FEW-BODY SYSTEMS UNDER EXTERNAL CONFINEMENT

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- Confinement-induced resonances: solution of the puzzle.
- **Outlook:** going beyond two particles.

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

- In many cases the wavefunction of a system consists of a complicated short-range and a "simple" long-range part.

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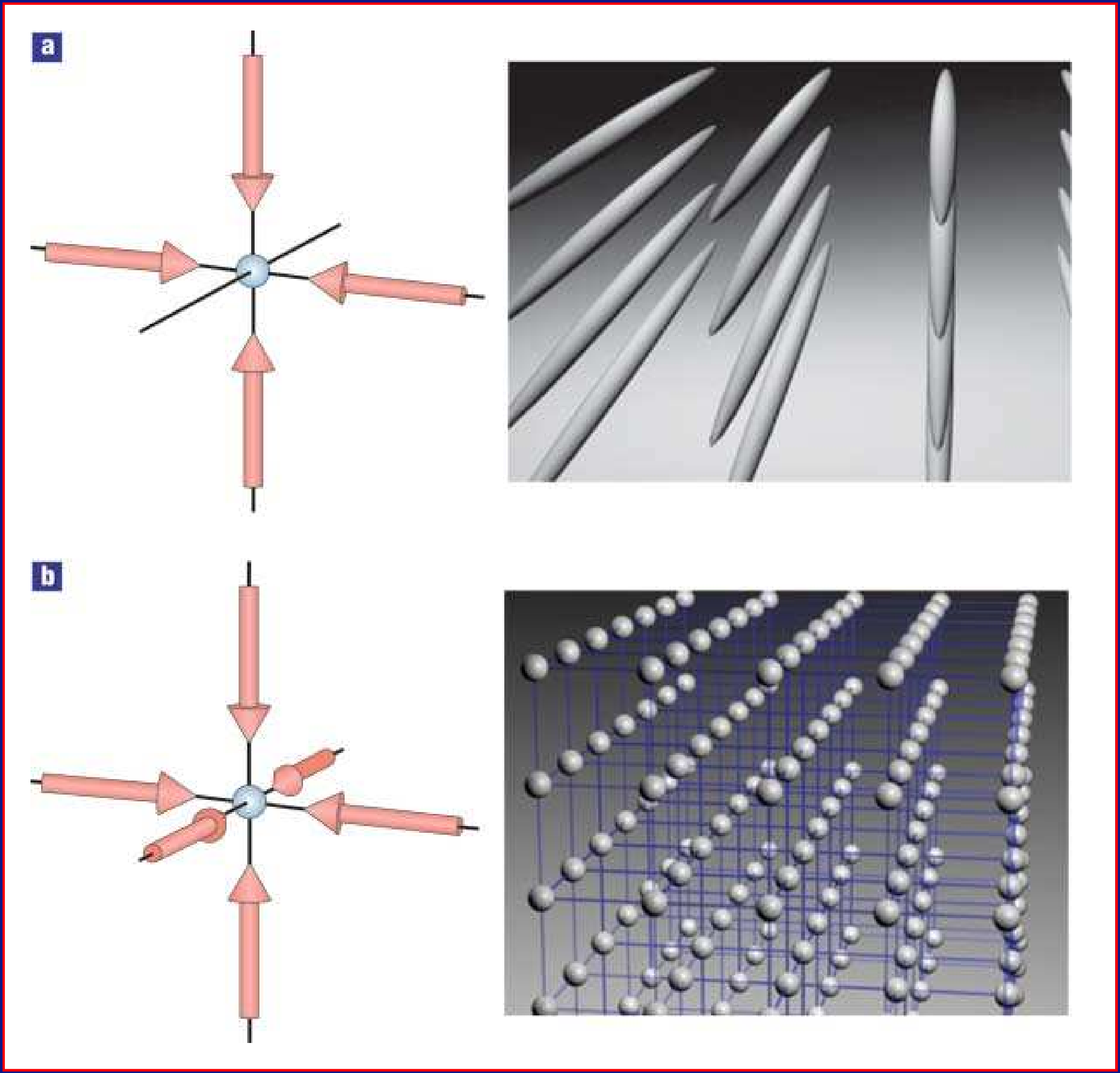
Note: V_{pseudo} is counterintuitive: long-range behaviour described by δ function!!!

Optical lattices: shaped (tight) confinement



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

Counterpropagating lasers:

$\longrightarrow$ standing light field.

Trap potential varies as

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

with

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

λ: laser wavelength.

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

with

laser intensity I and

atomic polarizability α.

