# FEW-BODY SYSTEMS UNDER CONFINEMENT

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**Acknowledgment:**

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# External trap potential and interatomic interaction

## Atom-atom interaction (in pseudo-potential approximation):

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

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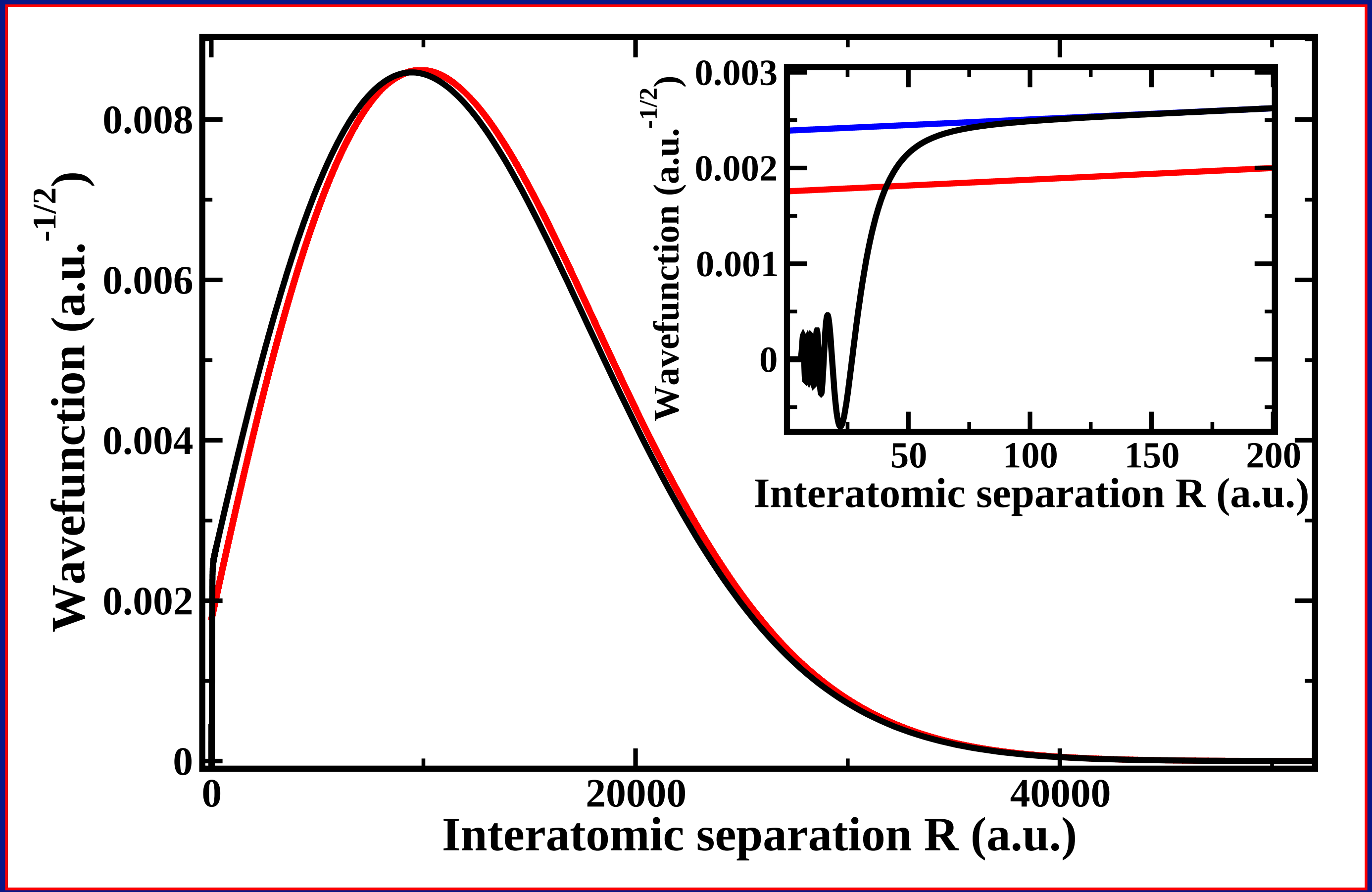
- As weaker the least bound state is bound, as closer the scales get to each other.

$\longrightarrow$ standard pseudo-potential approximation breaks down!

# Pseudopotential approximation (in a trap): wavefunctions




**Example:** spin-polarized $^6$Li atoms (a $^3\Sigma_u$) in a 10 kHz trap:

**"correct"** wavefunction (**black**, $a_{\rm sc} = -2030\, a_0$)

vs. standard **pseudo-potential** result (**red**, $a_{\rm sc} = -2030\, a_0$).

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- In a (tight) trap energy is (noticeably) quantized: zero-point energy.
- **Consequence:** Interception of $\psi$ with the $R$ axis $\neq a_{\rm sc}$.
  Present example $^6$Li (state a $^3\Sigma_u$) in 10 kHz trap:
  Effect for correct $\psi$ is small: interception at $-2023\,a_0$ for $a_{\rm sc} = -2030\,a_0$.
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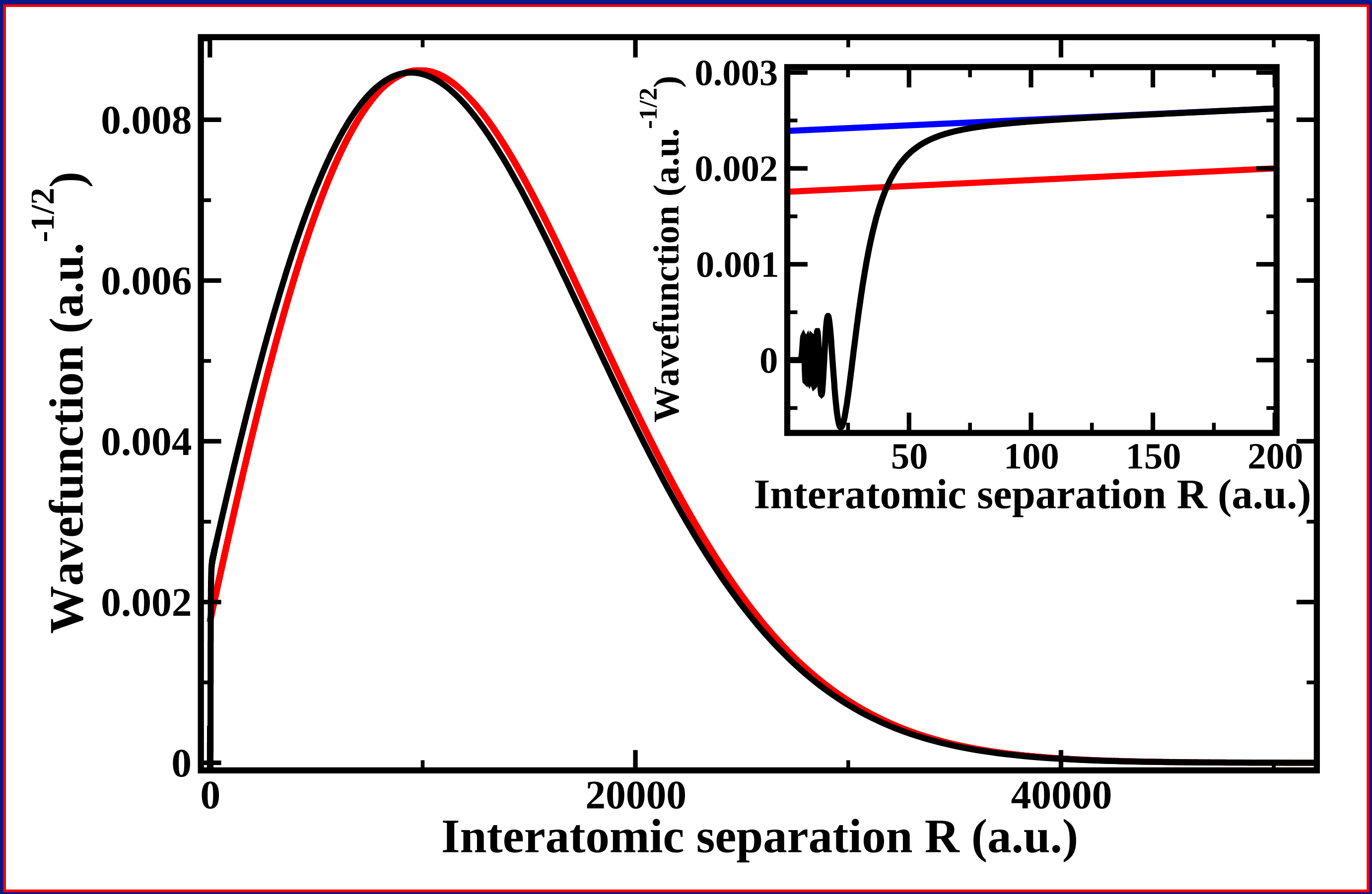
**Note:** In contrast to the physical $a_{\text{sc}}$ the empirical parameter $a_{\text{sc}}(E)$ follows only from the correct $\psi$ obtained with $V_{\text{mol}}(R)$!

$\longrightarrow$ knowledge of $V_{\text{mol}}(R)$ is essential!

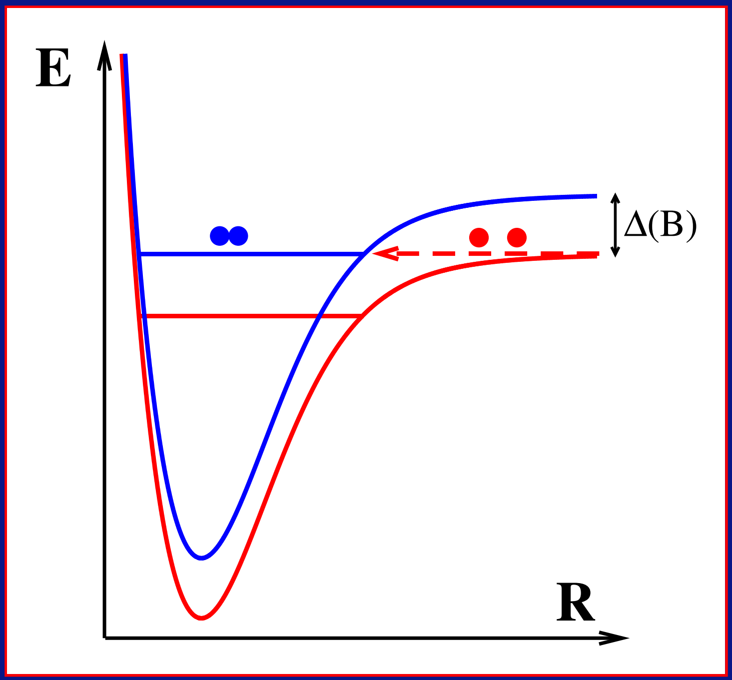
# Pseudopotential approximation (in a trap): wavefunctions




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 **energy-dependent (blue, $a_{\rm sc} = -2872\, a_0$) pseudo-potential** results.

# Tunable interaction: magnetic Feshbach resonances




## Simple picture:

Only **2 channels**:

– open (continuum) channel,

– closed (bound) channel.

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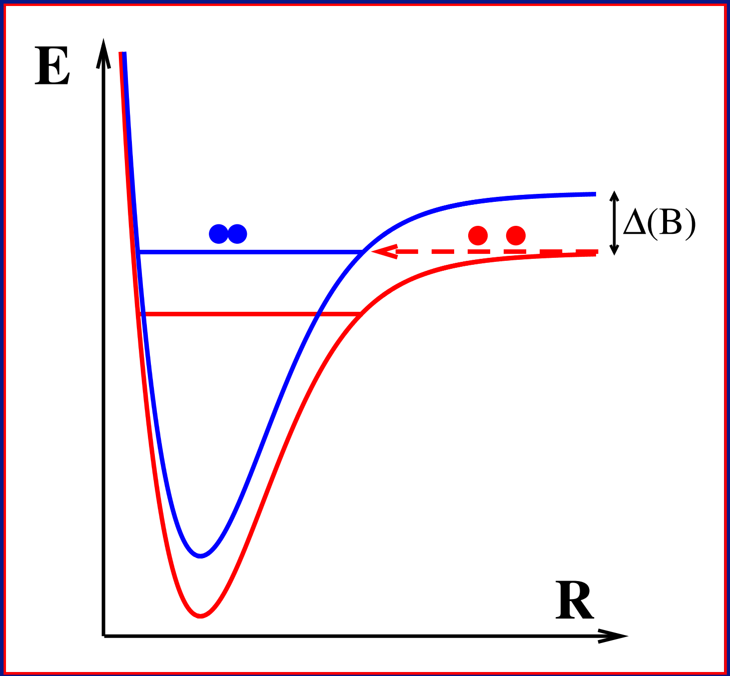


