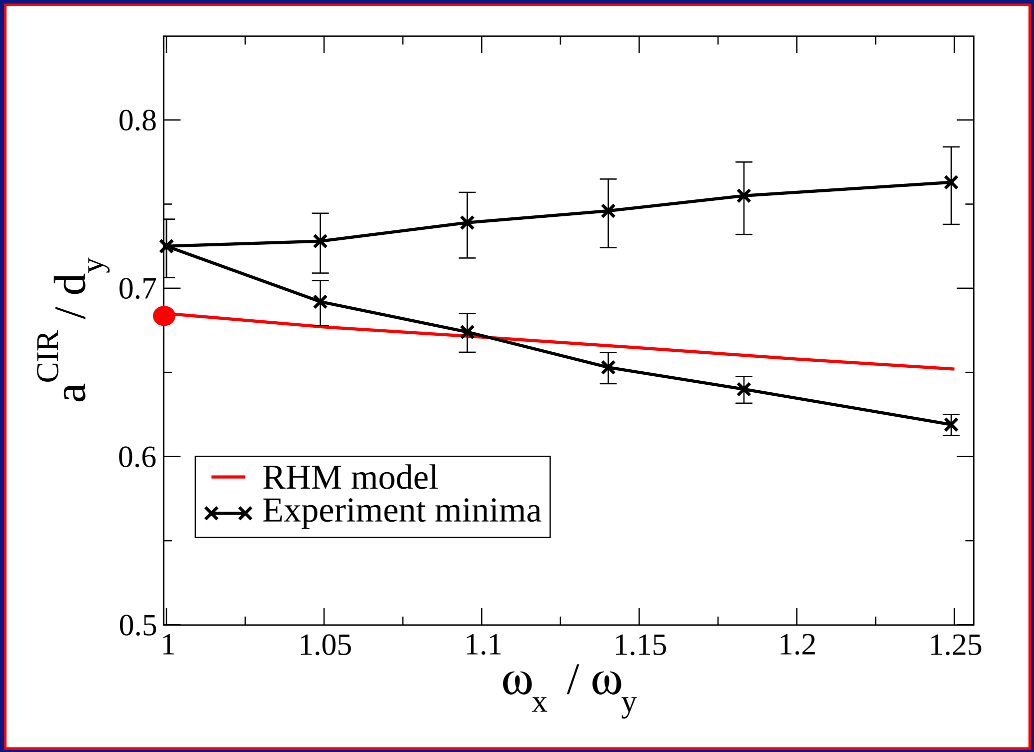

E. Haller et al., PRL, **104**, 153203 (2010)

⇒ 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.

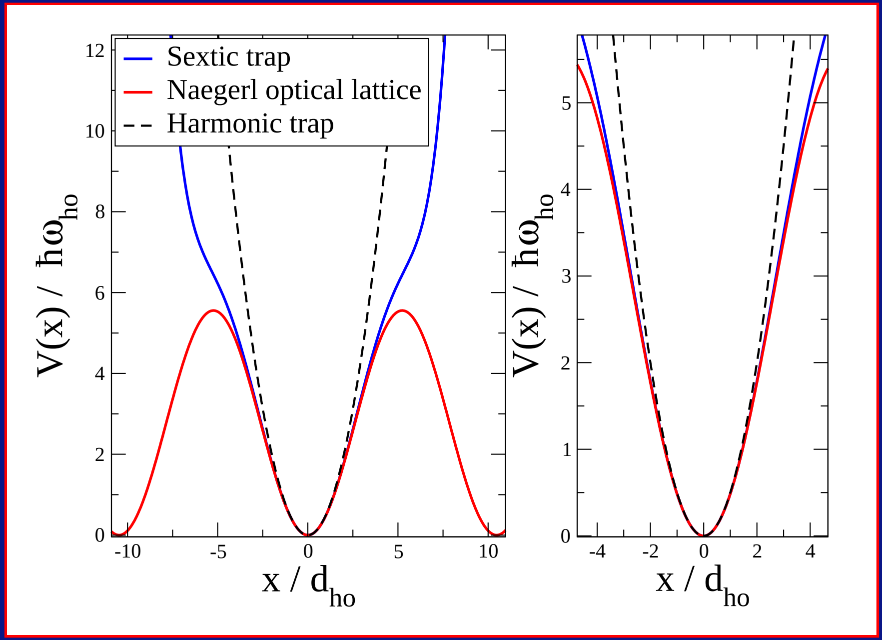
Full treatment of two atoms in quasi-1D trap:

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

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

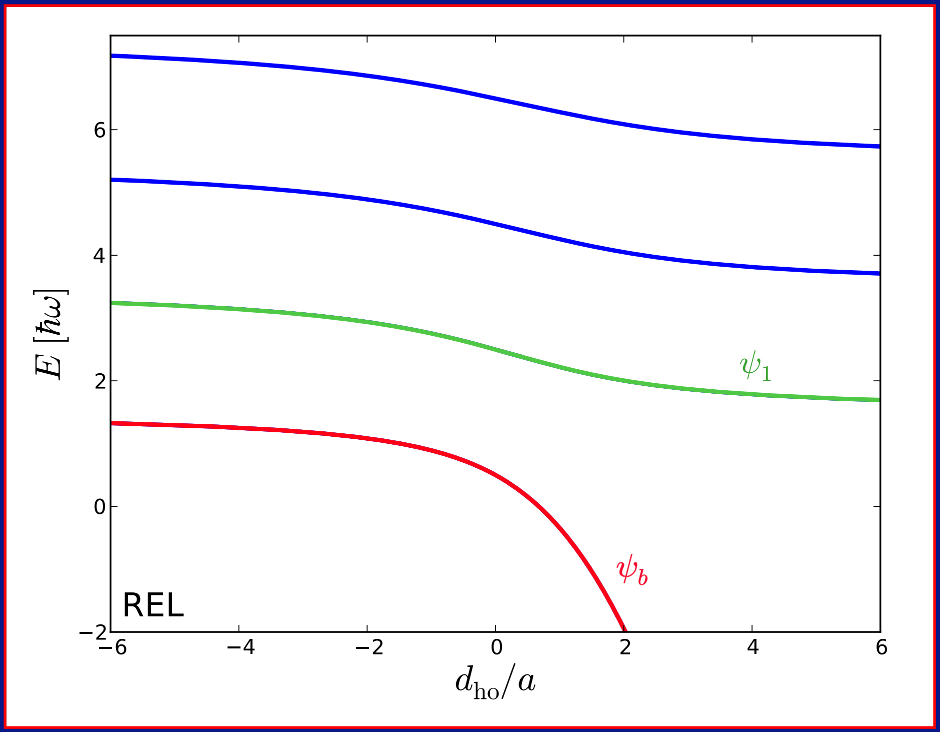
Note:

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



Energy spectra (cartoon)