External trap potential and interatomic interaction

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- This relation was derived for $k \to 0$ (limit of zero-collision energy).
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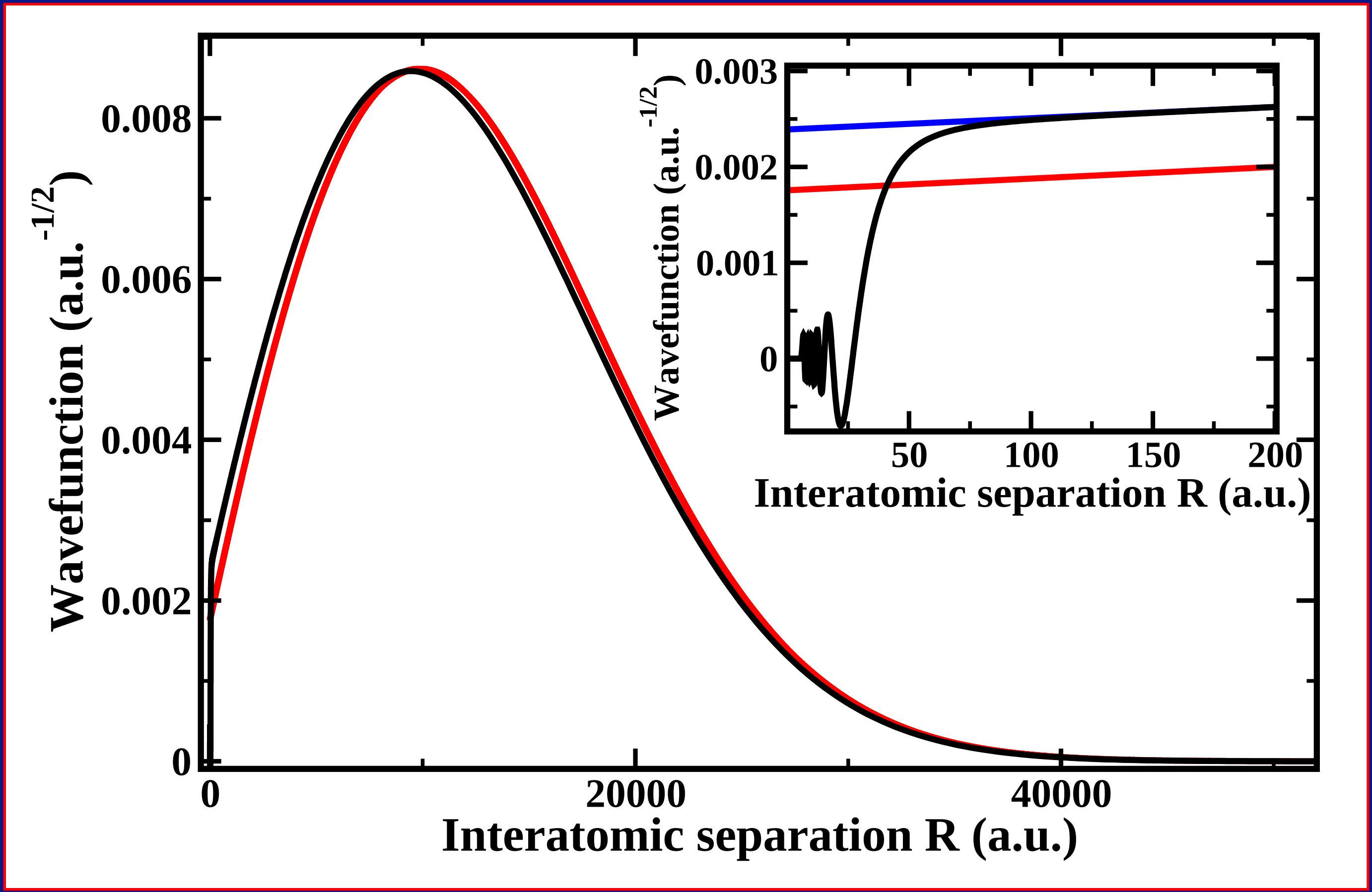
- As weaker the least bound state is bound, as closer the scales get to each other.

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 dependent (blue, $a_{\rm sc} = -2872\,a_0$) pseudopotential results.

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- Intercept of ψ on R axis does not agree with a_{sc}.
  Example ^{6}Li (state a $^3\Sigma_u$) in 10 kHz trap:
  Deviation for ψ small, intercept at -2023 for $a_{\mathrm{sc}} = -2030\,a_0$.
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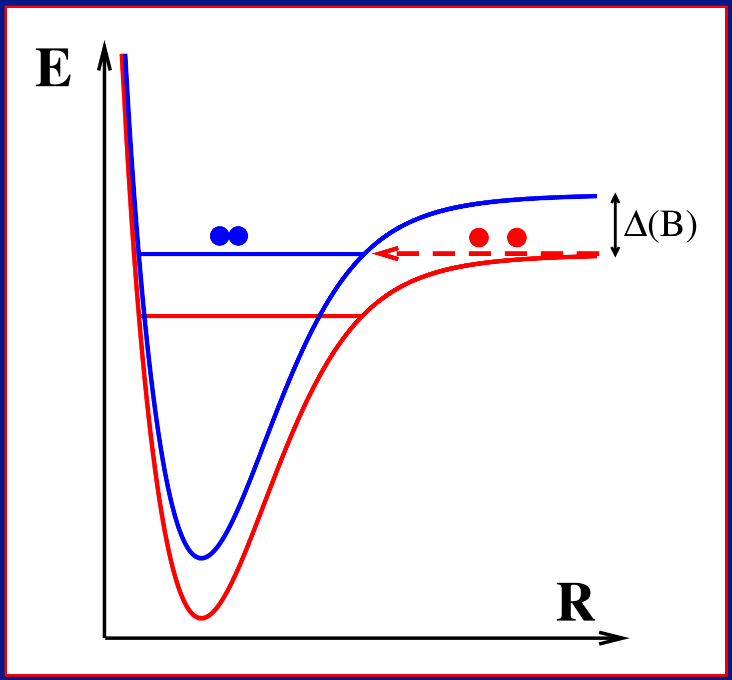
Note: In contrast to the physical $a_{\rm sc}$ the empirical parameter $a_{\rm sc}(E)$ follows only from the correct ψ obtained with $V_{\rm mol}(R)$!