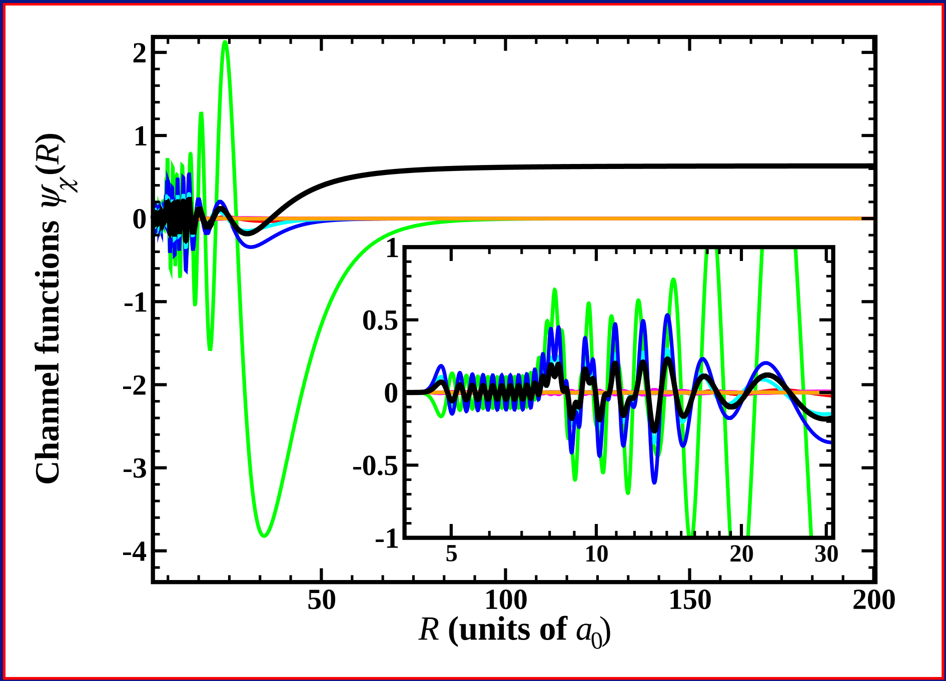


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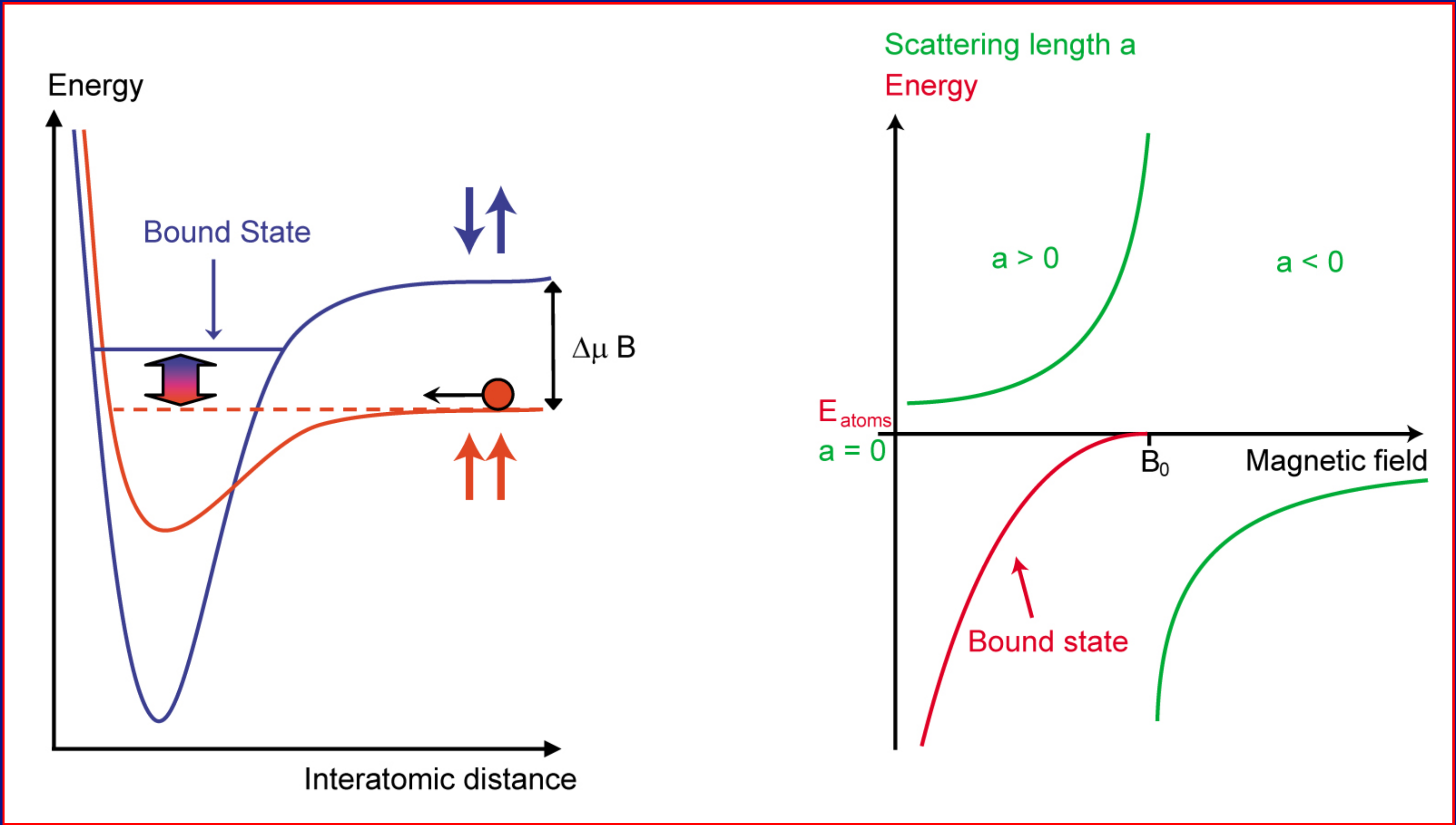
## Multichannel reality:

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!**

# Magnetic Feshbach resonances (MFRs) in a harmonic trap

- Description as coupled single open and closed channels ($|\Psi\rangle = C|\mathrm{open}\rangle + \mathrm{A}|\mathrm{closed}\rangle$)
- Use analytically known long-range behavior of the wave functions (parabolic cylinder fcts.)

[P.-I.Schneider, Y.V. Vanne, A.S., *Phys. Rev. A*, **83**, 030701 (*Rapid Comm.*) (2011)]

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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

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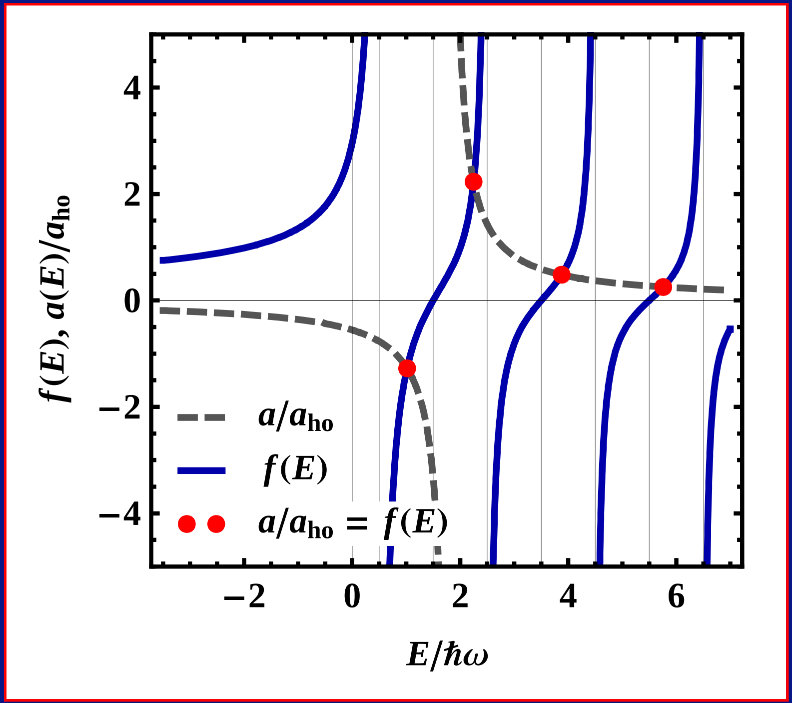


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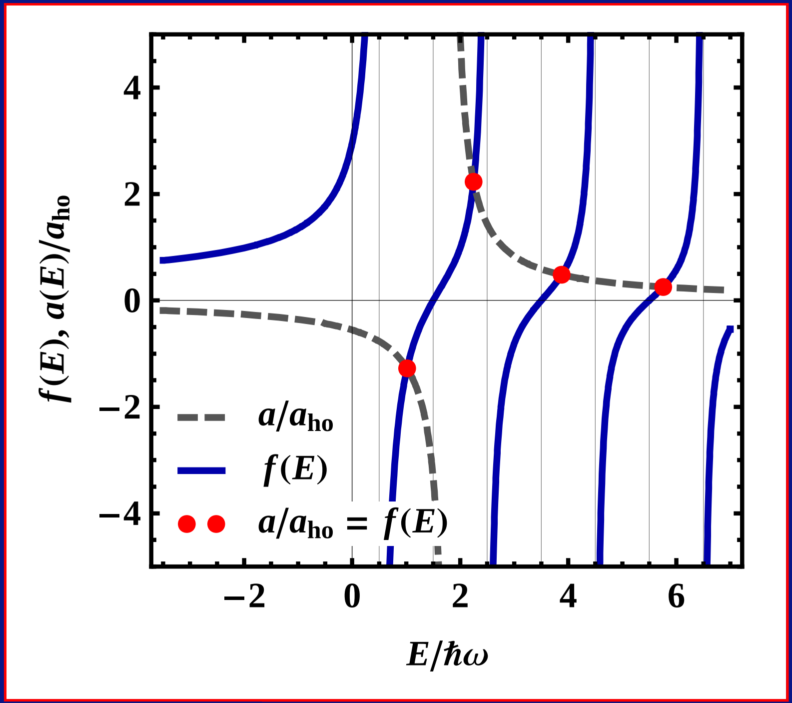


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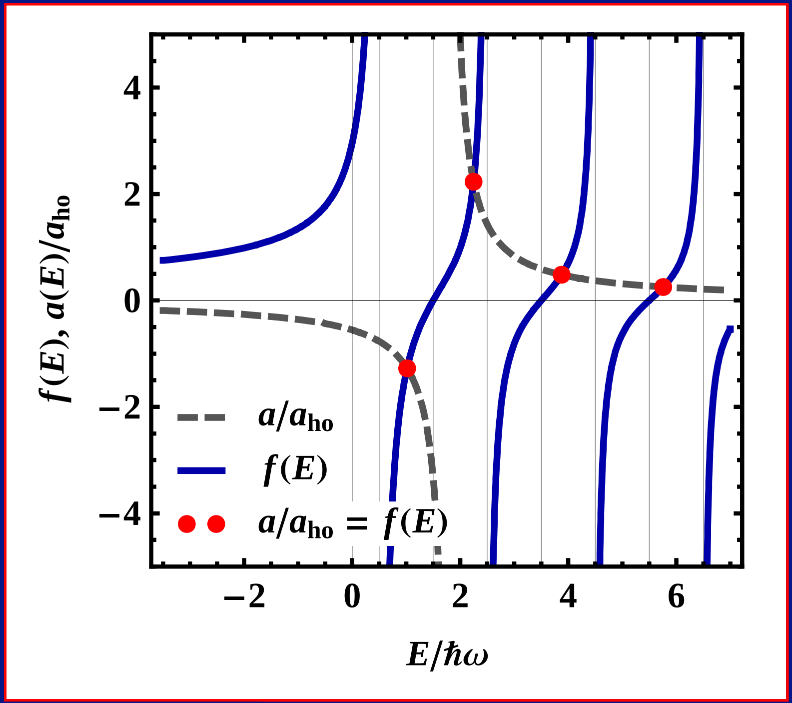
$$a(E,B) = a_{\text{bg}}\left(1 - \frac{\Delta B}{B - B_0 + \delta B - E/\mu}\right)$$

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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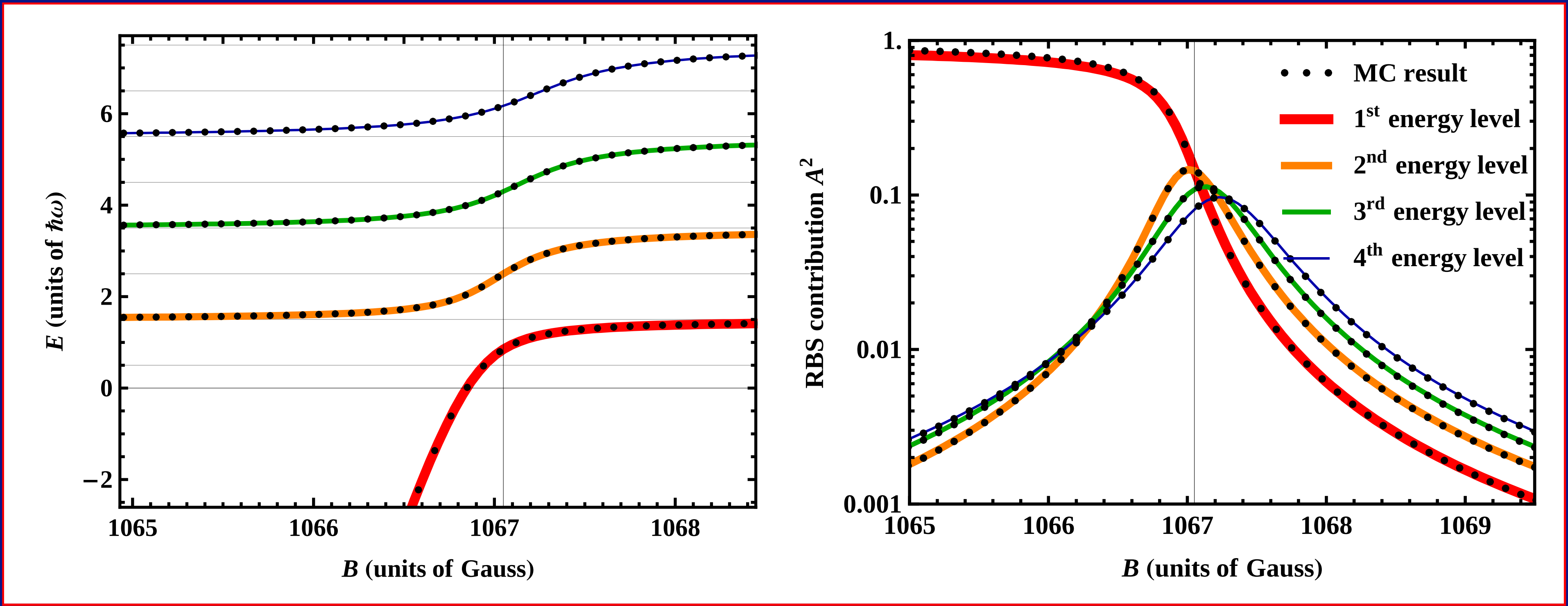
# How good is the model?