Relative-motion spectrum in harmonic trap vs. full (rel + com) spectrum



Relative motion only

ψ_b: (molecular) bound state

ψ_1: lowest-lying trap state

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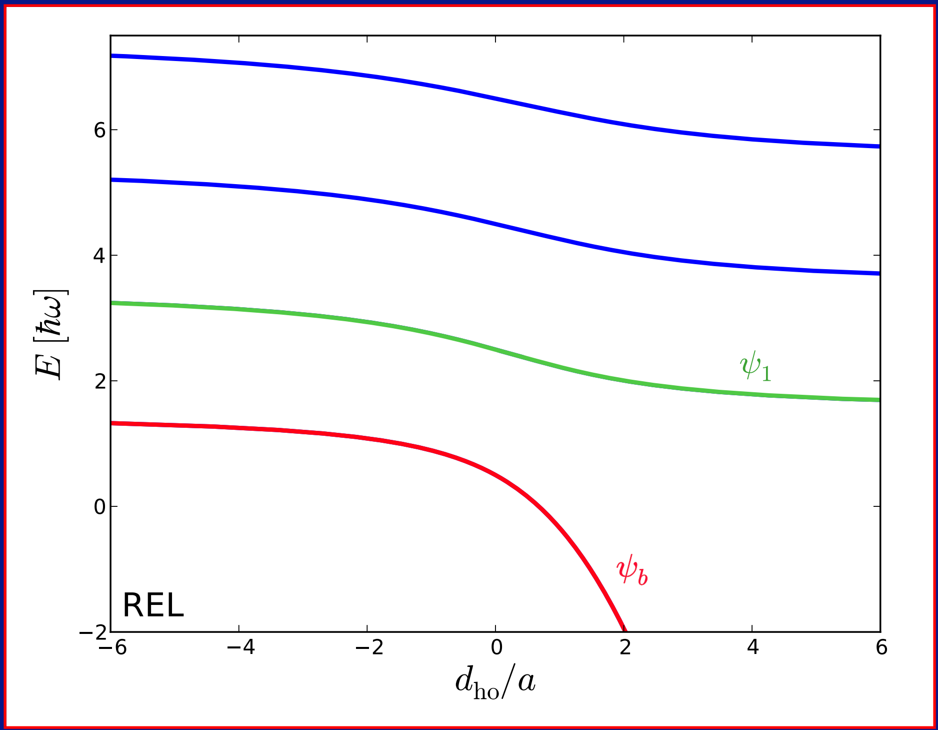

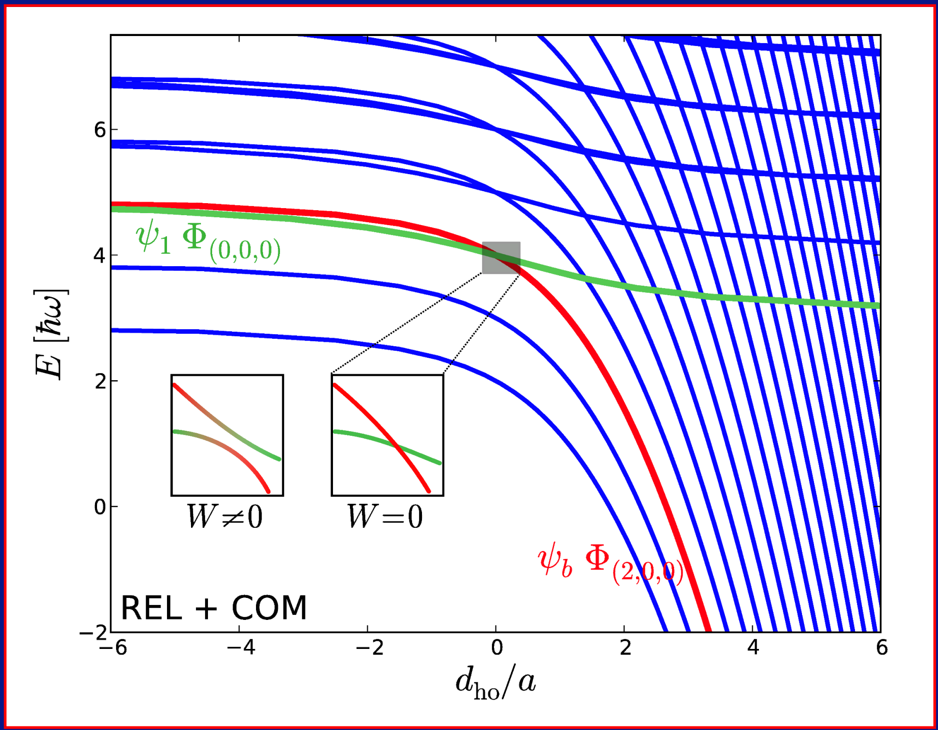

Relative motion only

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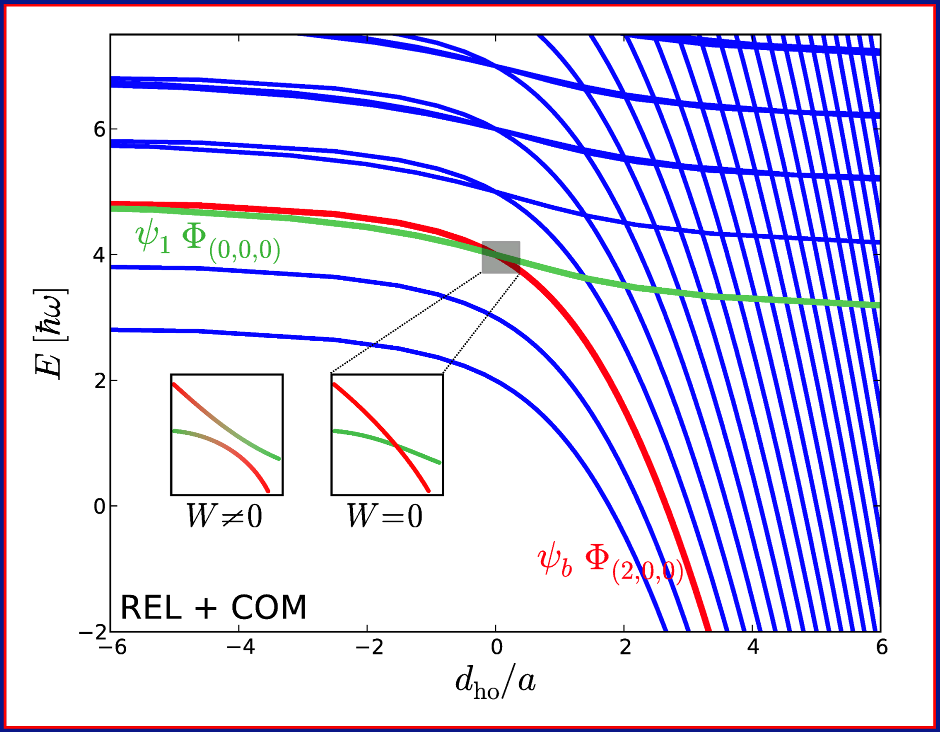
Full spectrum