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

Tunable interaction: magnetic Feshbach resonances



Simple picture:

Only **2 channels**:

– open (continuum) channel,

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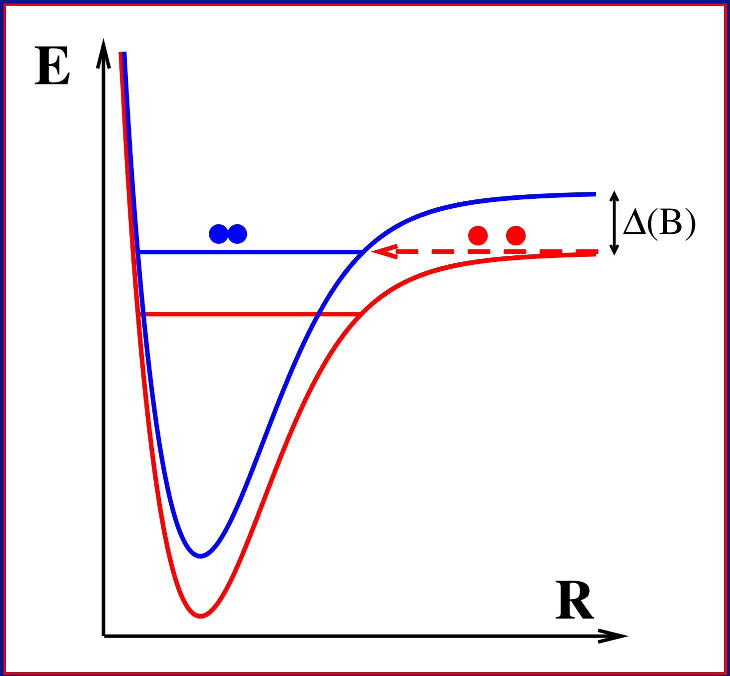

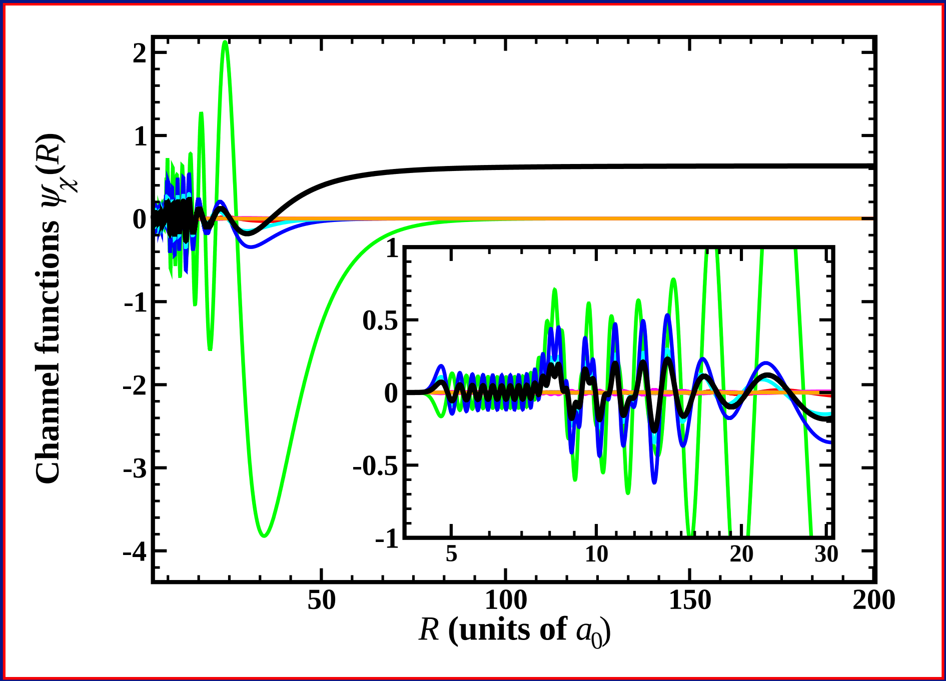

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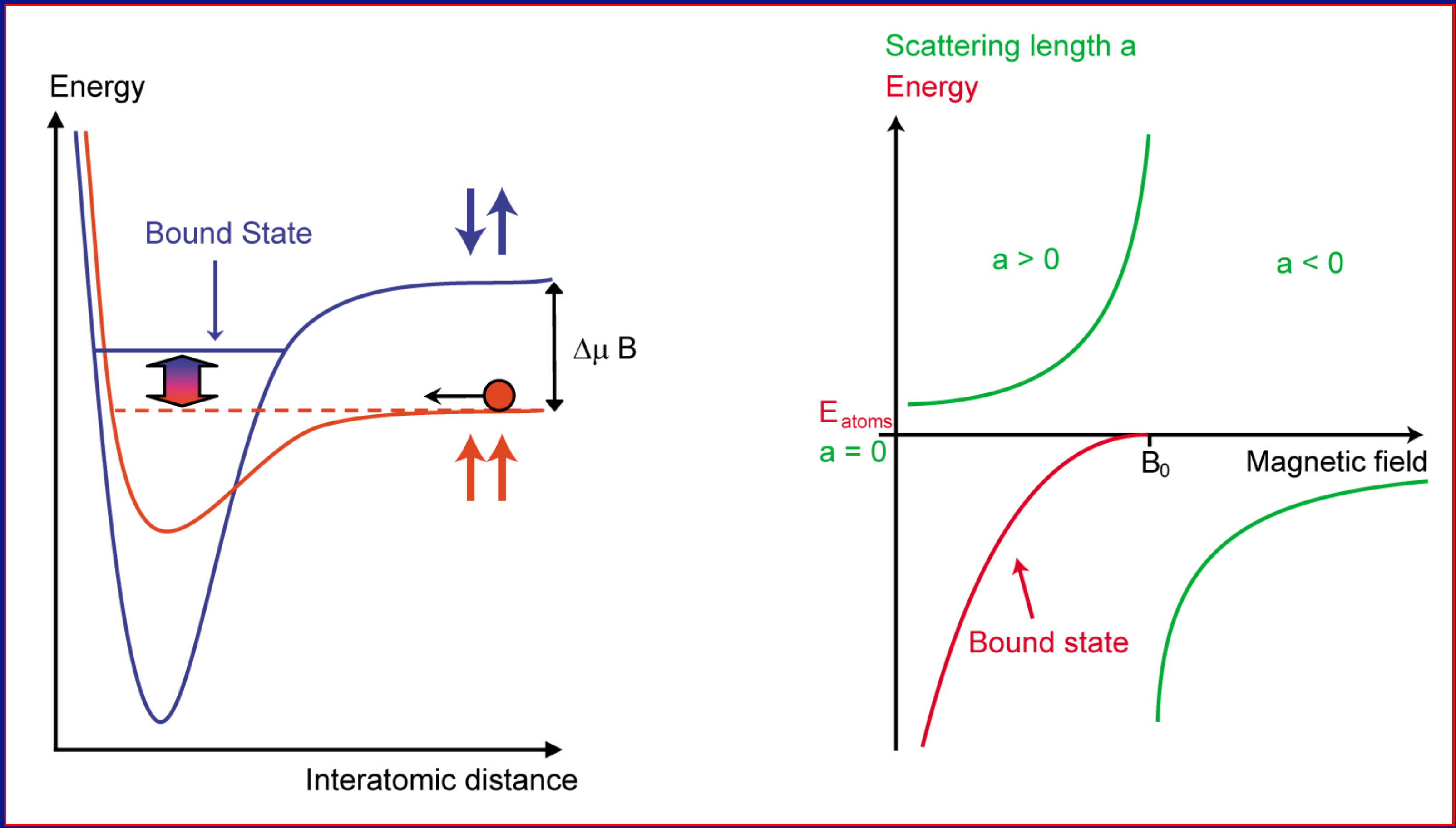
Multichannel reality:

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!**

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

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

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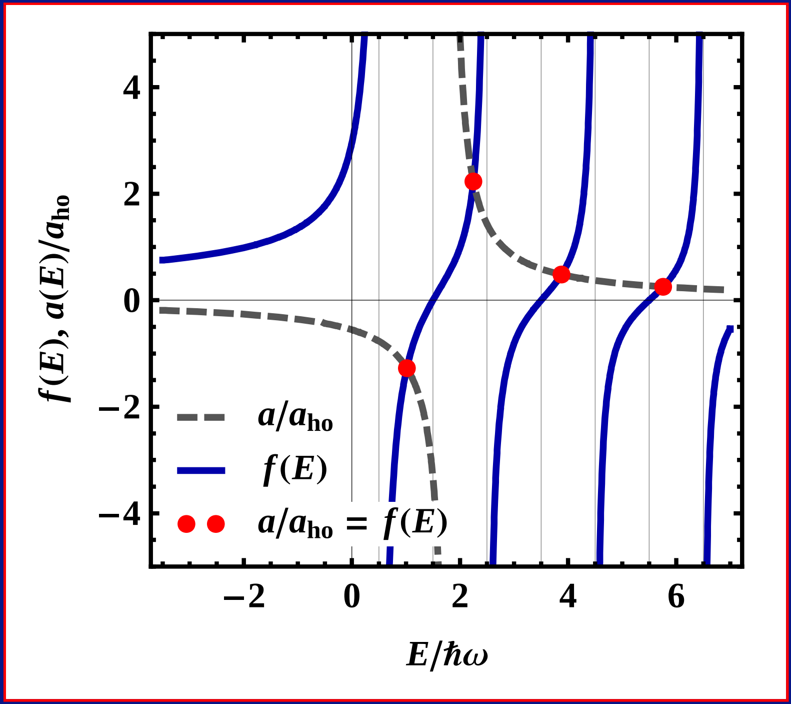

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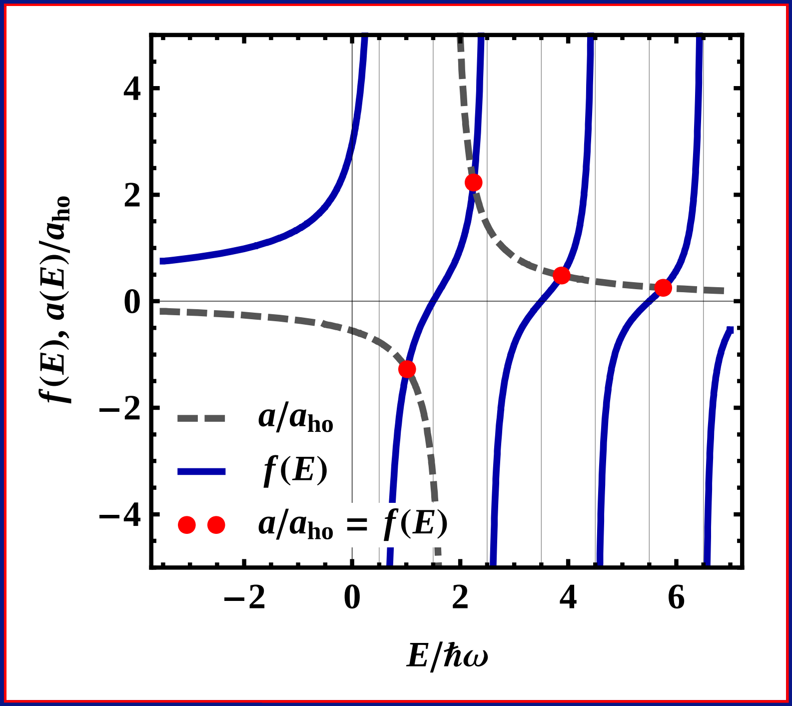