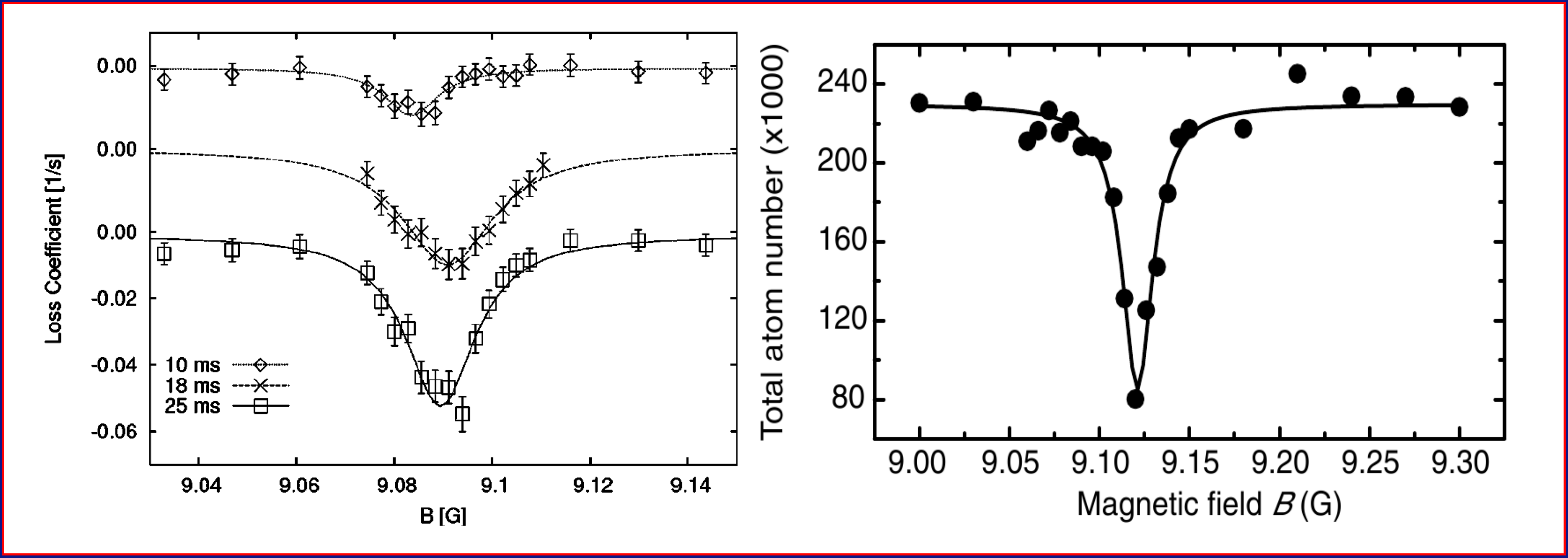
Comparison with full coupled-channel calculations for $^{6}$Li-$^{87}$Rb in a 200 kHz trap:




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

# Resolving a seven-year debate

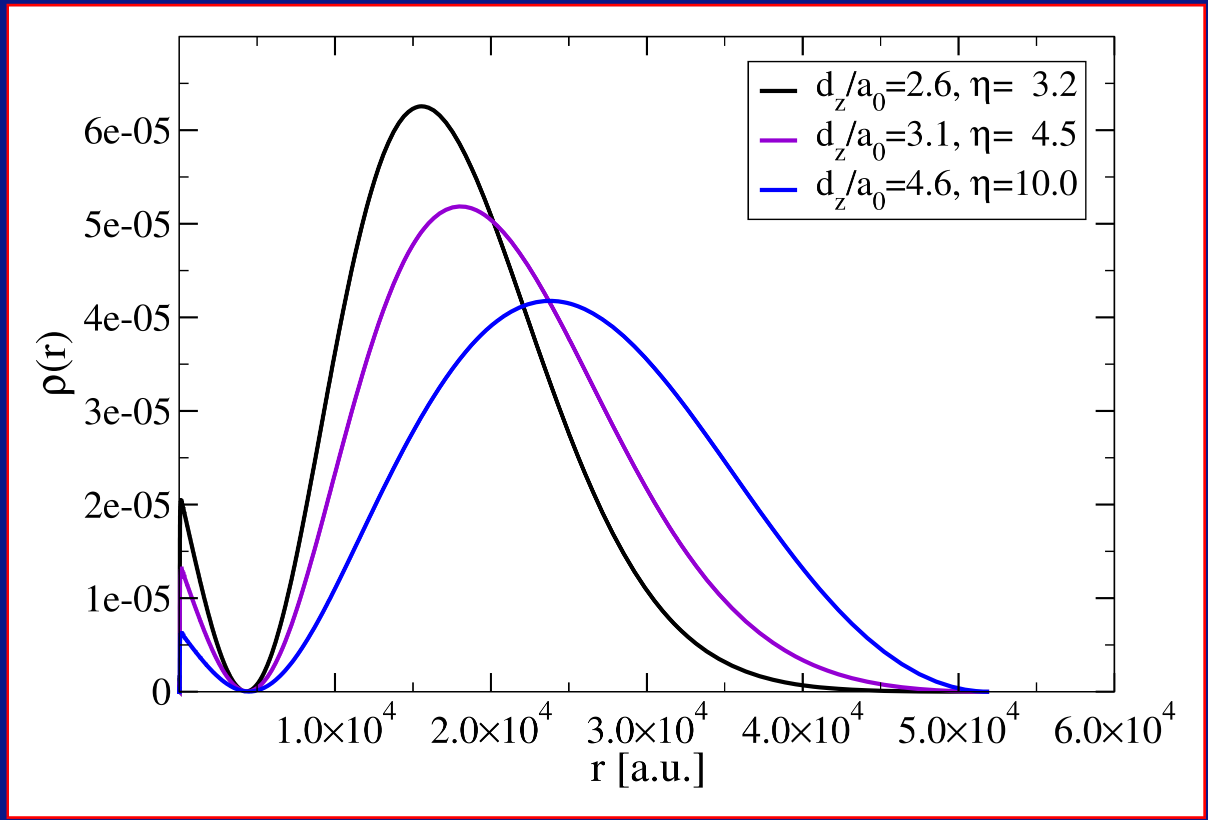
- Resonances of $a \propto f(E)$ are located at $E_{\rm res}^{(n)} = \hbar\omega(2n + \frac{1}{2}) \Rightarrow$ thus NOT at bare resonance position $B_R = B_0 - \delta B$, but at
$$B = B_{\rm res}^{(n)} = B_0 - \delta B + E_{\rm res}^{(n)}/\mu \,.$$
- This explained the disagreement of experimentally 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).

# 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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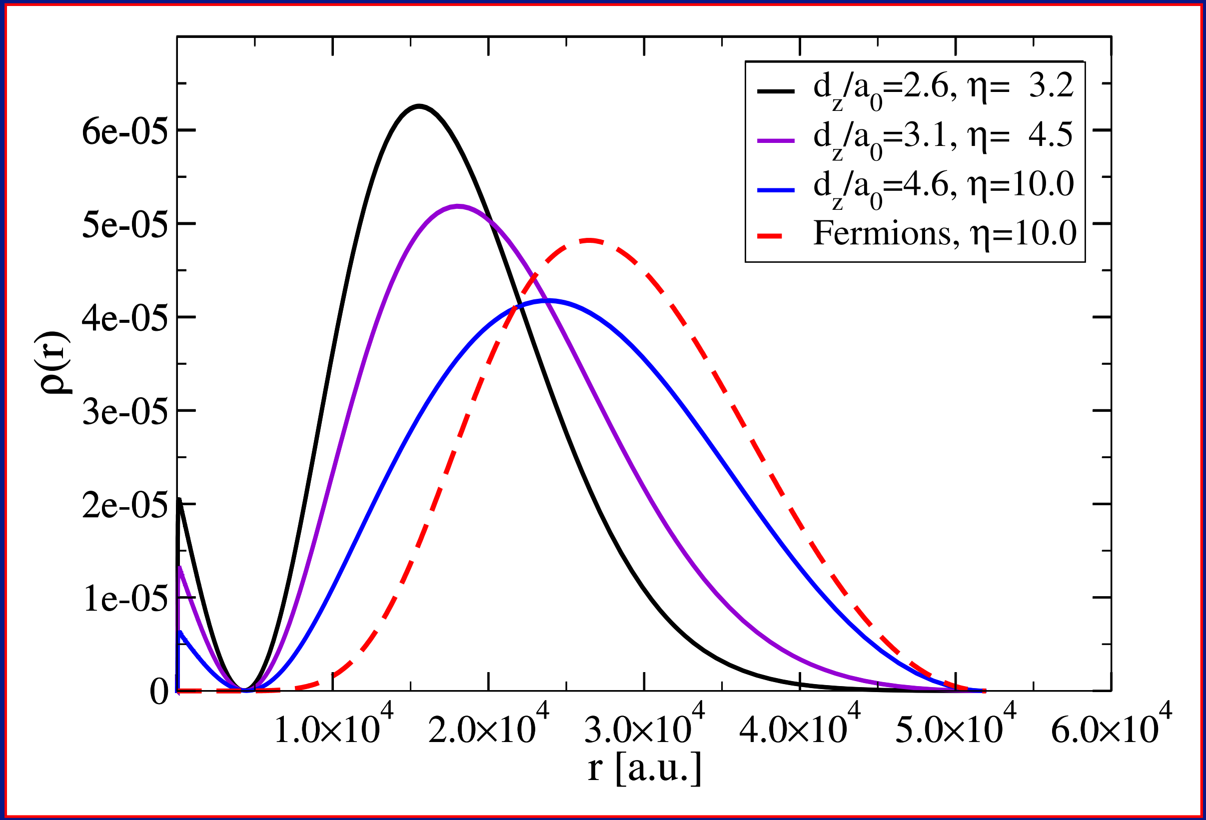


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# Confinement-induced resonances (CIR)

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

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

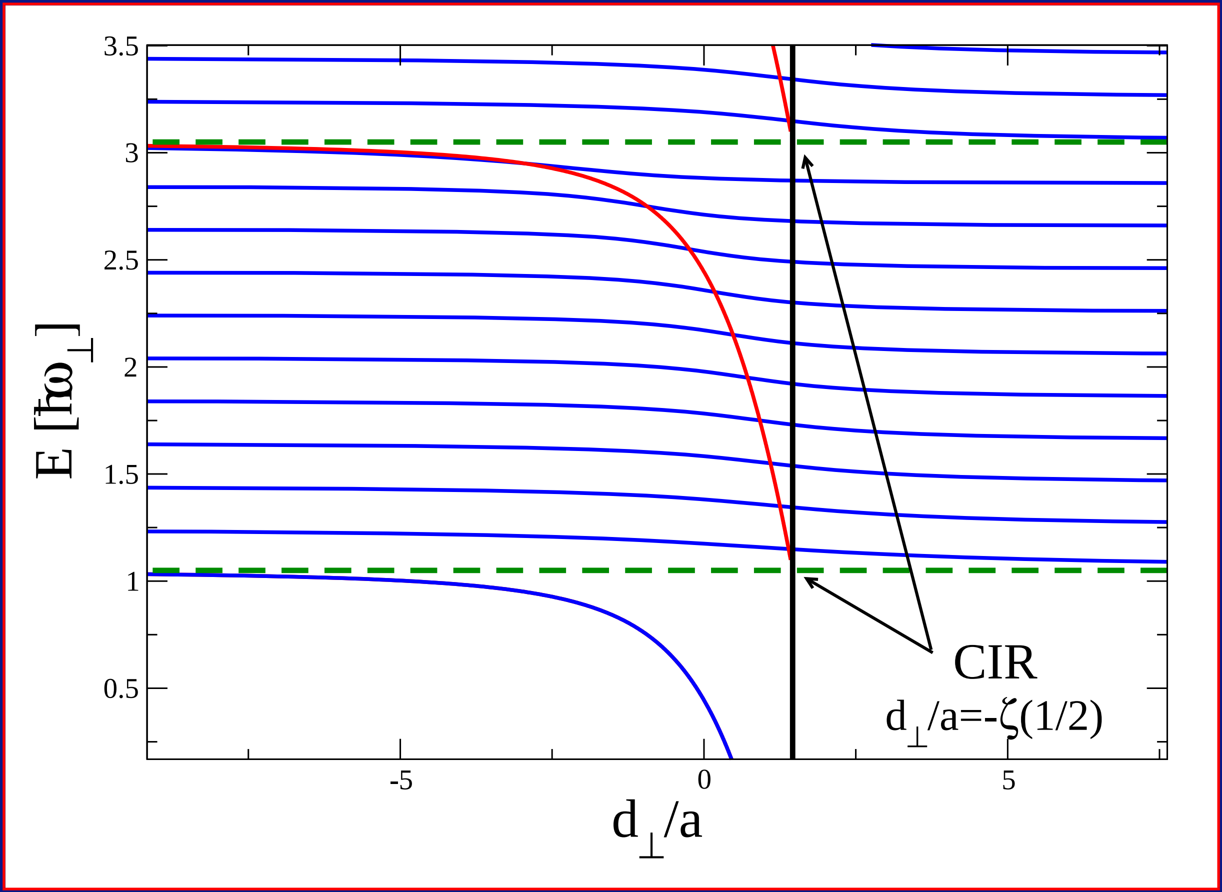
**Universal resonance:** $g_{1D} \to \infty$ for $\frac{d_\perp}{a} = -\zeta(\frac{1}{2}) \approx 1.46\ldots$