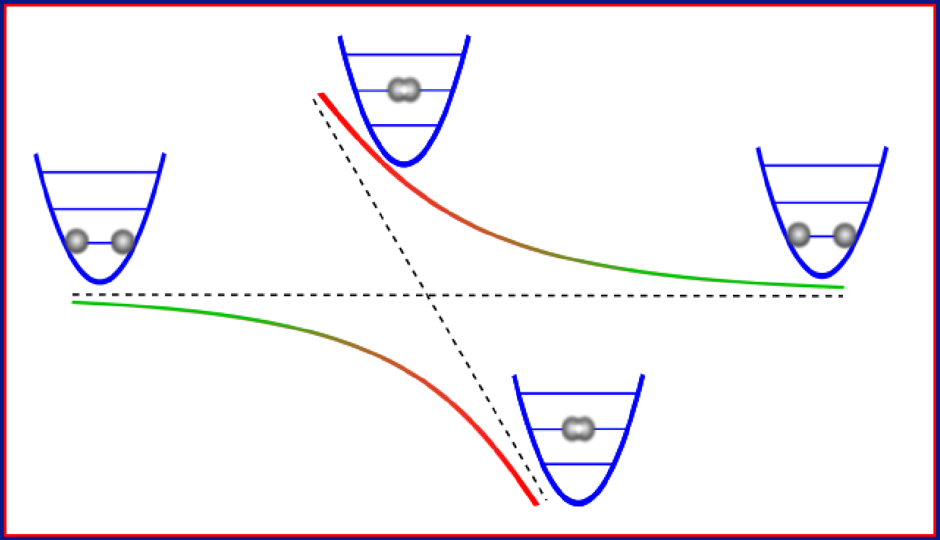
$\Phi_{(0,0,0)}$: ground com state

$\Phi_{(2,0,0)}$: excited com state

Molecule formation due to confinement



Full spectrum



Avoided crossing

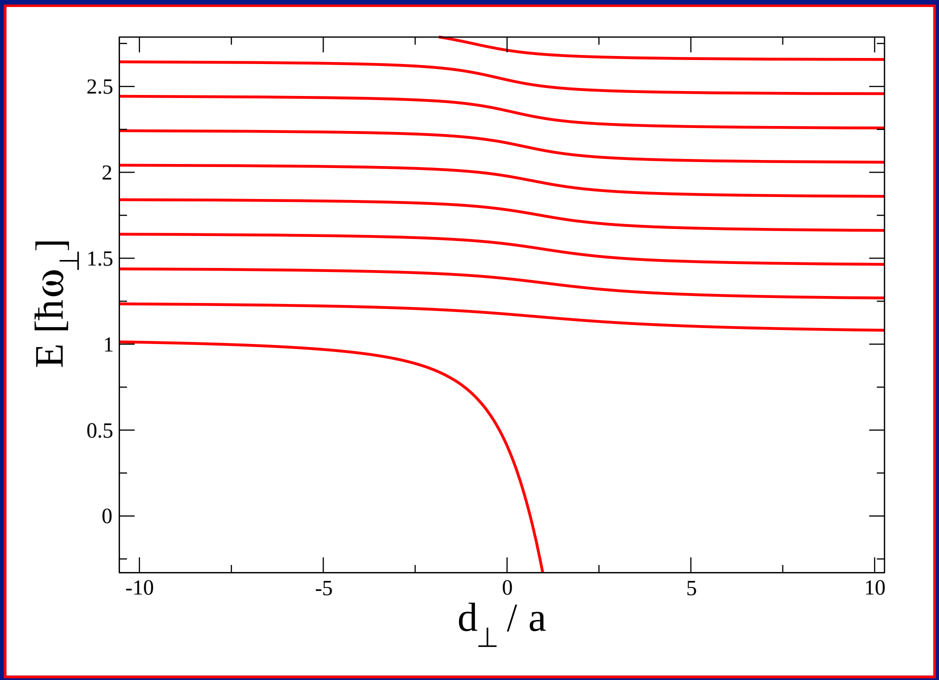
Coupling of center-of-mass (com) and relative (rel) motion ($W \neq 0$):

$\longrightarrow$ avoided crossing

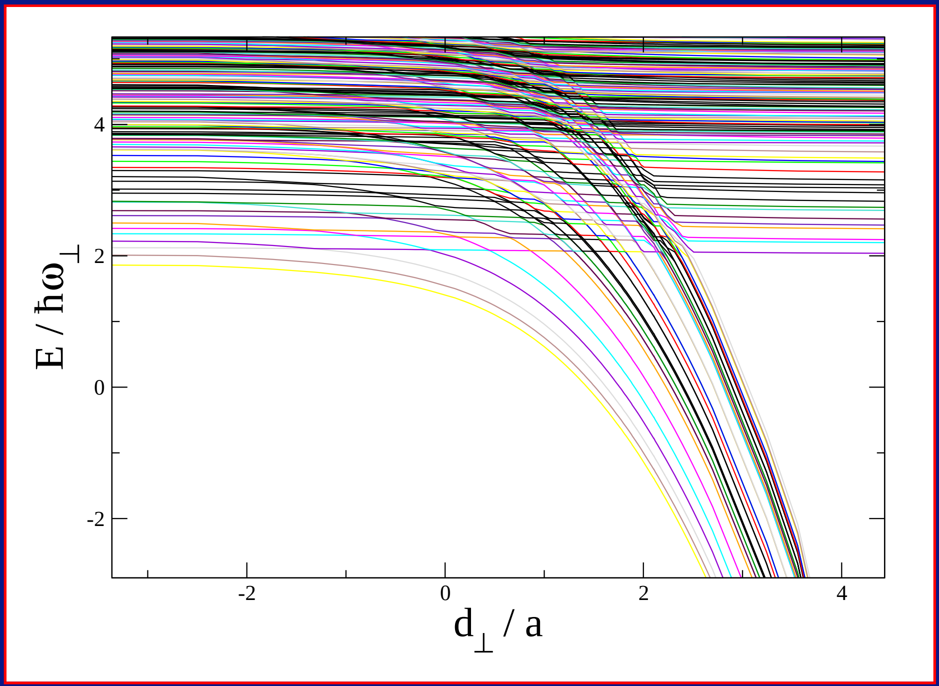
$\longrightarrow$ **molecule formation possible!**

Energy spectra (ab initio results)