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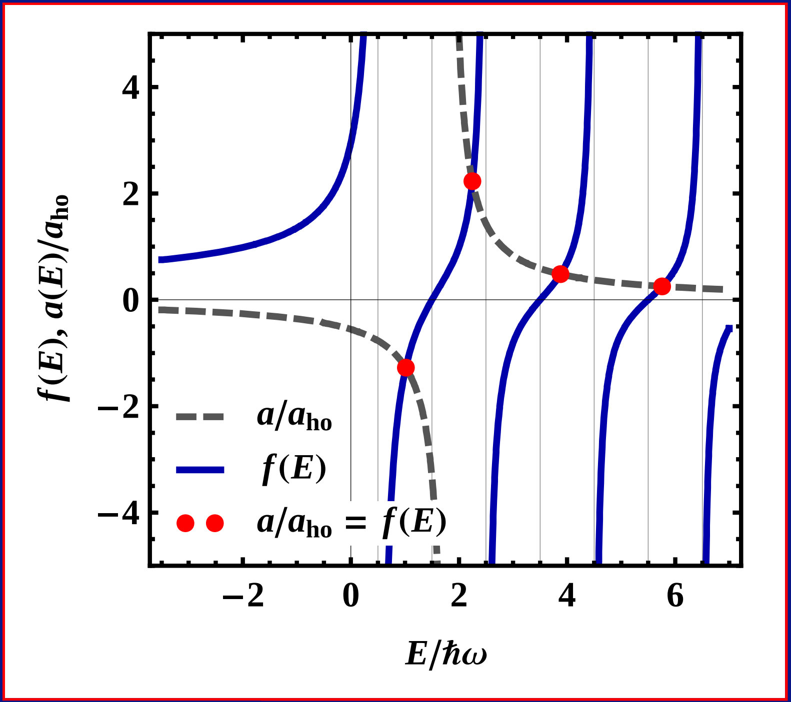
$$a(E,B) = a_{\mathrm{bg}} \left(1 - \frac{\Delta B}{B - B_0 + \delta B - E/\mu} \right)$$

3. derive the admixture of the closed channel

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



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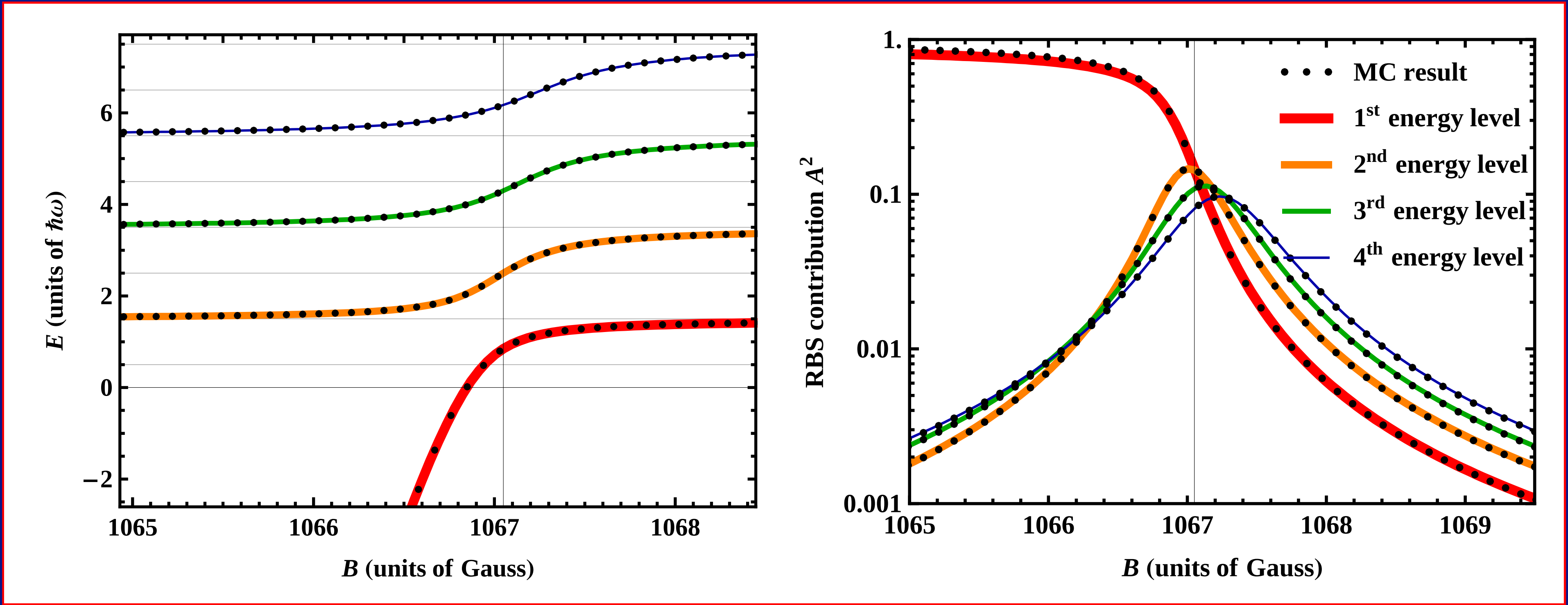
How good is the model?