**Analogously: confinement-induced 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:

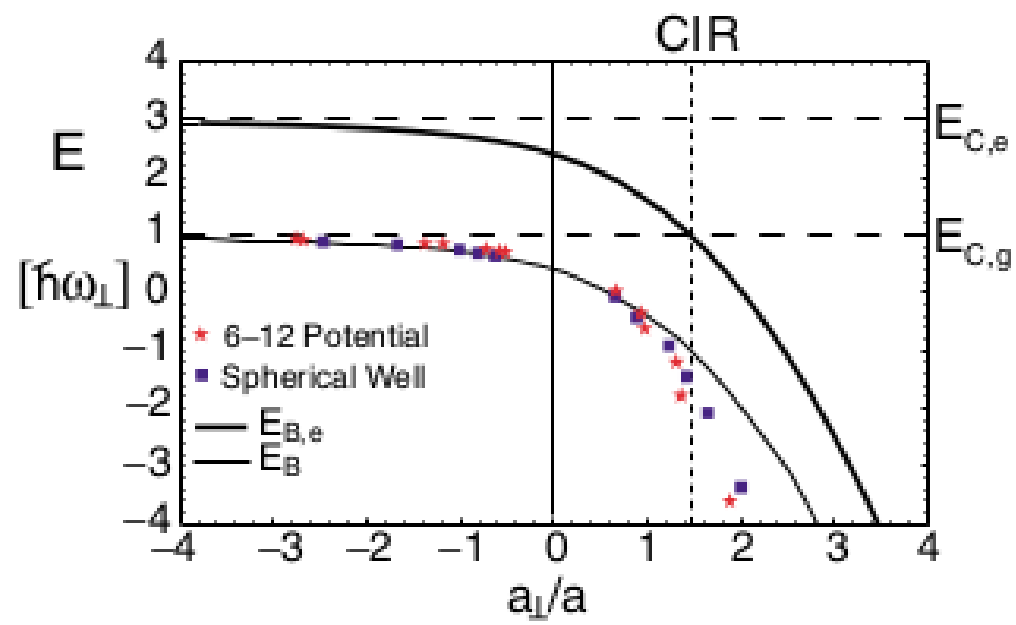



Blue: quasi 1D spectrum

Red: artificially(!) excited bound state

Green: quasi continuum threshold

# Olshanii's model (II)



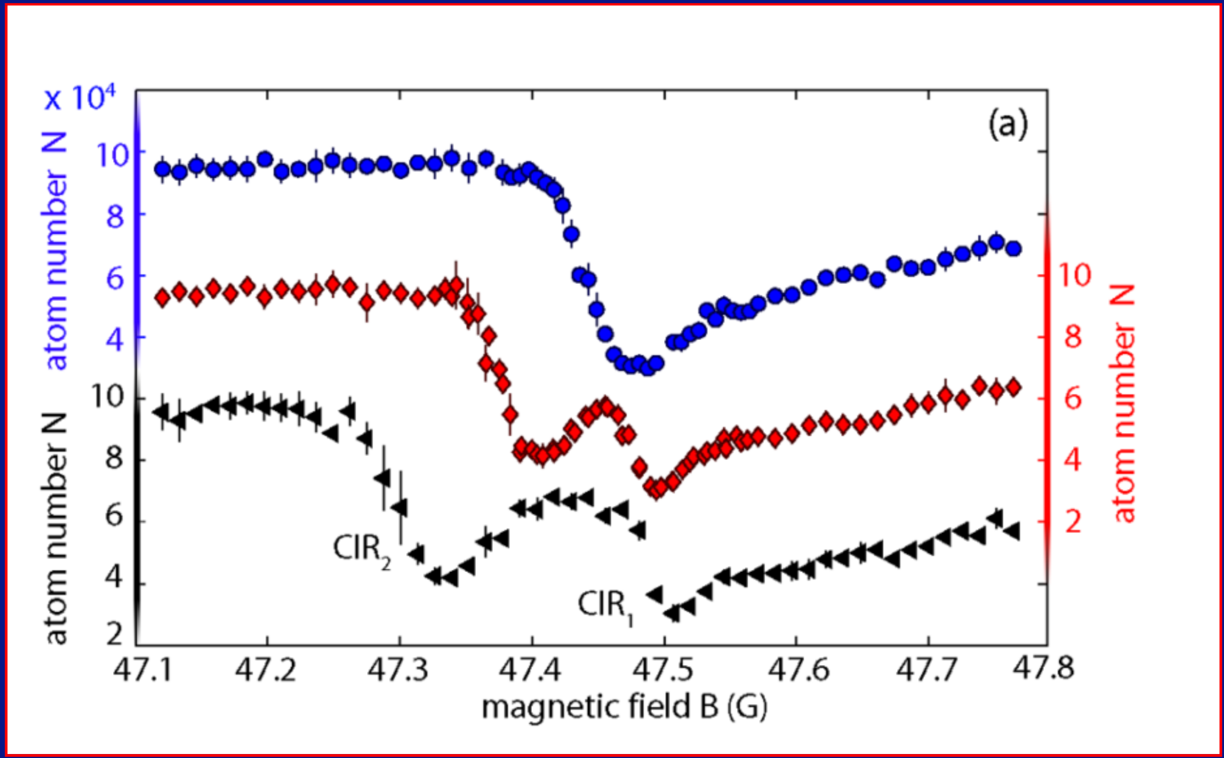

T. Bergeman et al., PRL **91**, 163201 (2003)

**Result:**

Confinement-induced resonances (CIR) are not an artefact of the $\delta$ potential.

**Note:** No data points on the artificially shifted curve!

# Innsbruck experiment (Cs atoms)

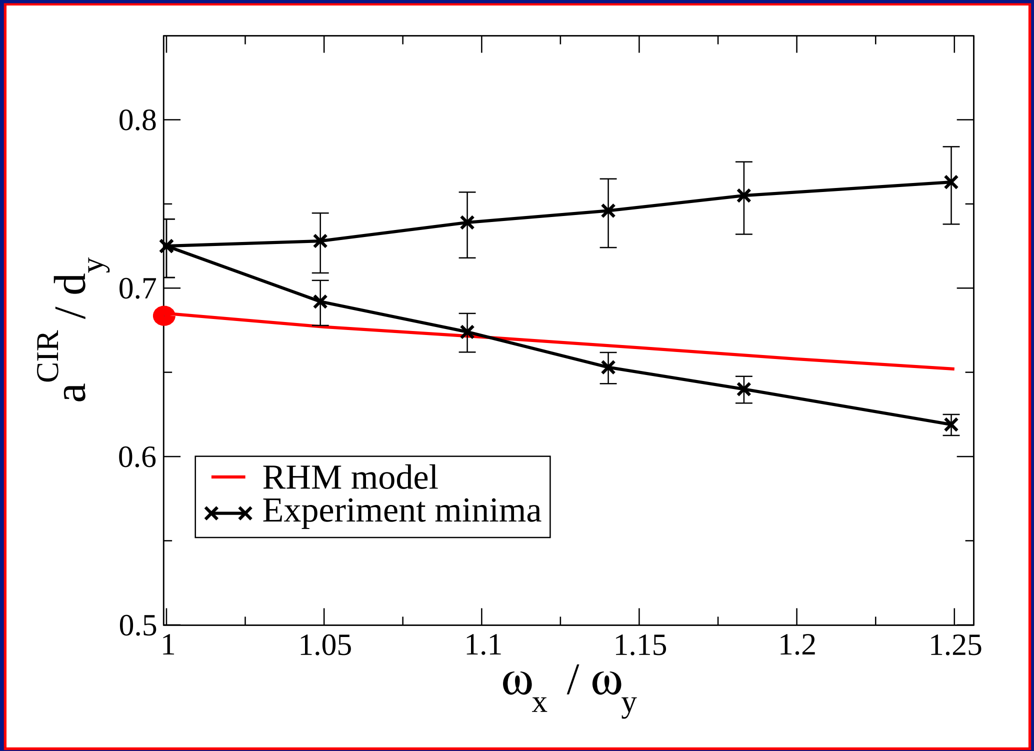



**Blue curve:** Atom losses for $\omega_x = \omega_y \gg \omega_z$ (anisotropy fixed, $a$ varied).

**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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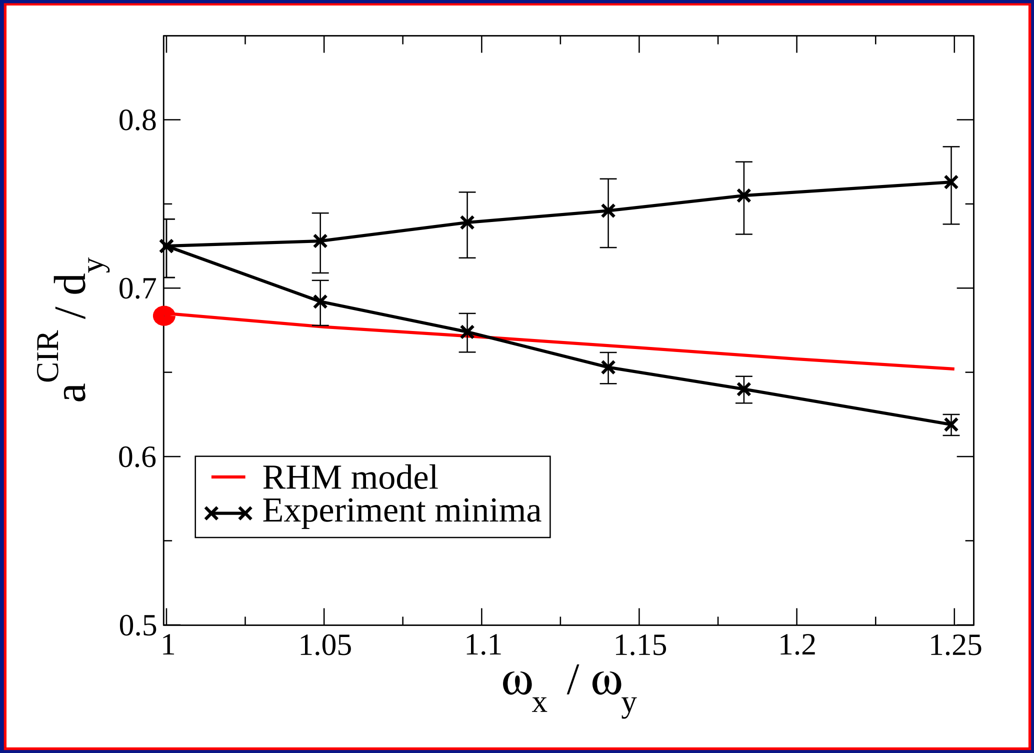


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⇒ Good agreement with Olshanii prediction for single anisotropy ($\omega_x = \omega_y$)

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

# Complete confusion:

## Innsbruck loss experiment (Haller et al.):

- **Position of 1D CIR agrees** with Olshanii prediction for $\omega_x = \omega_y$.

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- **Quasi-2D:** No losses at the "correct" value of $a$.

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- **Position of 1D CIR agrees** with Olshanii prediction for $\omega_x = \omega_y$.
- **Splitting of 1D CIR** for $\omega_x \neq \omega_y$ seems trivial, but **conflicts** with Olshanii theory.
- **Quasi-2D:** CIR appears for $a$ with **"wrong"** sign compared to Petrov, Holzmann, Shlyapnikov prediction.
- **Quasi-2D:** No losses at the "correct" value of $a$.

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

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

# 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 $a_{\mathrm{sc}}$),
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## However, coupling of center-of-mass (COM) and relative (REL) motion

- for the (correct) $\sin^2$ potential of an optical lattice,
- in fact for any **realistic** trap potential,
- even in harmonic traps, if the two atoms experience different trap potentials
  - ⋆ heteronuclear atom pairs or
  - ⋆ atoms in different electronic states (if polarisability differs).

# Our 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 (orthorhombic) 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 orthorhombic lattice symmetry (and possible indistinguishability of atoms).

# Our theoretical approach (extensions)

- Inclusion of **time-dependent external potential** (fully non-perturbative), so far: additional linear or harmonic potential (extension straightforward).
  [P.I. Schneider, S. Grishkevich, A.S., *Phys. Rev. A* **87**, 053413 (2013).]

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- Generalization to **arbitrary polynomial trapping potentials**.

  [F. Revuelta, S. Onyango, B. Schulz, A.S., *in preparation*]

- **Off-set between the traps/lattices** of the two atoms, especially for atom-ion pairs.

  [S. Onyango, F. Revuelta, A.S., *in preparation*]

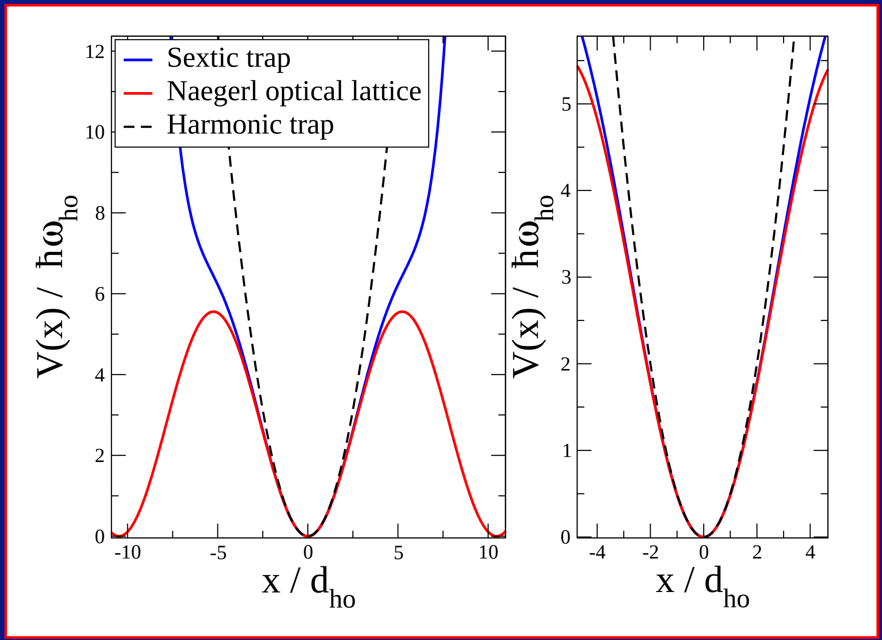
# Full treatment of two atoms in quasi-1D trap:

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

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

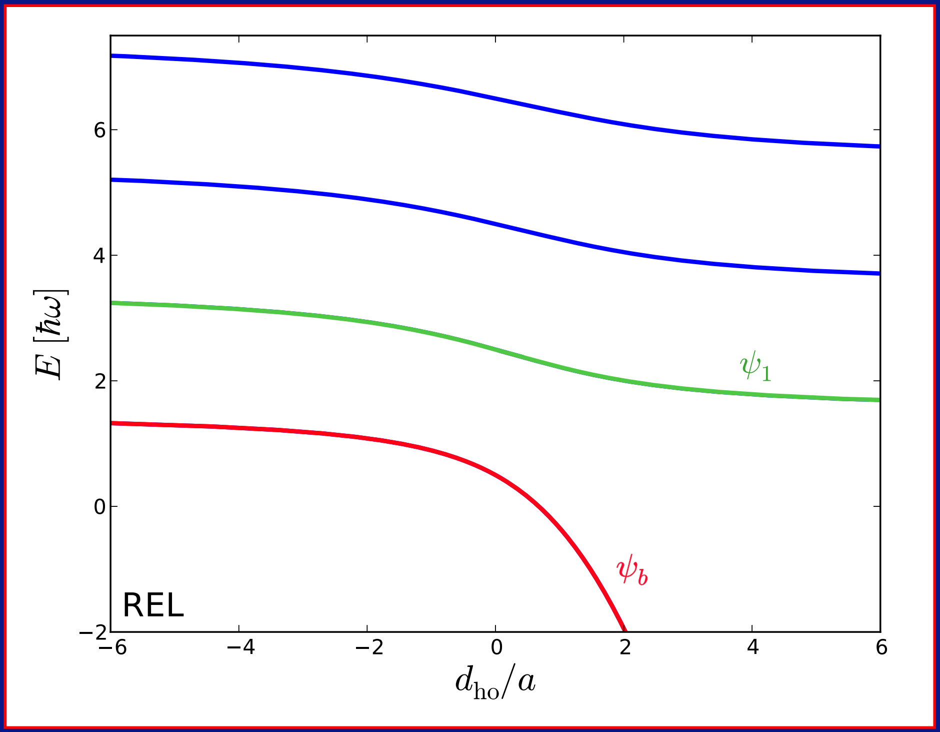
**Note:**

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

$\psi_b$: (molecular) bound state

$\psi_1$: lowest-lying trap state

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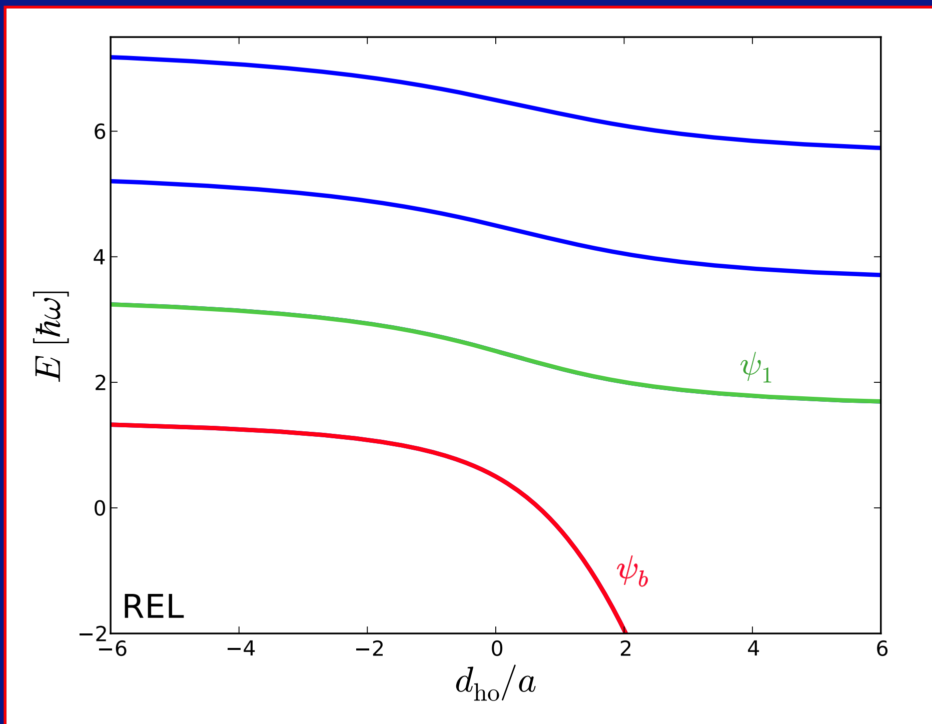
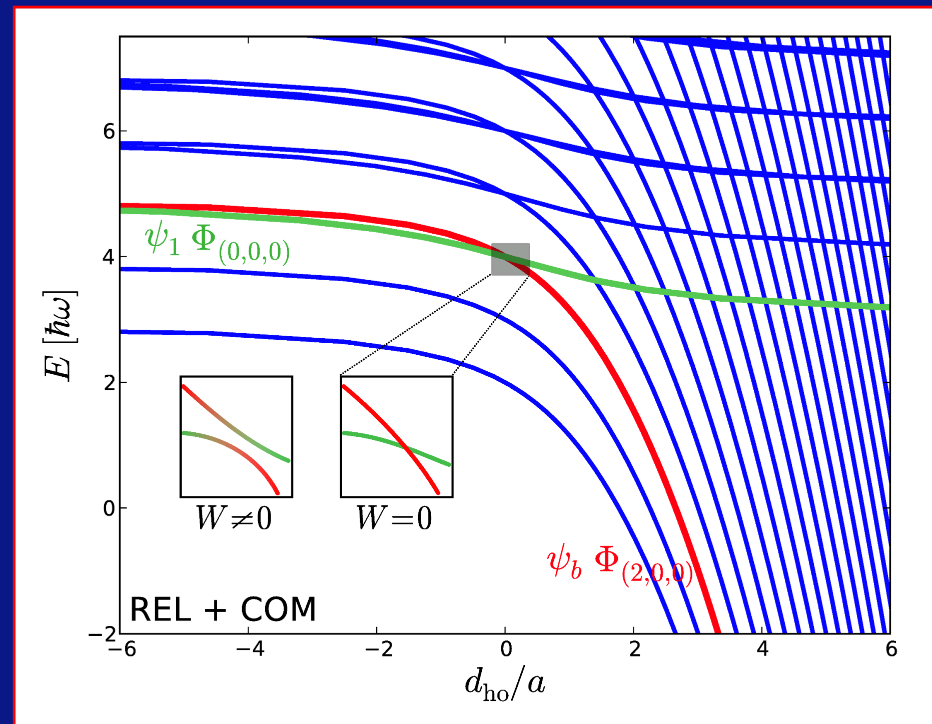



Relative motion only

$\psi_b$: (molecular) bound state

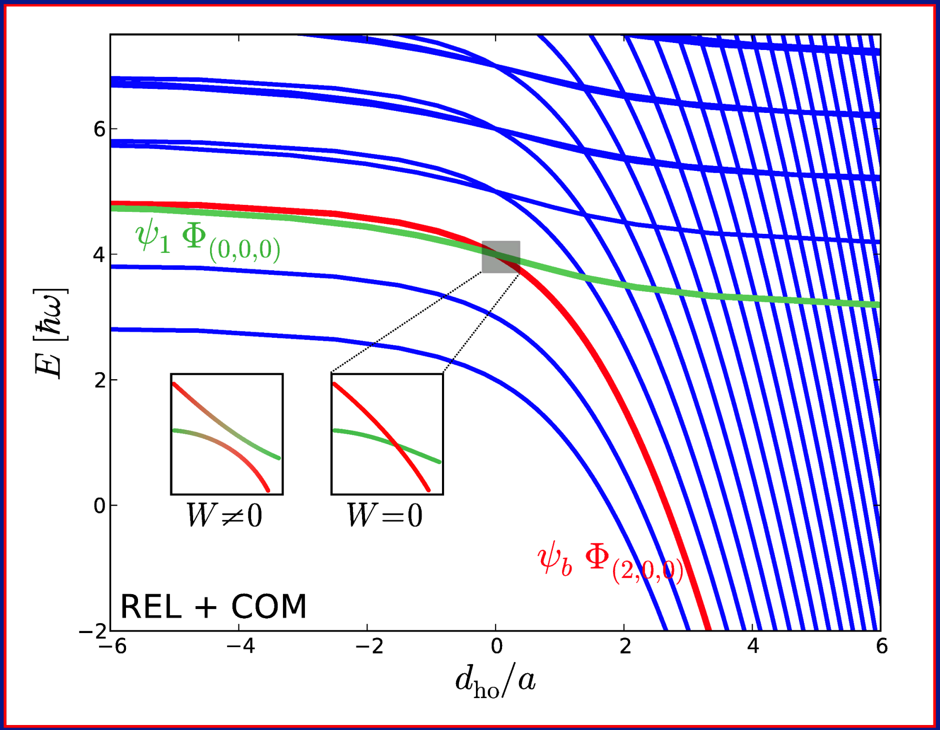
$\psi_1$: lowest-lying trap state

Full spectrum

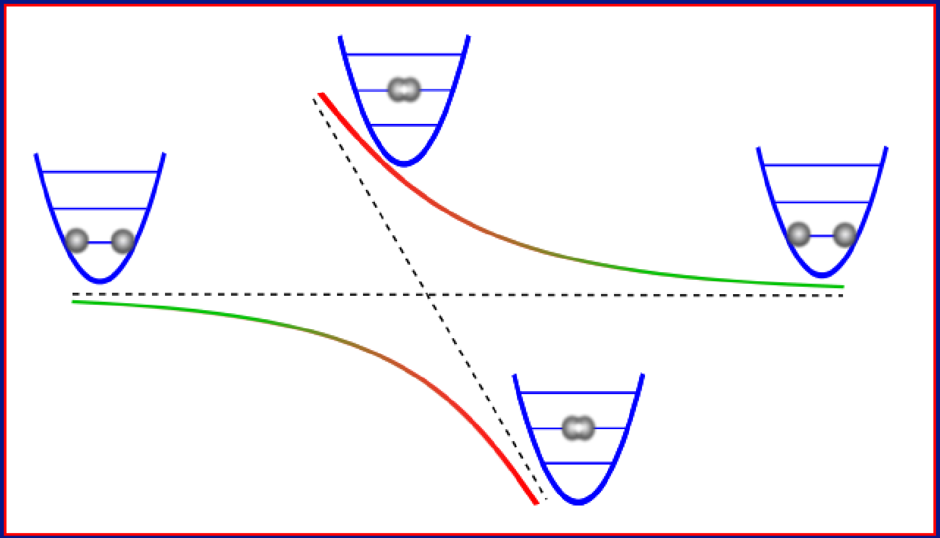
$\Phi_{(0,0,0)}$: ground com state

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

# Molecule formation due to confinement




Full spectrum



Avoided crossing

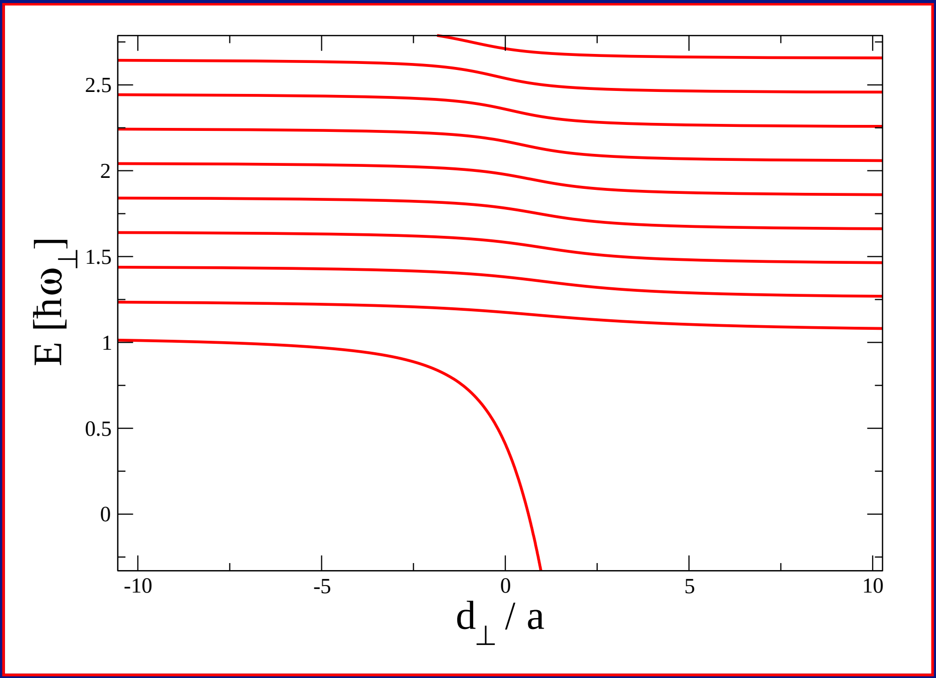
Coupling of center-of-mass (com) and relative (rel) motion ($W \neq 0$):

$\longrightarrow$ avoided crossing

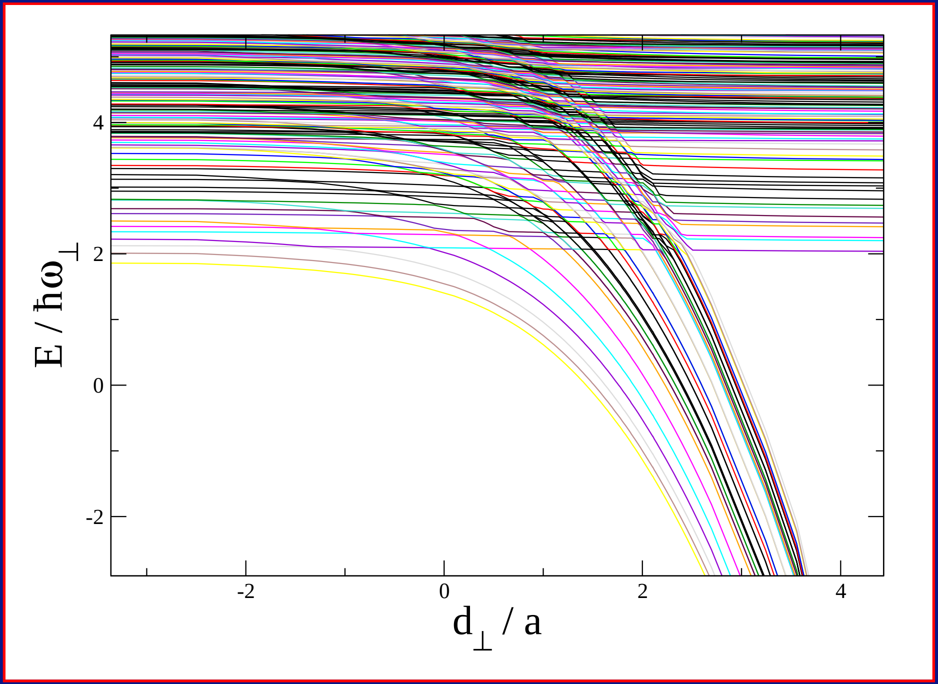
$\longrightarrow$ **molecule formation possible!**

# Energy spectra (ab initio results)

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




REL

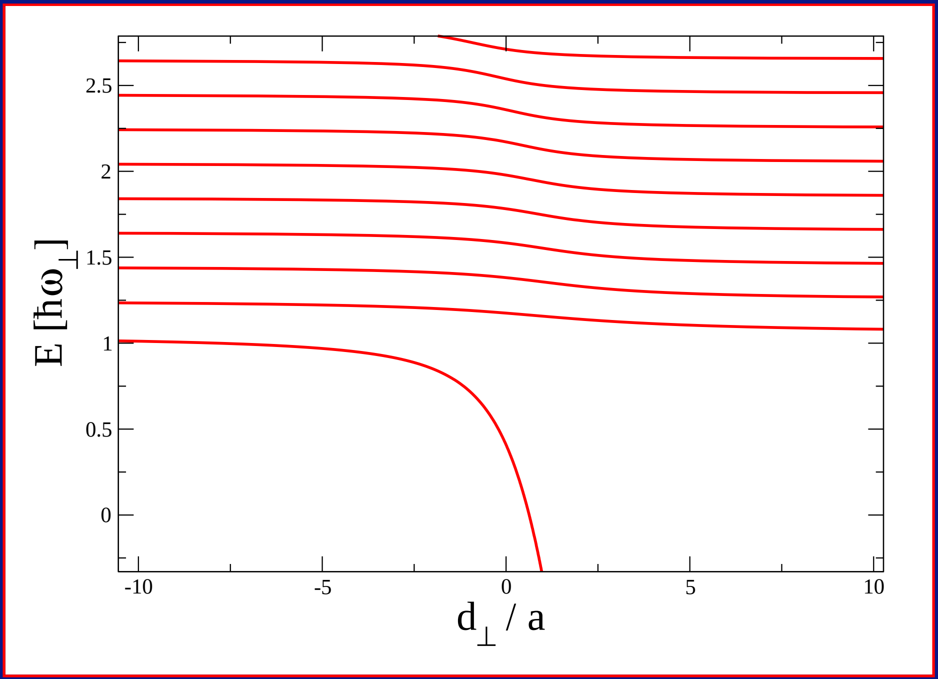



REL + COM + COUPLING

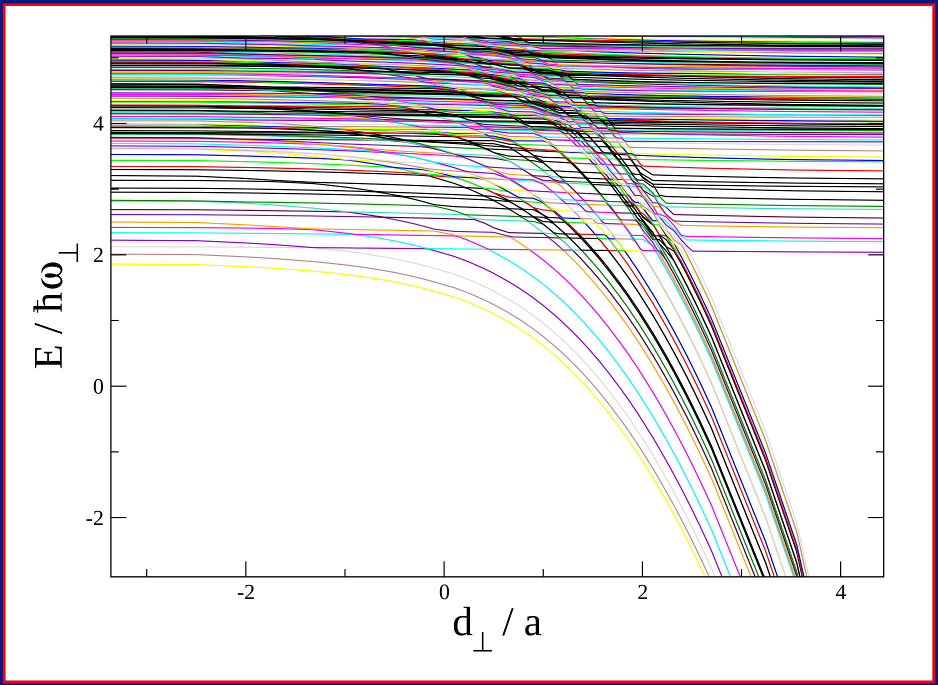
Many crossings are found in the coupled model,