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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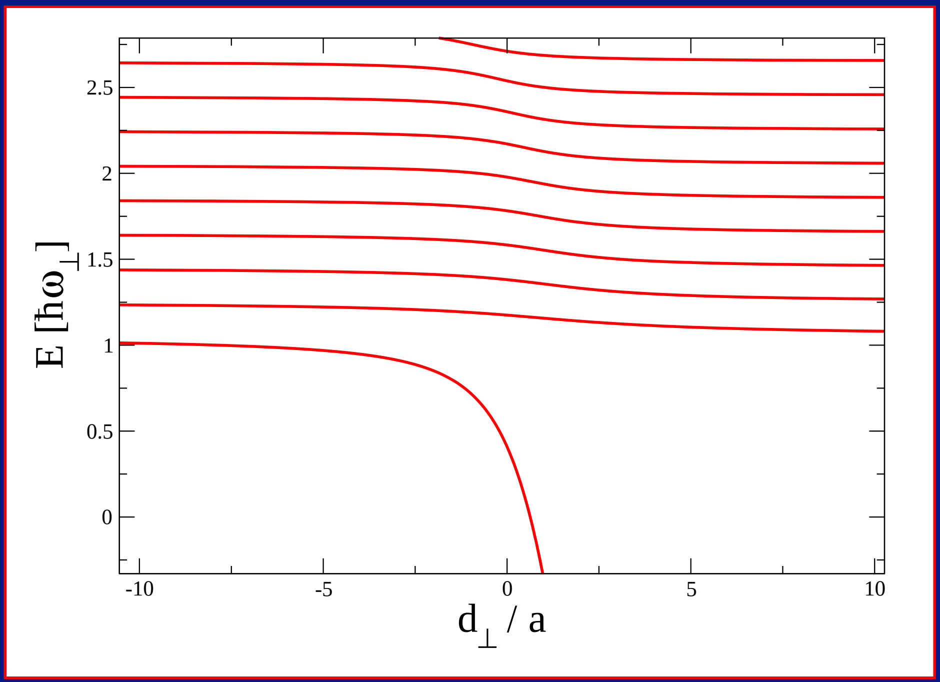
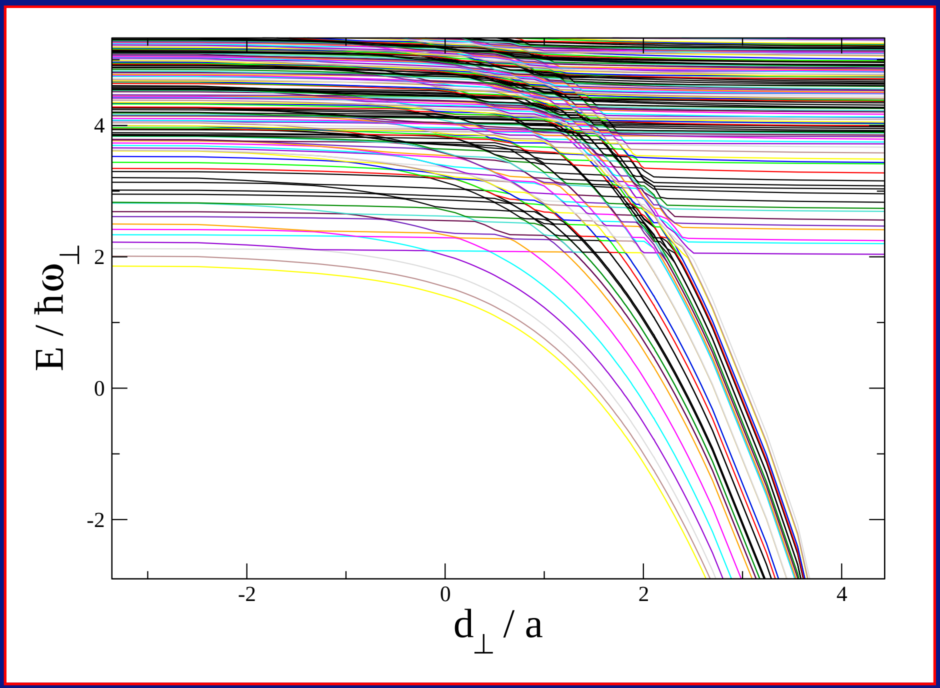


REL



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

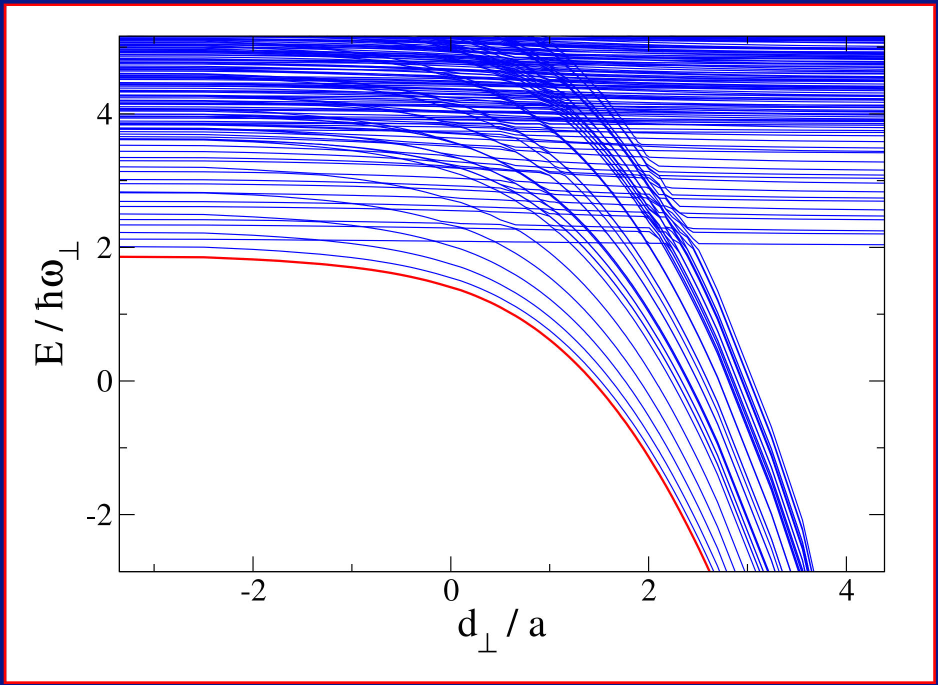
Ultracold: only ground trap state populated $\Longrightarrow m = k = 0$.

Resonances:

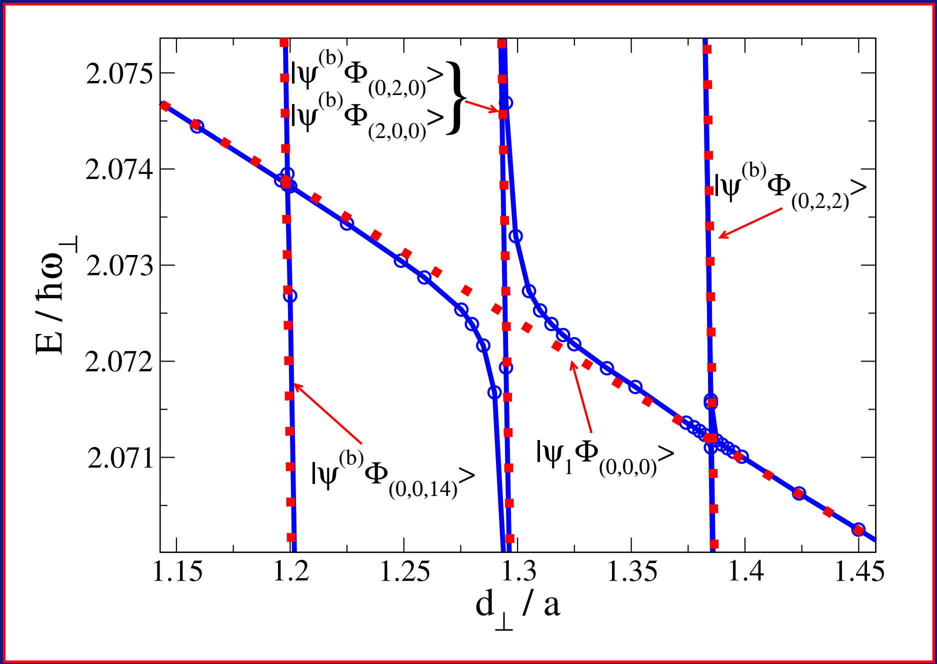
Crossing of transversally COM excited REL bound state with ground (COM and REL) trap state.