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

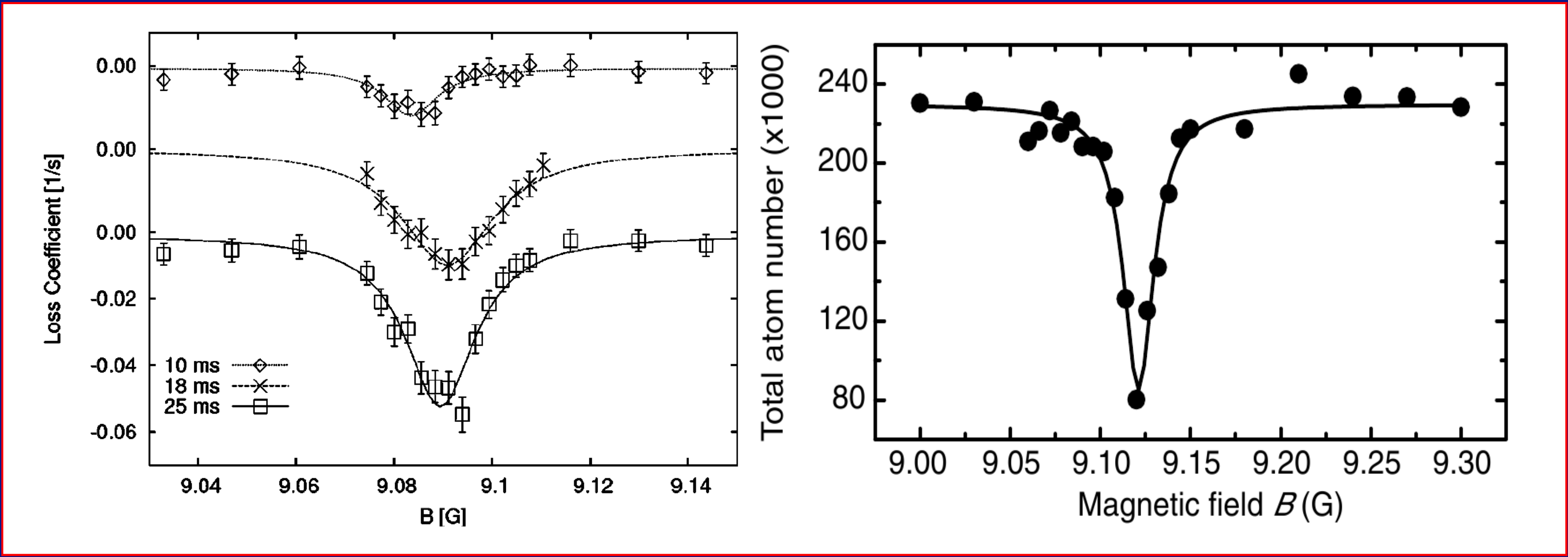


- **Energy deviation** $< 0.003\,\hbar\omega$.
- **Closed-channel admixture deviation** $< 0.1\%$.

[Schneider, Vanne, A.S., Phys. Rev. A **83**, 030701(R) (2011).]

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 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).

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 (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 lattice symmetry (and possible indistinguishability of atoms).

Present 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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- **Anisotropic dipole-dipole interparticle interaction** (field-aligned dipoles along one of the orthorhombic crystal axes).

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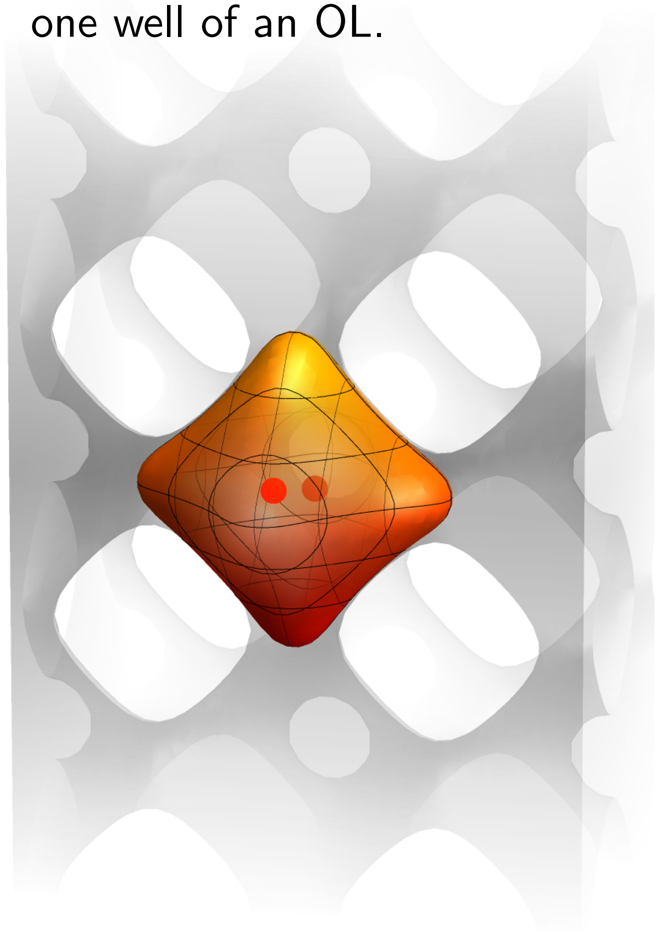
- **Off-set between the traps/lattices** of the two atoms, especially for atom-ion pairs.