# 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,

**but which of them lead to resonances?**

# Approximate selection rules

## Coupling matrix element:

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

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

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

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

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

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

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

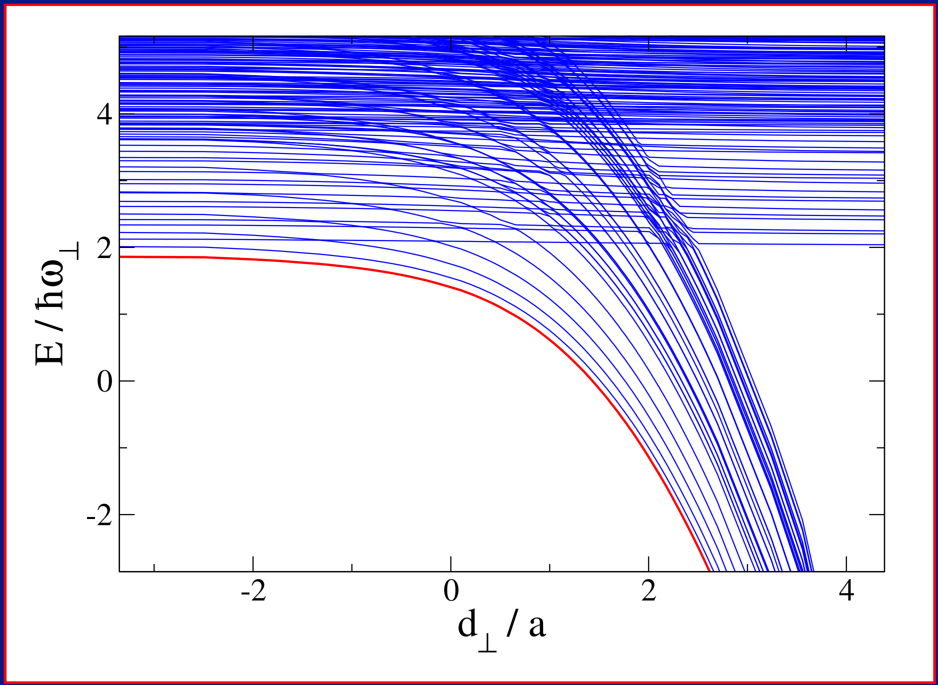
Ultracold: only ground trap state populated $\Longrightarrow m = k = 0$.

Resonances:

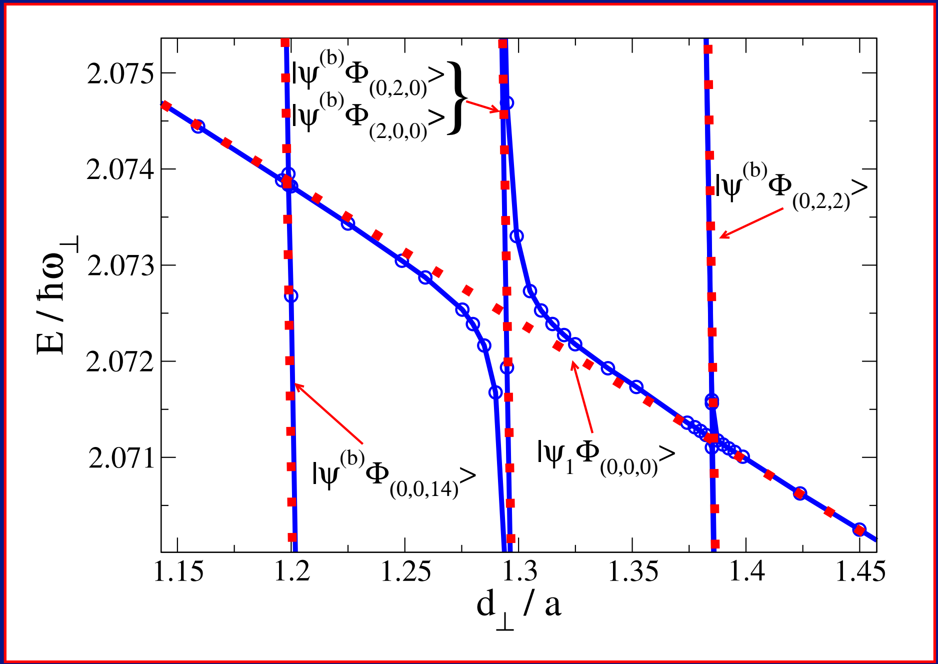
Crossing of transversally COM excited REL bound state with ground (COM and REL) trap state.

# Avoided Crossings (I)

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



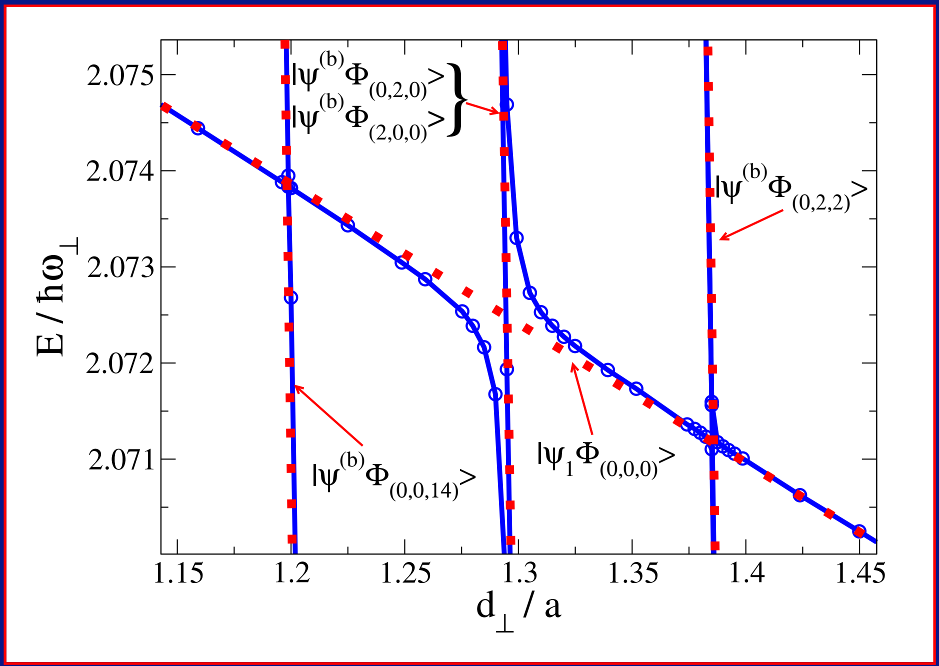

Large part of spectrum



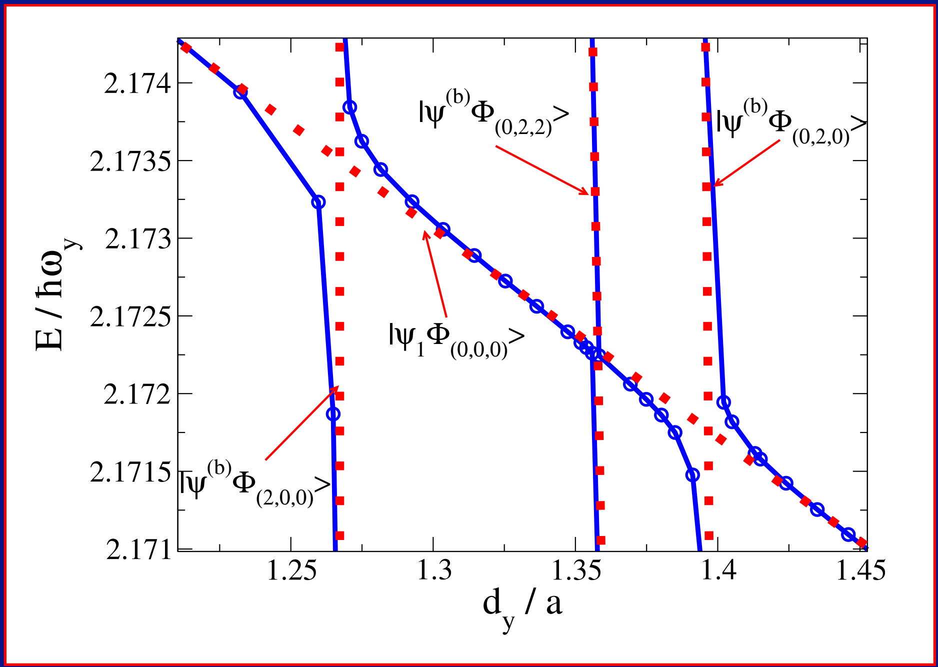

Zoom-in in spectrum.

# Avoided Crossings (II)

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




$\omega_x = \omega_y \gg \omega_z$



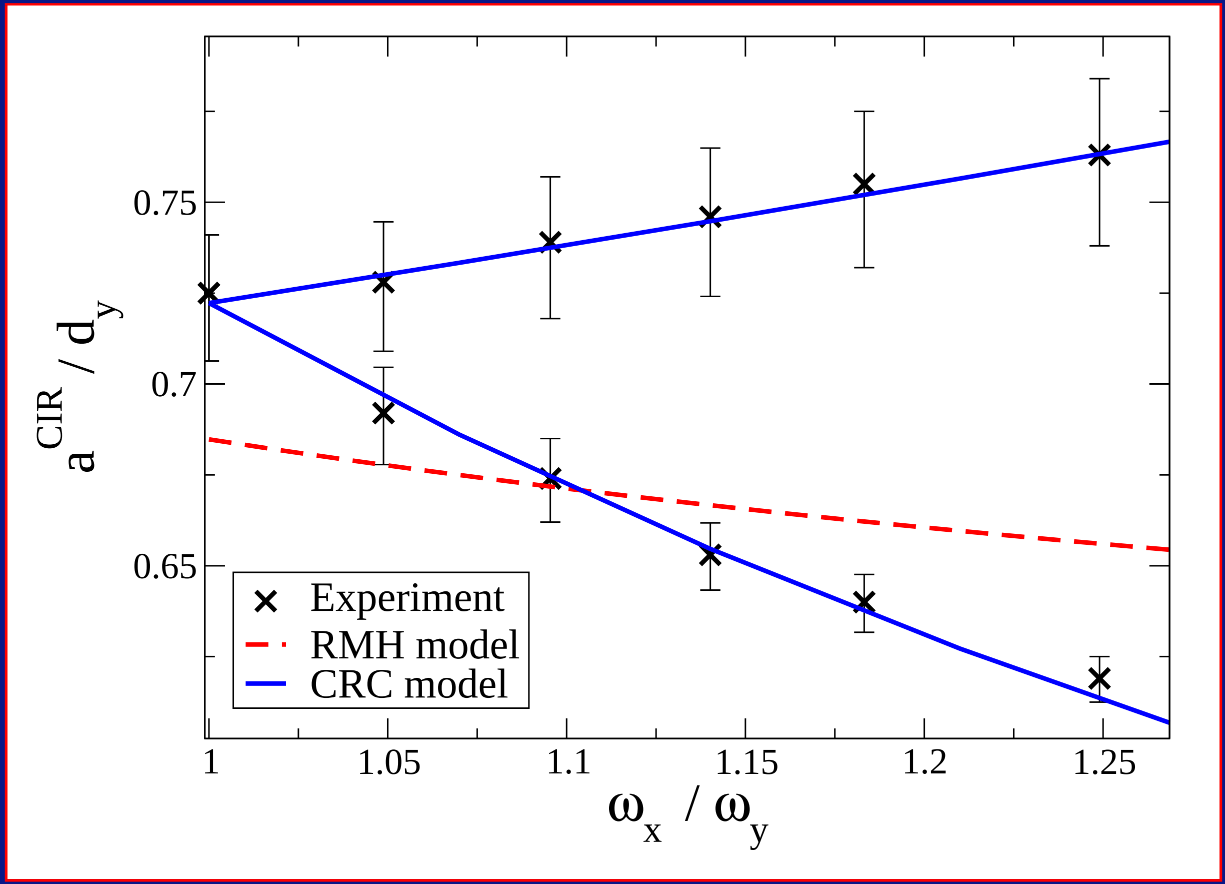

$\omega_x \neq \omega_y \gg \omega_z$

$\Rightarrow$ 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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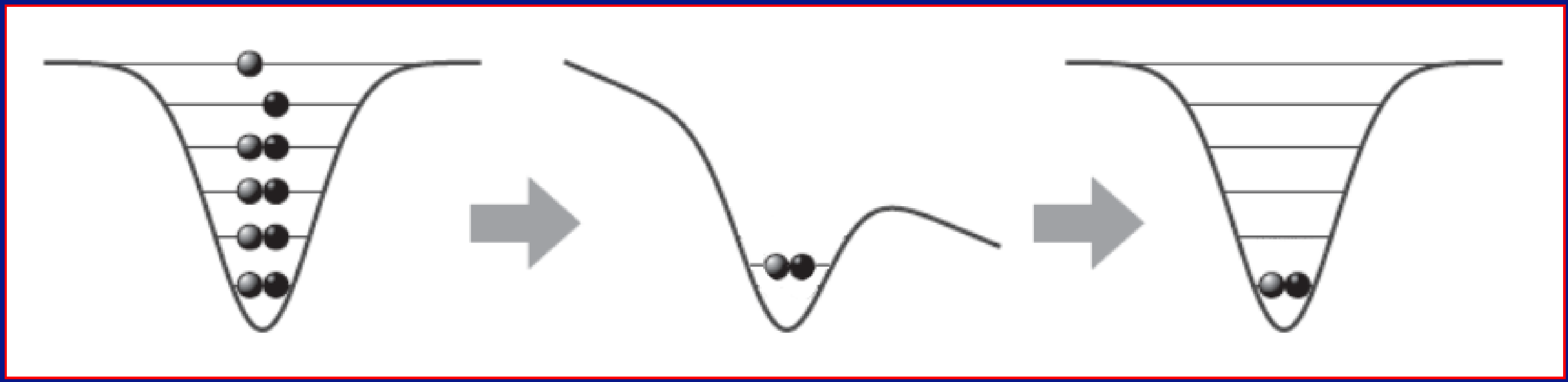
**However, are the losses in the Innsbruck experiment really due to molecule formation?**