Avoided Crossings (I)

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



Large part of spectrum



Zoom-in in spectrum.

Avoided Crossings (II)

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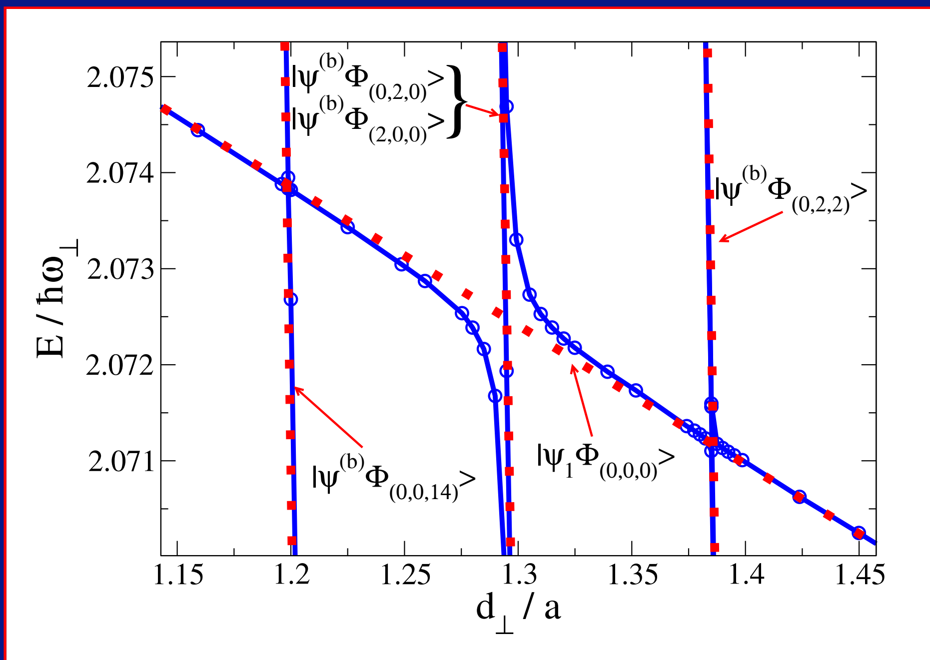
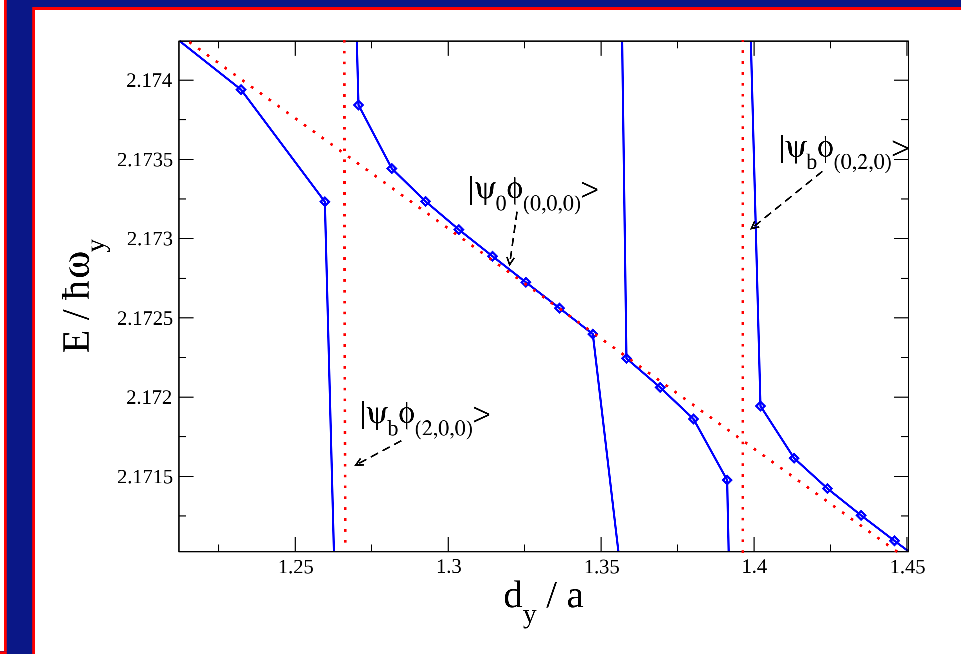


$\omega_x = \omega_y \gg \omega_z$



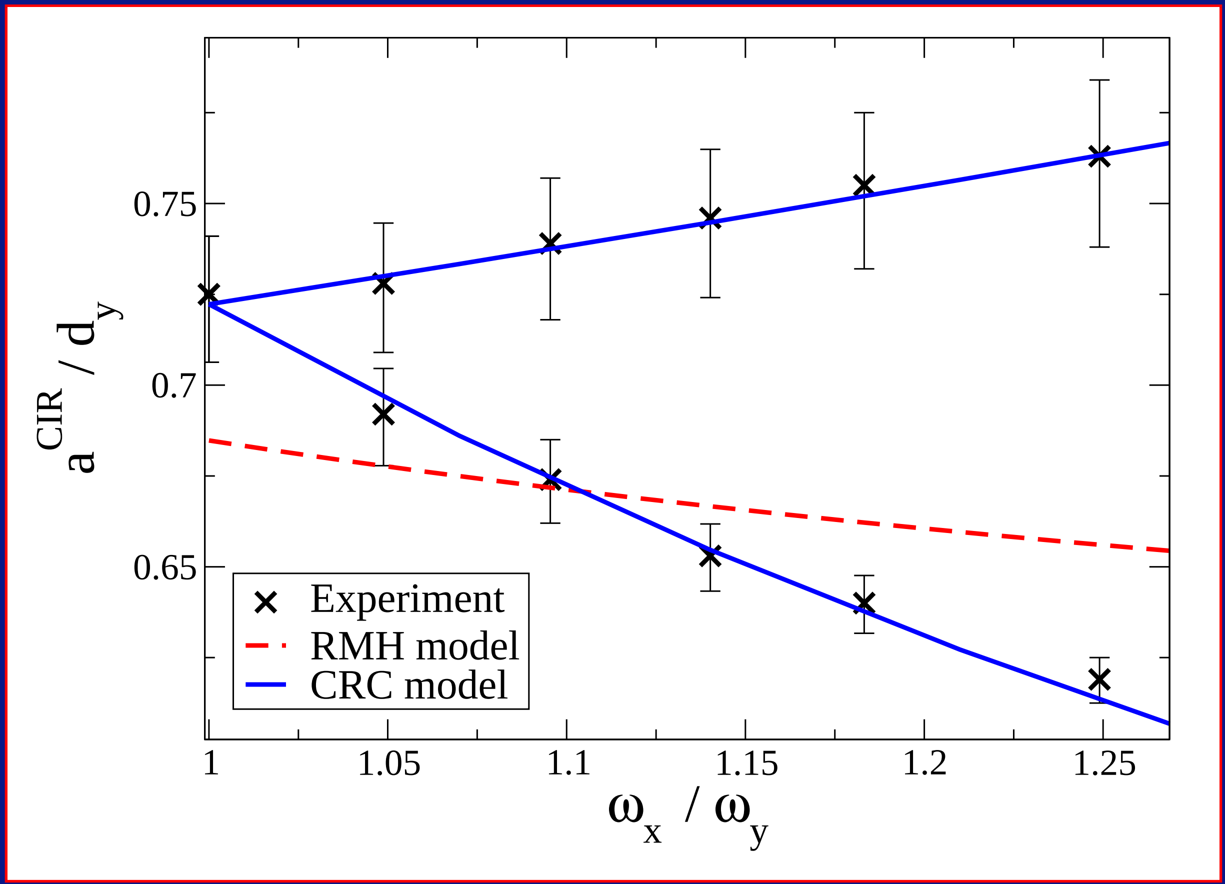
$\omega_x \neq \omega_y \gg \omega_z$

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

$\Rightarrow$ 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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However, not everyone (e.g. 2 out of 3 referees) was convinced!