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

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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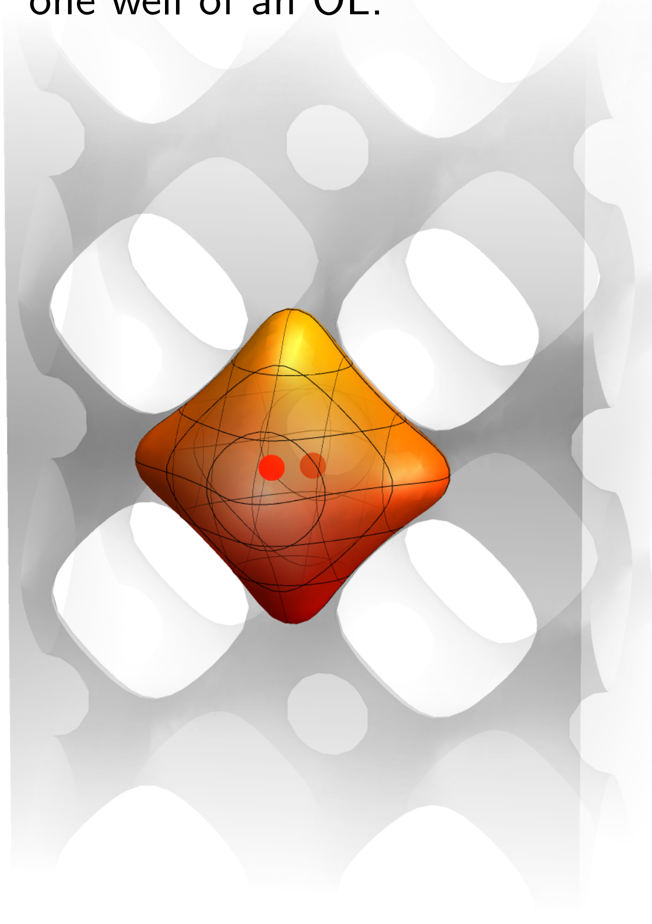
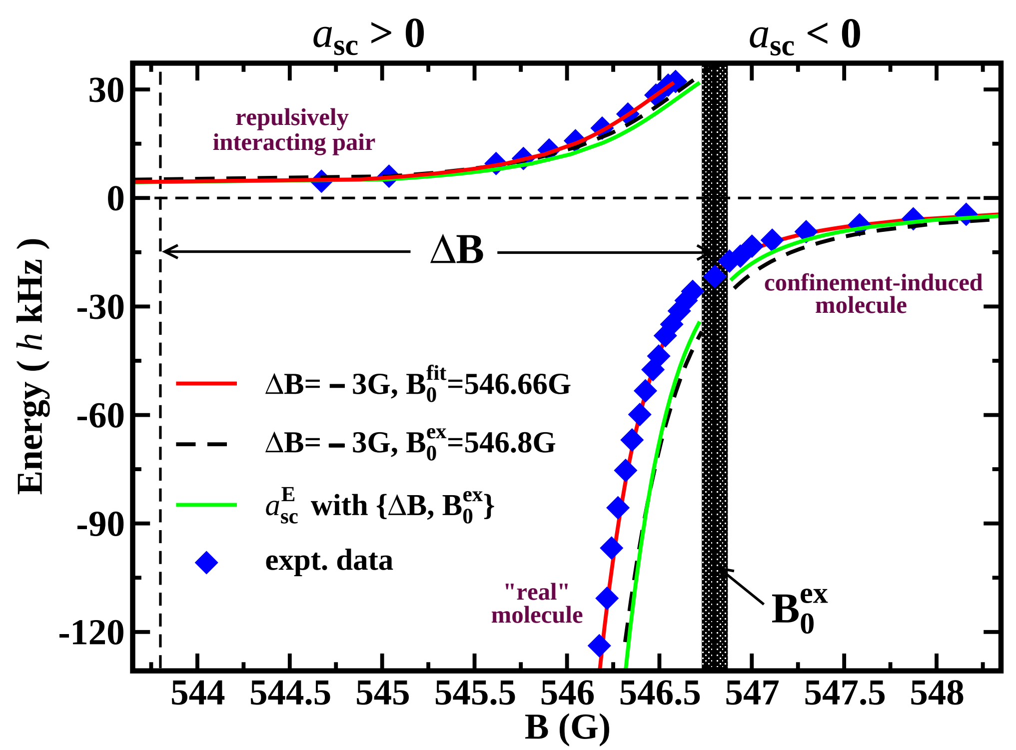


Agreement with experiment on **kHz level**

$\rightarrow$ improved resonance parameters by fit?

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

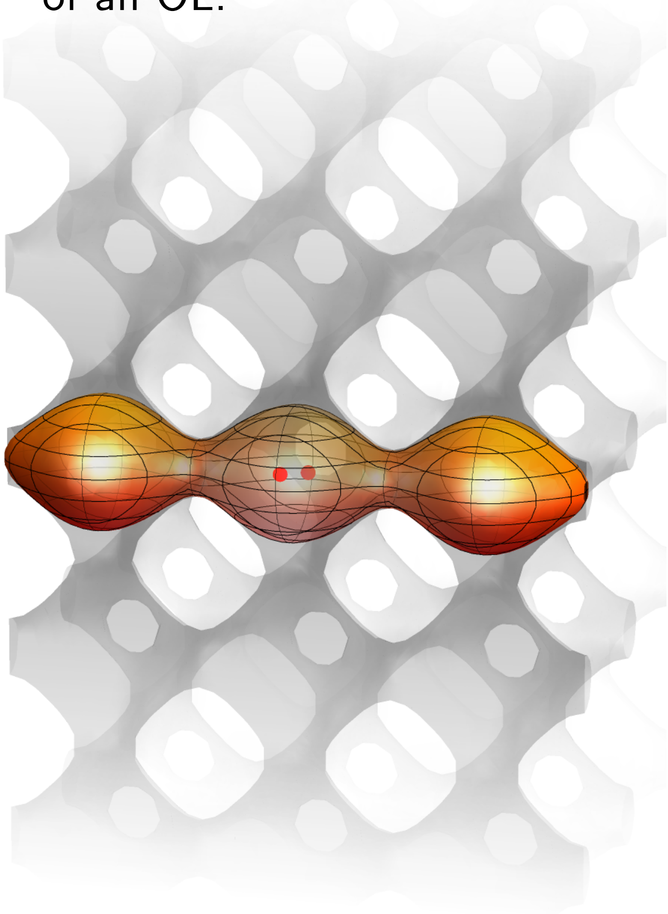
$\rightarrow$ **coupling of COM and REL motion important!**