# Experimental validation (with group of S. Jochim)

Exclusion of many-body and multi-channel effects:

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

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



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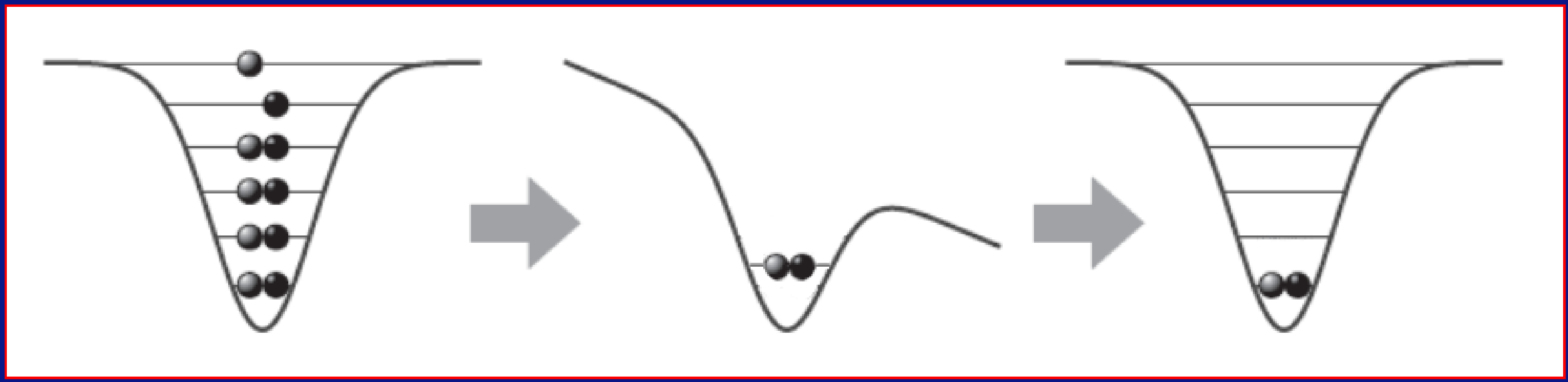

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Interaction energy shifts two-atom ground state ⇒ modified **atomic** tunnel rate.

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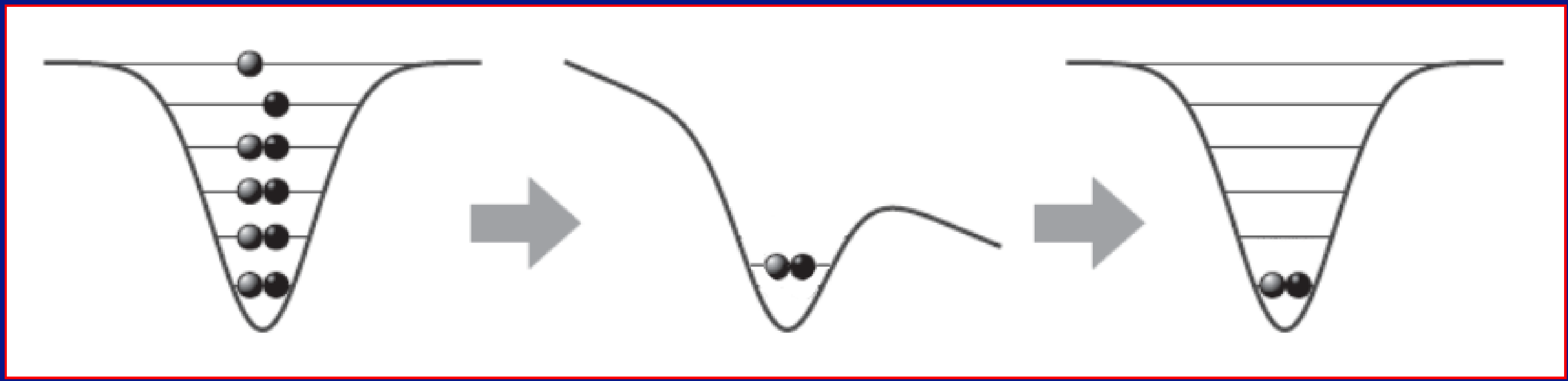

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Interaction energy shifts two-atom ground state ⇒ modified **atomic** tunnel rate.

**2. Detection of molecules created by inelastic CIRs:** measurement of tunneling atoms at $B$ field where bound molecules do not tunnel (doubled mass).

[Sala, Zürn, Lompe, Wenz, Murmann, Serwane, Jochim, A.S., *PRL* **110**, 203202 (2013).]

# Universality of confinement-induced resonances:

## 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.

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**Ion-atom pairs:** [S. Onyango, F. Revuelta, A.S., *in preparation*]

## 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.S., New J. Phys. **17**, 065002 (2015)]

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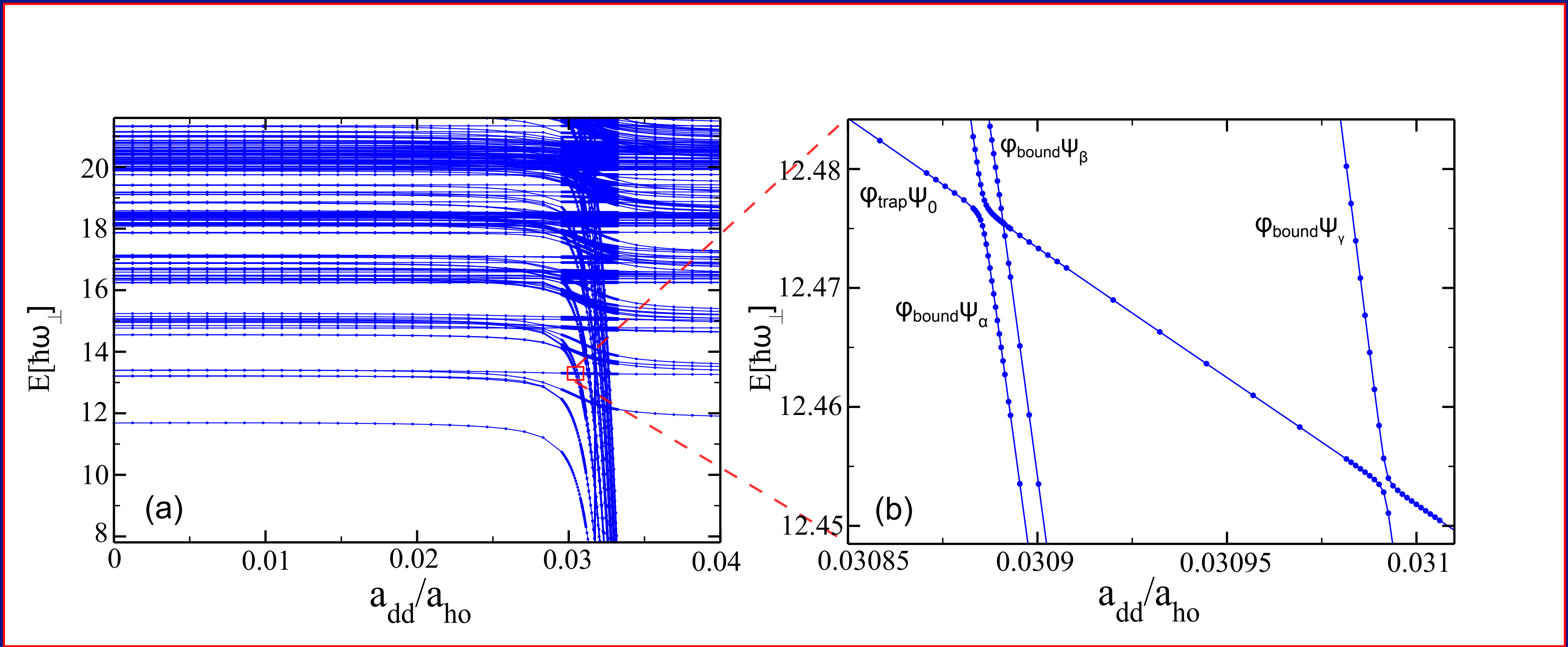
# Inelastic confinement-induced dipolar resonances (ICIDR)




**Note:** In this case, tuning is achieved via the dipolar interaction (external electric or magnetic fields).

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

[More resonances in dipolar gases and double-well potentials:
B. Schulz, A.S., *ChemPhysChem* **17**, 3747 (2016)]

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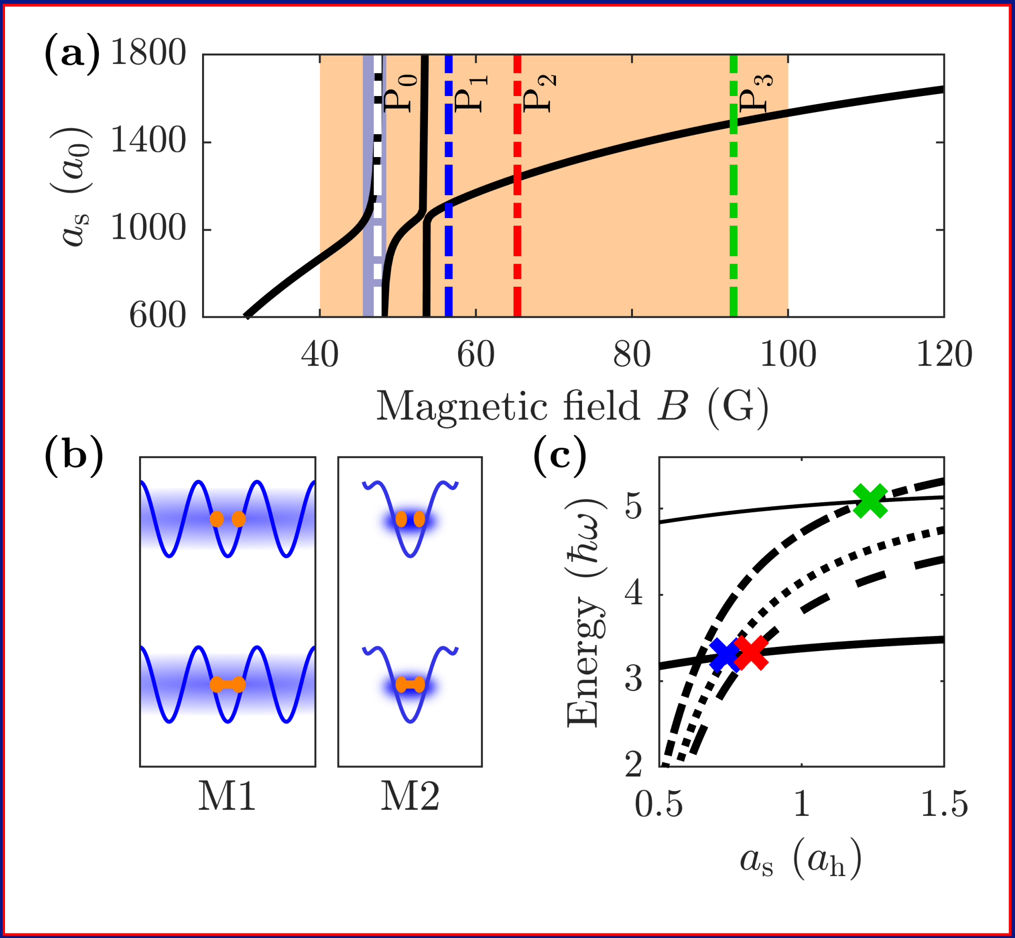
## Inlastic CIRs:

- caused by center-of-mass / relative-motion coupling
- allow for molecule (dimer) formation or break-up
- resonance position and strength can be tuned
- should occur in all dimensions, i. e. also under 3d (0d) confinement.

# Observation of ICIRs in 3d confinement




(a) Scattering length $a_s$ for Cs $(F = 3, m_f = 3)$ as a function of the magnetic field $B$.

The dashed lines labeled P0, P1, P2, and P3 mark the positions of the experimentally observed resonant features.