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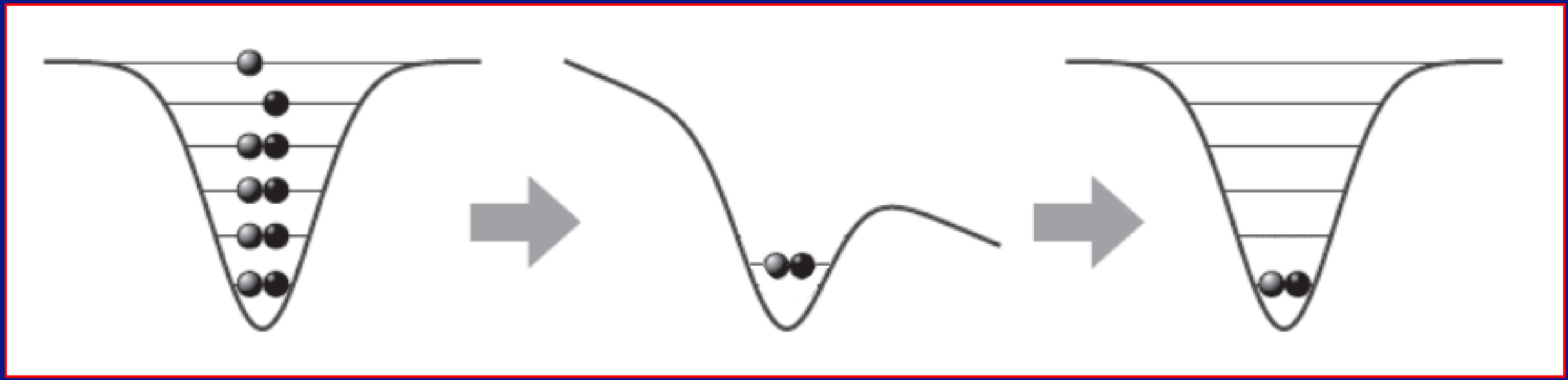
- Losses in a many-body system (Innsbruck experiment) are very unspecific, in contrast to Cambridge rf experiment.

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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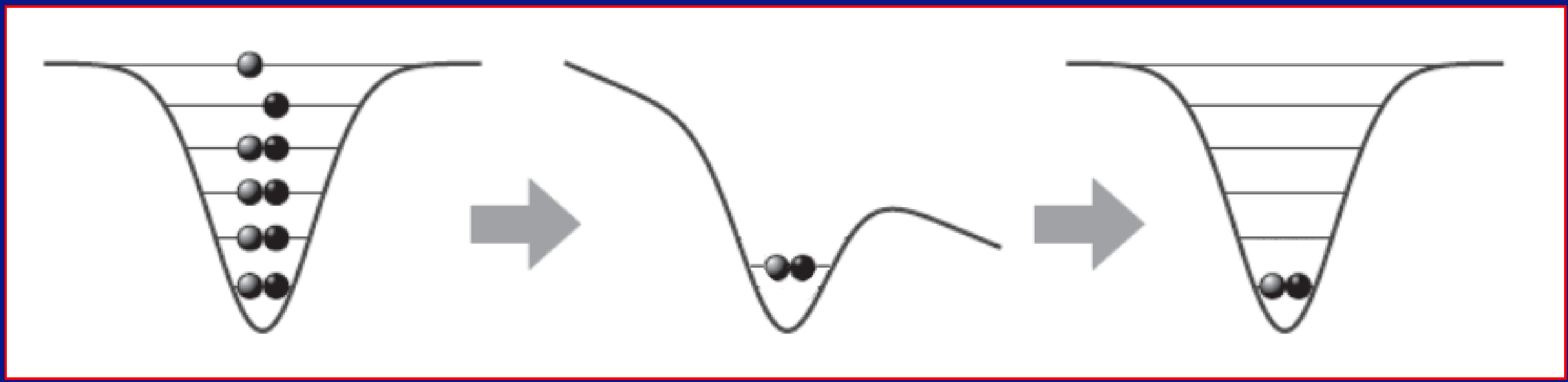

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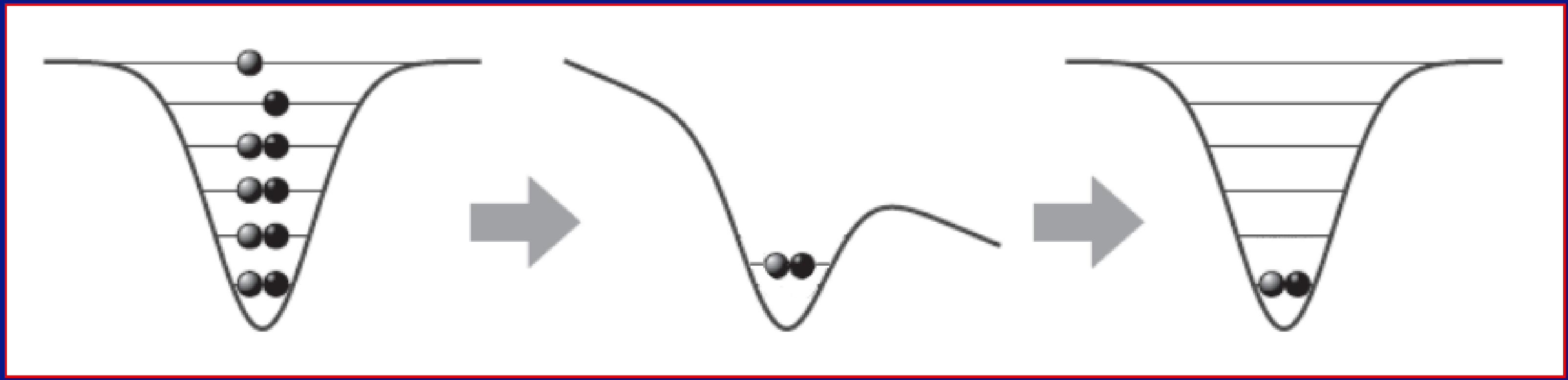

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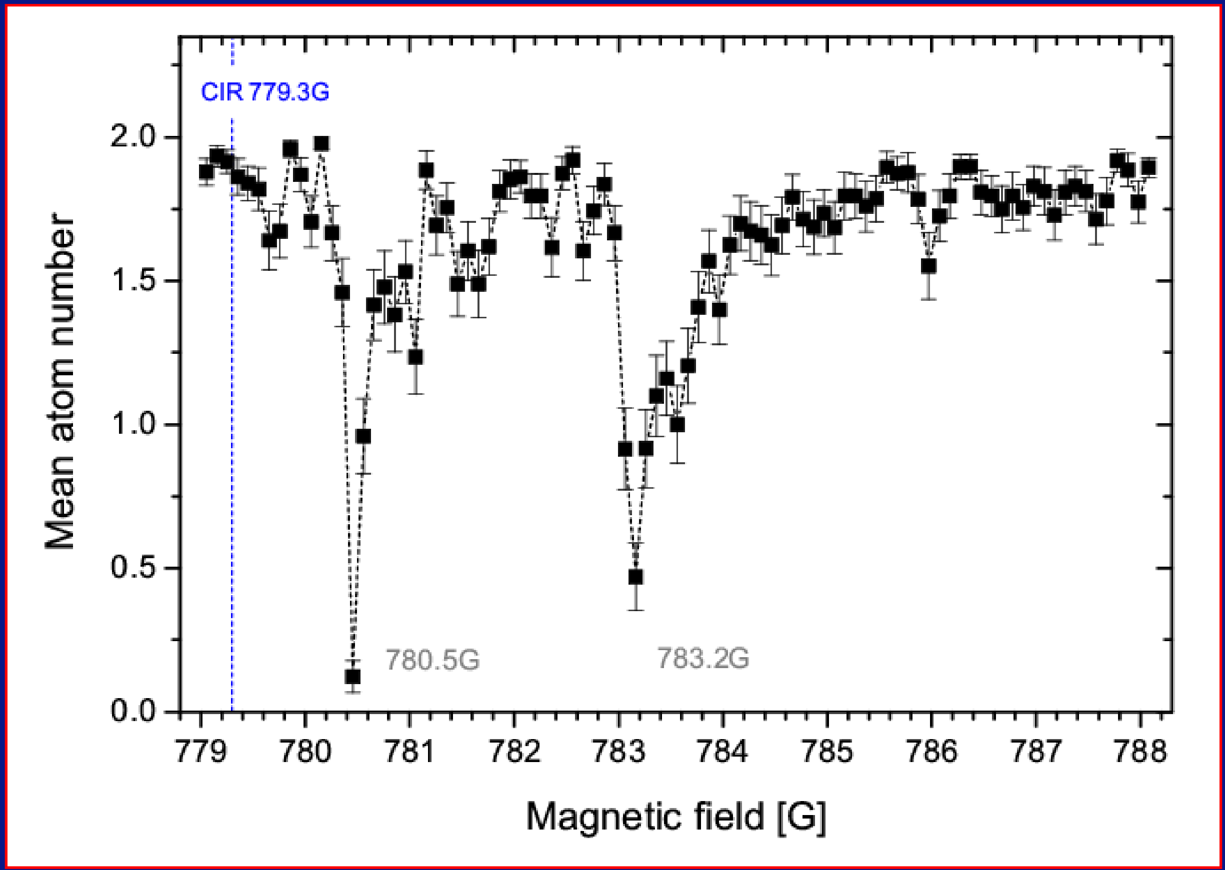
2. Detection of molecules: measurement of tunneling atoms at a B field where deeply bound molecules do not tunnel.