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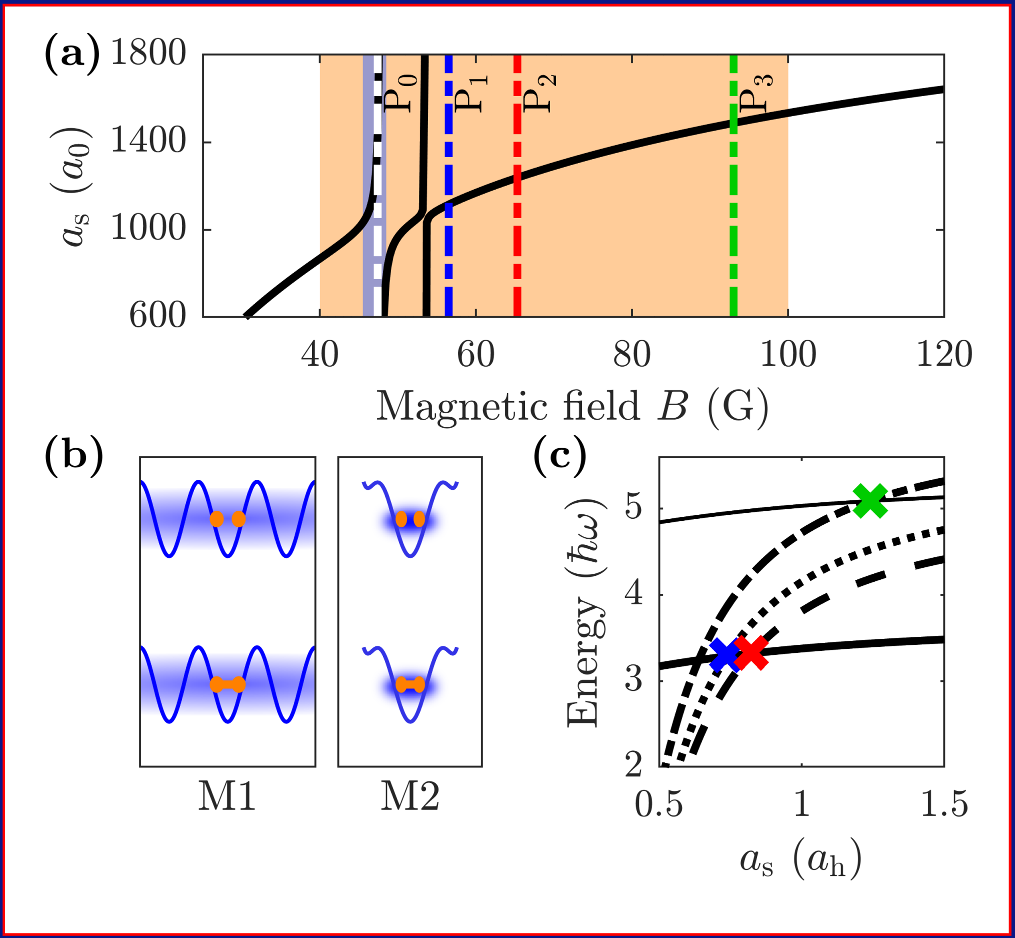
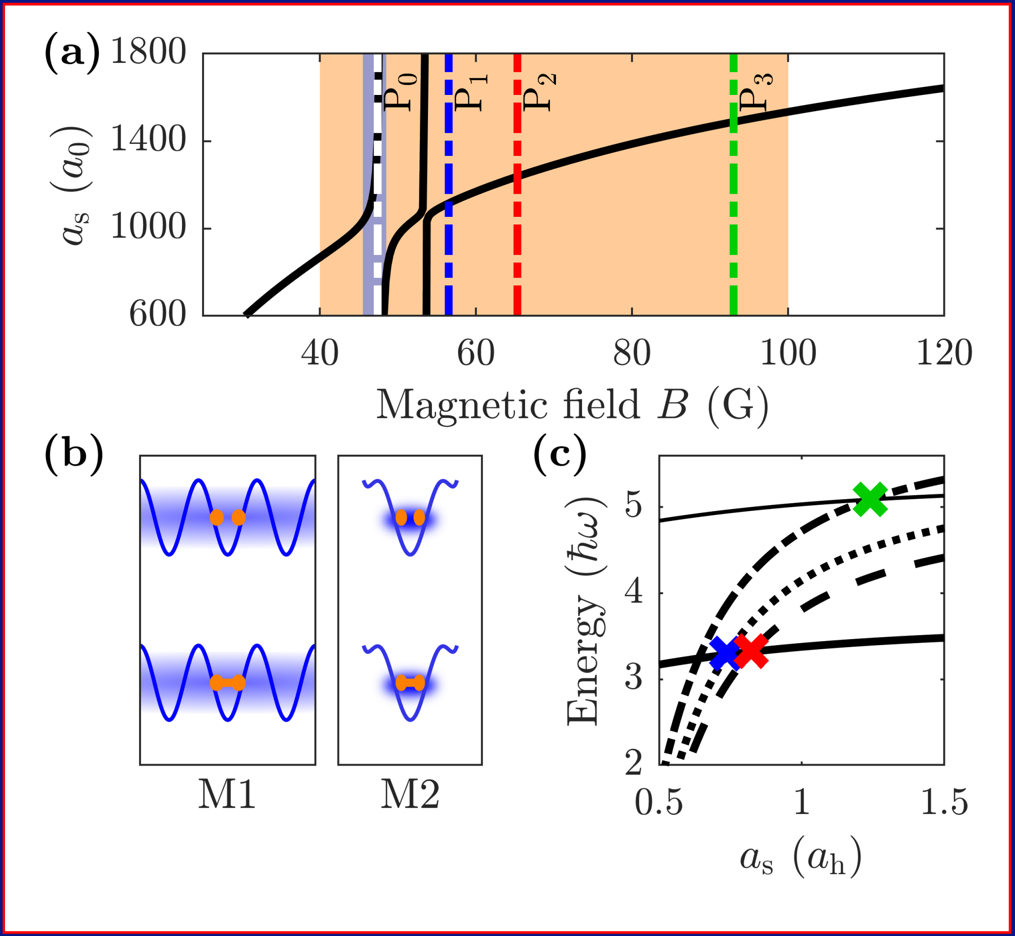



(b) Schematic representation of the states involved in the ICIRs: unbound trap state without COM exciation (upper) and bound (lower) states without COM excitation.

A lattice model M1 and a single-well (sextic) model M2 are used for theoretaical modeling of the experimental results.

# Observation of ICIRs in 3d confinement

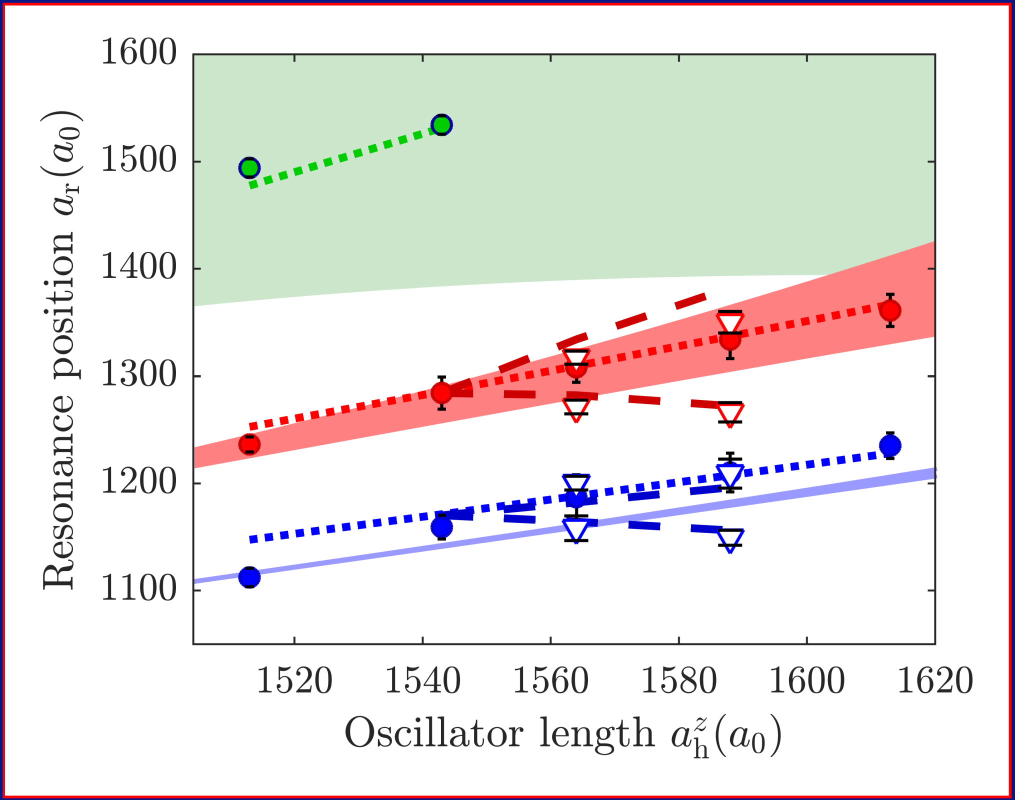



(c) Schematic energy diagram (for isotropic trap).

The thick and thin solid lines correspond to $\psi_t^{RM}\phi_{iso}^{CM}(0,0,0)$ and $\psi_t^{RM}\phi_{iso}^{CM}(2,0,0)$, respectively, whereas the dashed, dotted, and dashed-dotted curves represent $\psi_b^{RM}\phi_{iso}^{CM}(4,0,0)$, $\psi_b^{RM}\phi_{iso}^{CM}(2,2,0)$, and $\psi_b^{RM}\phi_{iso}^{CM}(6,0,0)$, respectively.

Intersections causing the ICIRs of the present work are indicated by crosses [color coding as in (a)].

# Resonance assignment




Resonance positions for $P_1$ (blue), $P_2$ (red), and $P_3$ (green) for the isotropic (circles) and the anisotropic (triangles) case.

For the isotropic case, $V_x = V_y = V_z$ was set to $20.0(3), 18.5(3), 17.5(3), 16.5(3)$, and $15.5(3)$ $E_R$ for the data from left to right.

For the anisotropic case, $V_x = V_y = 18.5(3)$ $E_R$ was chosen for $V_z = 17.5(3)$ $E_R$ (left triangles) and $16.5(3)$ $E_R$ (right triangles).

The results from M1 (only isotropic case) are shown as the blue, red, and green areas.

The predictions of M2 are plotted as dotted (dashed) lines for the isotropic (anisotropic) case.

[D. Capecchi *et al.* , arXiv2209.12504 (under review in *Phys. Rev. Lett.*]

# Lattice-induced resonances (delocalized ICIRs)

## Spin dynamics dominated by resonant tunneling into molecular states

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Optical lattices and Feshbach resonances are two of the most ubiquitously-used tools in atomic physics, allowing for the precise control, discrete confinement, and broad tunability of interacting atomic systems. Using a quantum simulator of lithium-7 atoms in an optical lattice, we investigate Heisenberg spin dynamics near a Feshbach resonance. We find novel resonance features in spin-spin interactions that can only be explained by lattice-induced resonances, which have never been observed before. We use these resonances to adiabatically convert atoms into molecules in excited bands. Lattice-induced resonances should be of general importance for studying strongly-interacting quantum many-body systems in optical lattices.

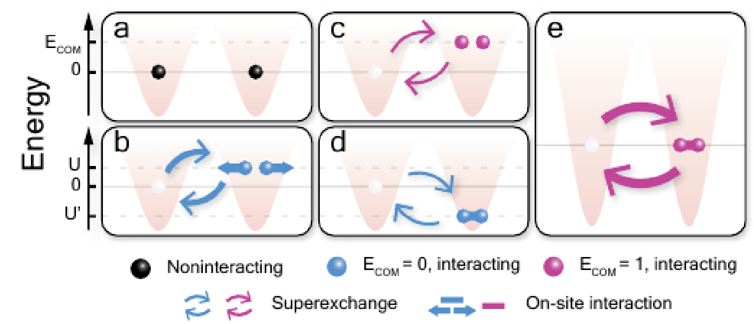


FIG. 1. **Resonant tunneling into molecular states**. An optical lattice in the Mott insulating regime with one atom per site (**a**) can host different virtual states, such as two atoms per site with repulsive interaction $U$ (**b**); two atoms in an excited c.m. mode (**c**); or a molecule with negative binding energy $U'$ (**d**). Both states **c** and **d** are typically far detuned from state **a**. However, positive c.m. energy (**c**) can be combined with negative binding energy (**d**), bringing a molecule in an excited c.m. mode into resonance with the Mott insulator (**e**). State **a** is connected to **e** via a resonant tunneling process. These are lattice-induced resonances, observed here for a quasi-1D lattice.

[arXiv:2208.06054, *Phys. Rev. Lett. (in print)*]

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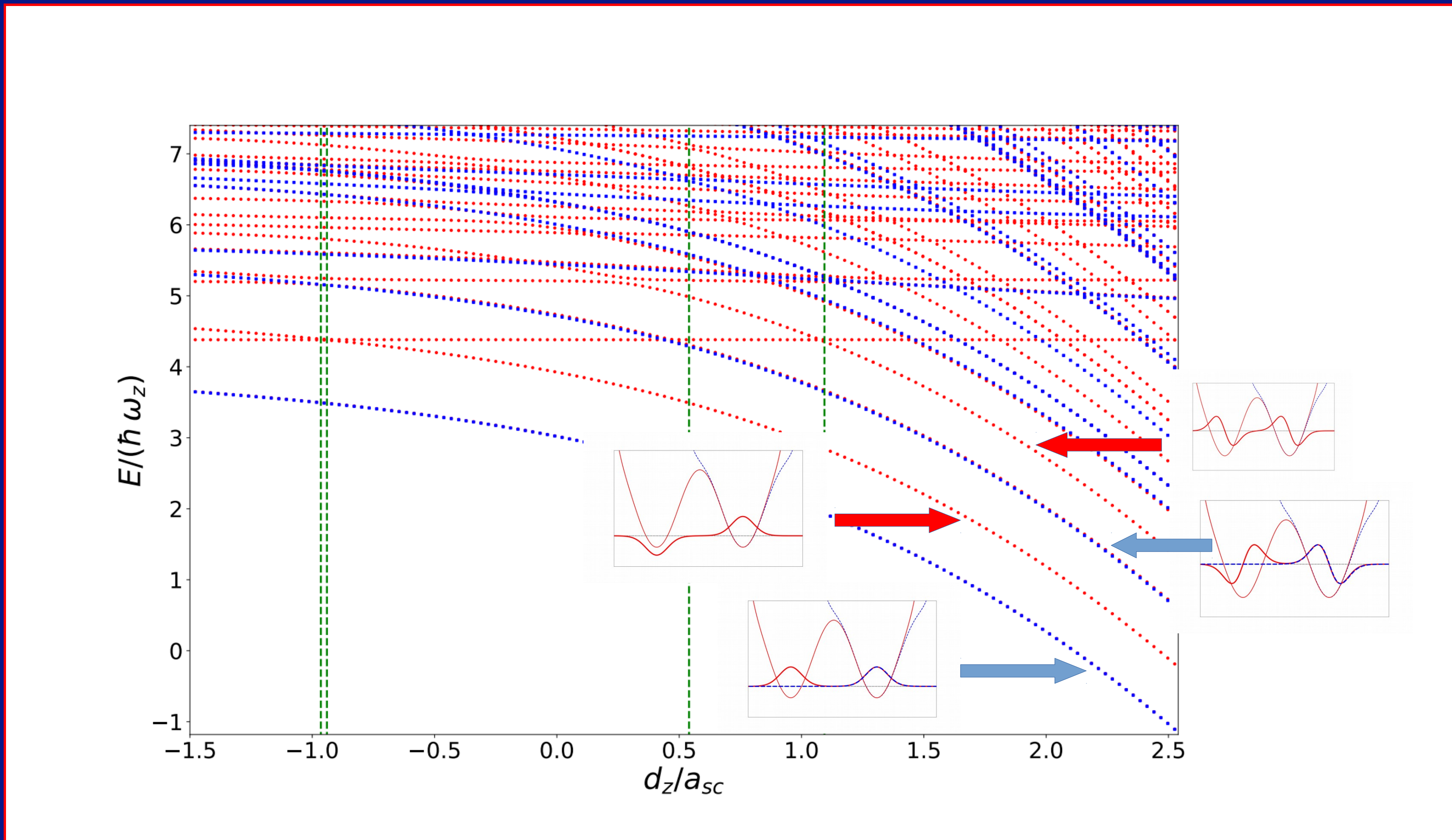


Our double-well simulation (and comparison to single-well results) agrees very well with the experimentally found resonance positions and confirms delocalized ICIRs.

[F. Revuelta, A.S., *in preparation*]

# Summary

- Ultracold quantum gases are in most cases trapped: the influence of the confinement (possibly reduced dimensionality, anharmonicity) is important.

- Resonances may be useful (modification of the interaction strength, molecule formation) or harmful (losses, unwanted effects overlaying the wanted ones).

- The microscopic few-body effects are not only relevant for few-body, but also for understanding many-body systems.

- If artificial confinement is adopted for computational convenience, the influence of the confinement needs to be understood.