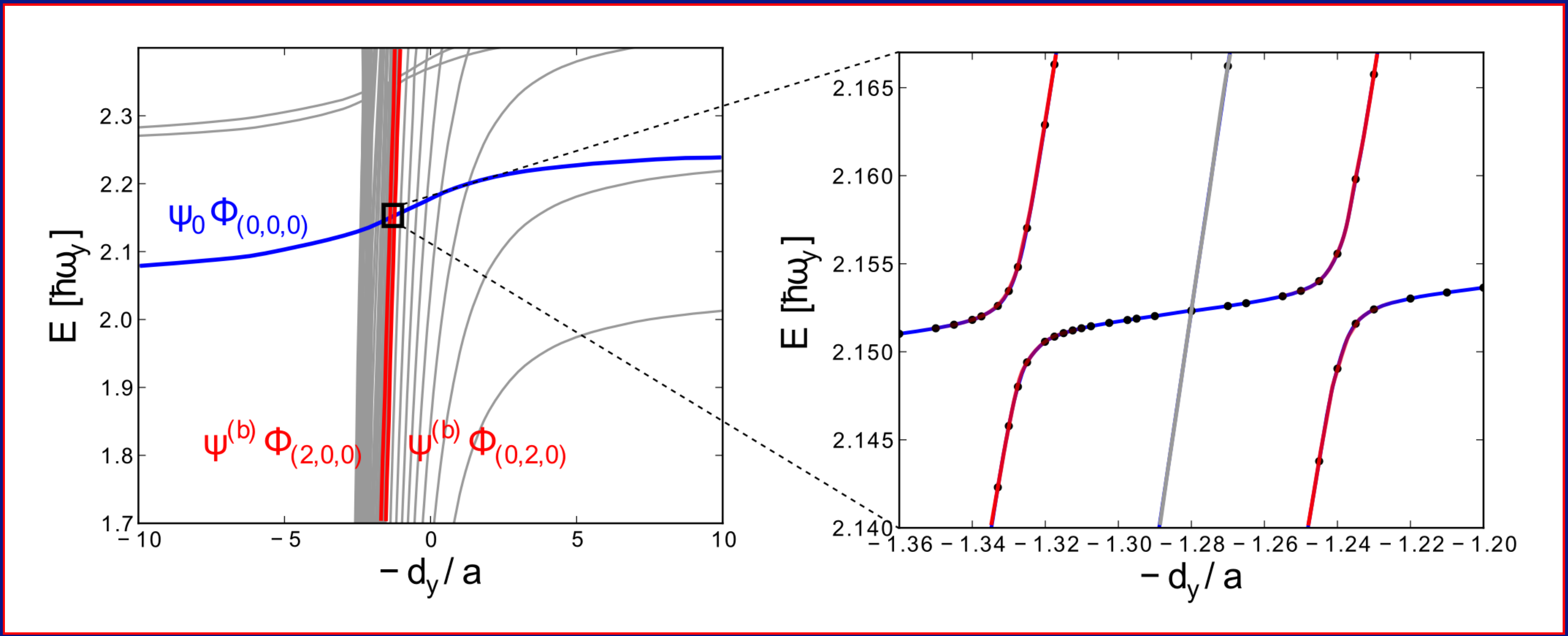
Measurement of the mean atom number



Positions for molecule formation: 776.01 G & 779.02 G

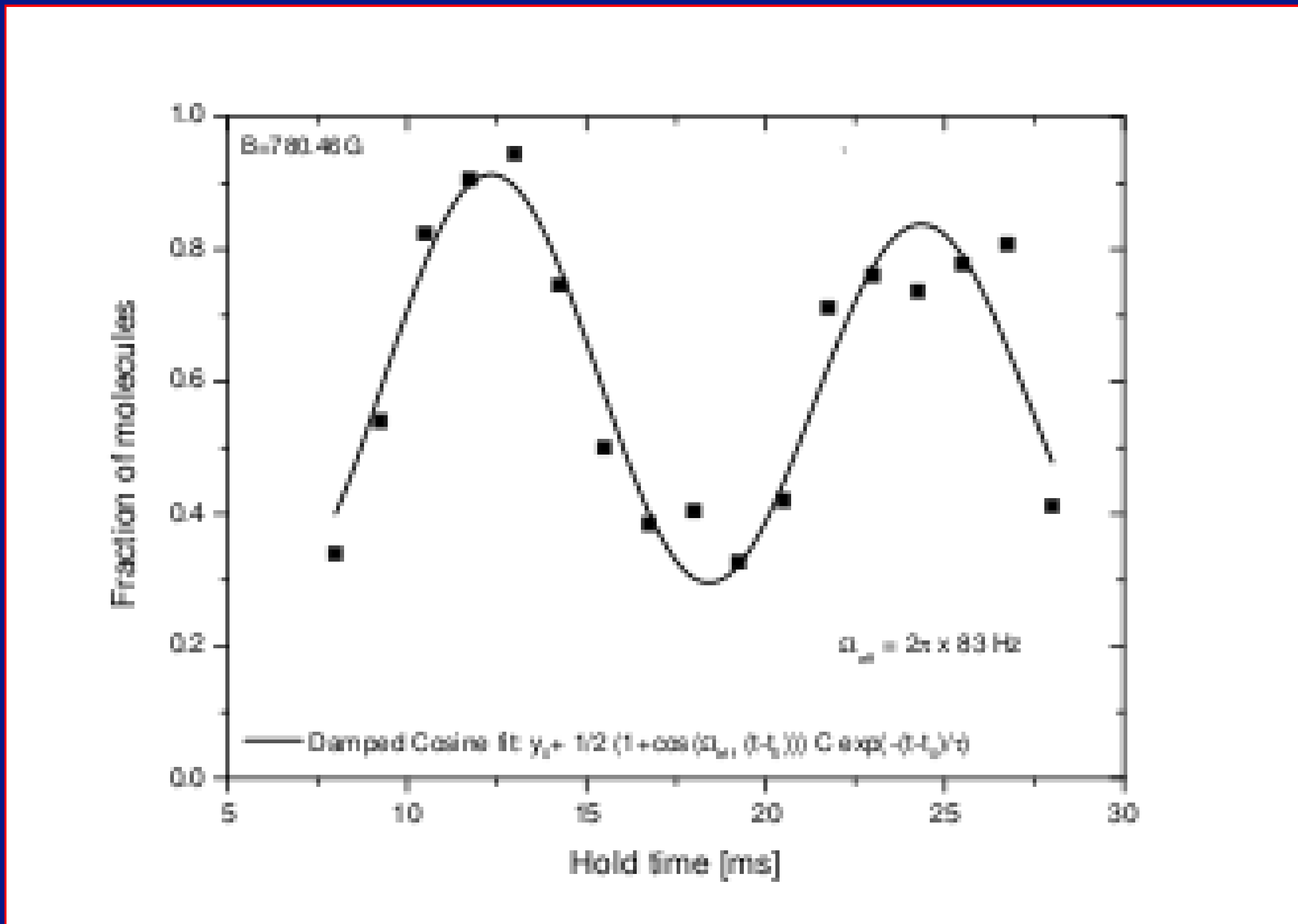
Ab initio calculation

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



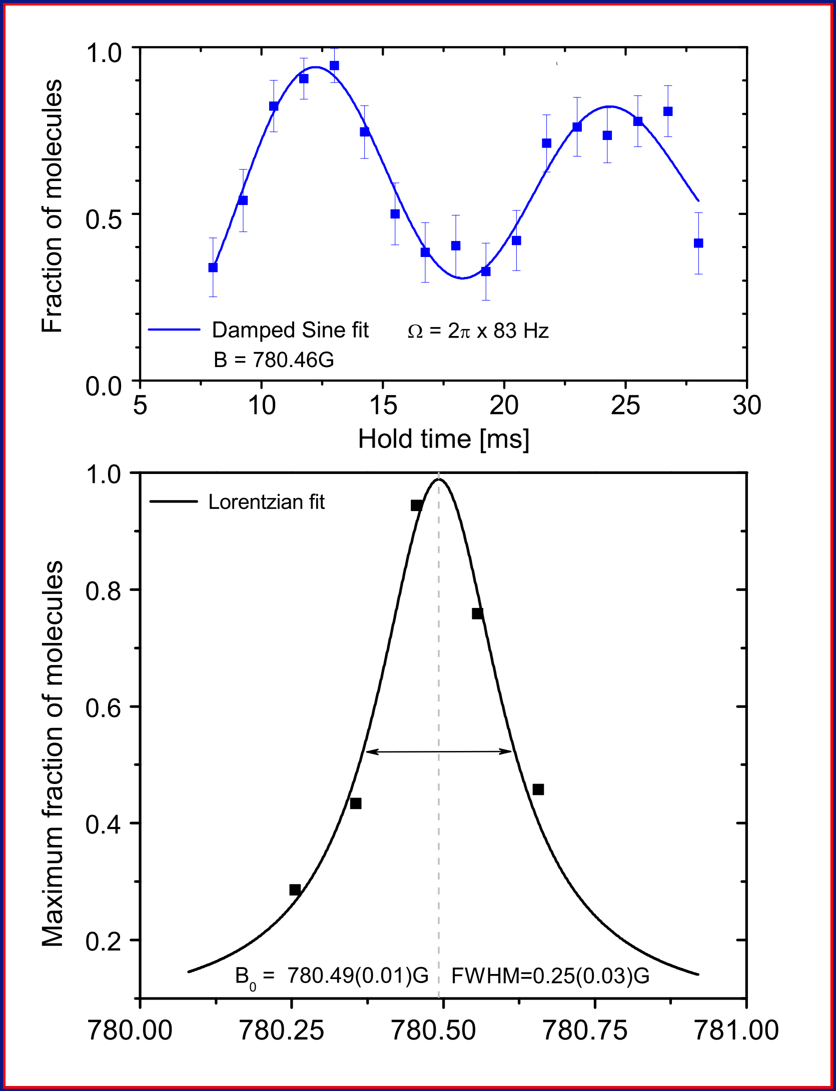
Due to anisotropy ($\omega_x \neq \omega_y \gg \omega_z$) two inelastic CIR (avoided crossings) expected.

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.,
Phys. Rev. Lett. **110**, 203202 (2013) .

Universality of confinement-induced resonances:

Dipolar gases (heteronuclear molecules, Rydberg atoms):

Inelastic confinement-induced resonances seen in ab initio calculations.

They are tunable by varying the dipole-coupling strength!

[B. Schulz, S. Sala, and A. Saenz, New J. Phys. **17**, 065002 (2015)]

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Quantum-dot systems (electron pairs or excitons):

Inelastic confinement-induced resonances occur also for Coulomb interaction.

For electron pairs (no bound state) (smaller) change of density.

For excitons (electron-hole pairs) larger change of density.

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$\longrightarrow$ on-demand single-photon source!

[M. Troppenz, S. Sala, P.-I. Schneider, and A. Saenz submitted to *Phys. Rev. B*; arXiv:1509.01159]

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Inelastic CIRs and molecule formation:

see *Phys. Rev. Lett.* **109**, 073201 (2012); *Phys. Rev. Lett.* **110**, 203202 (2013)

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