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

Few-body physics for improving many-body models

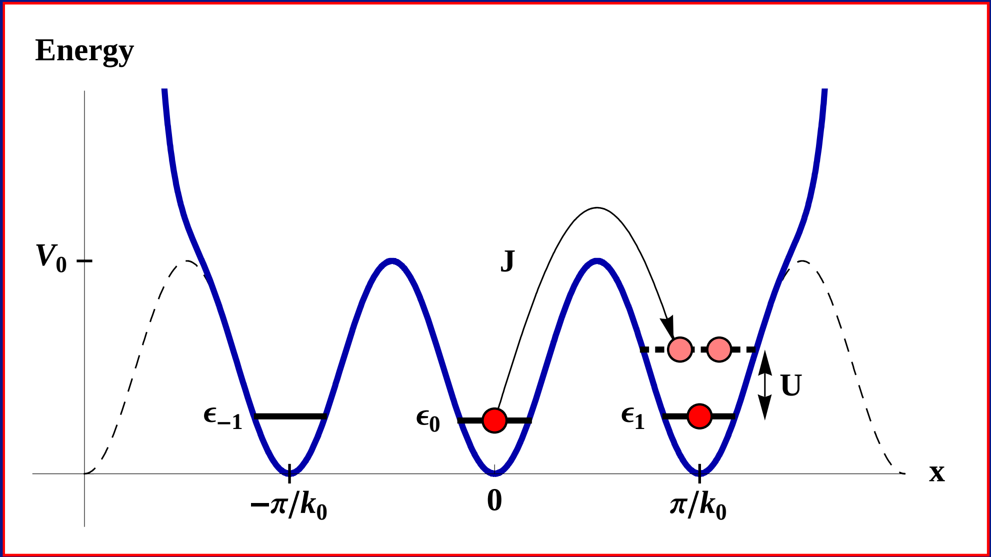
We obtain **exact solutions** for two interacting atoms in 3 wells of an OL.



- Comparison with **BH model** with Hamiltonian

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

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



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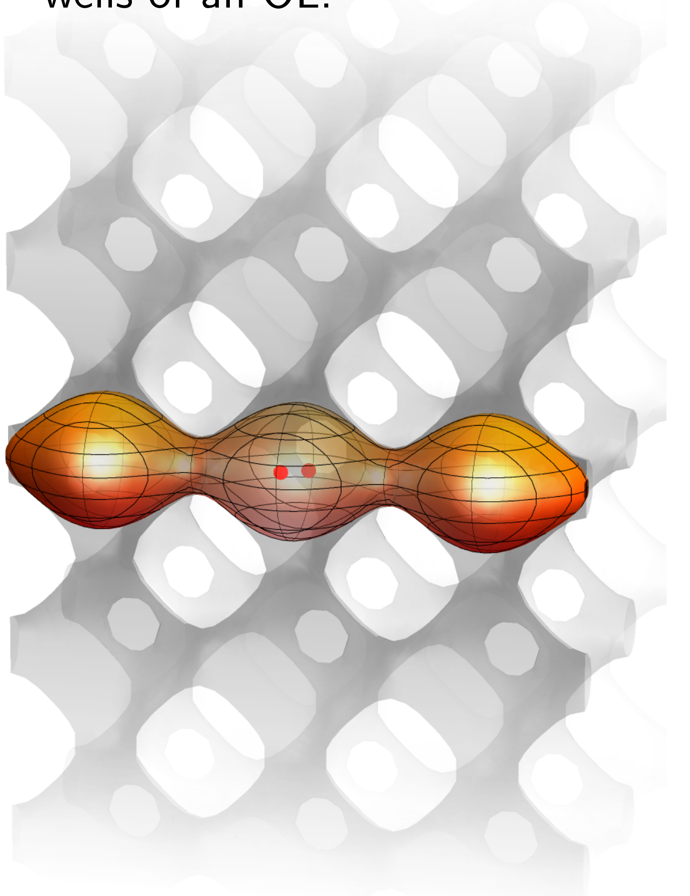
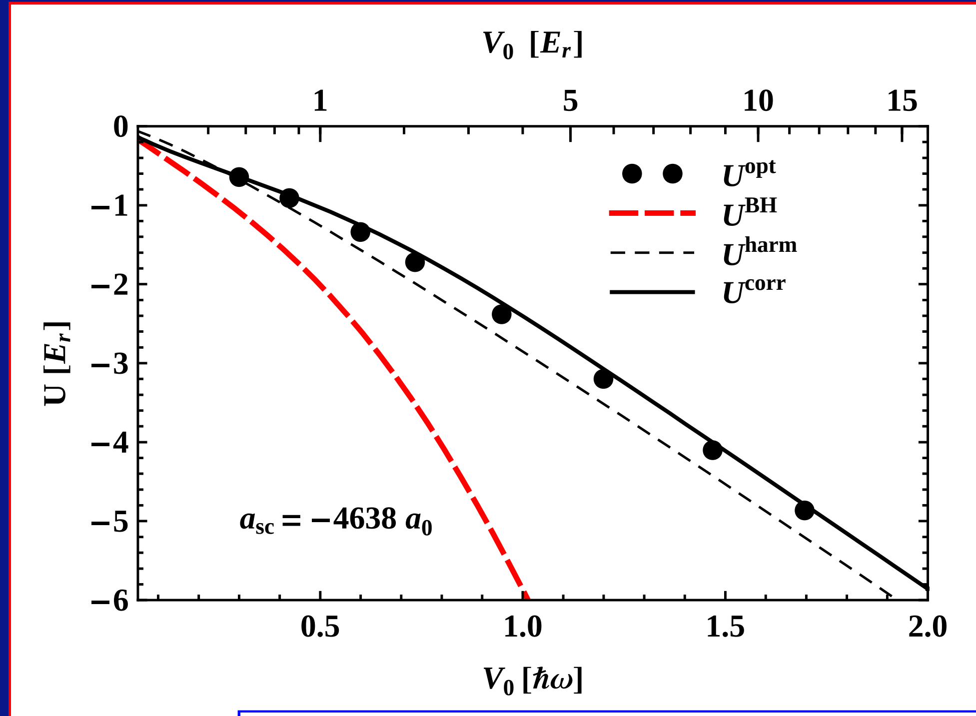


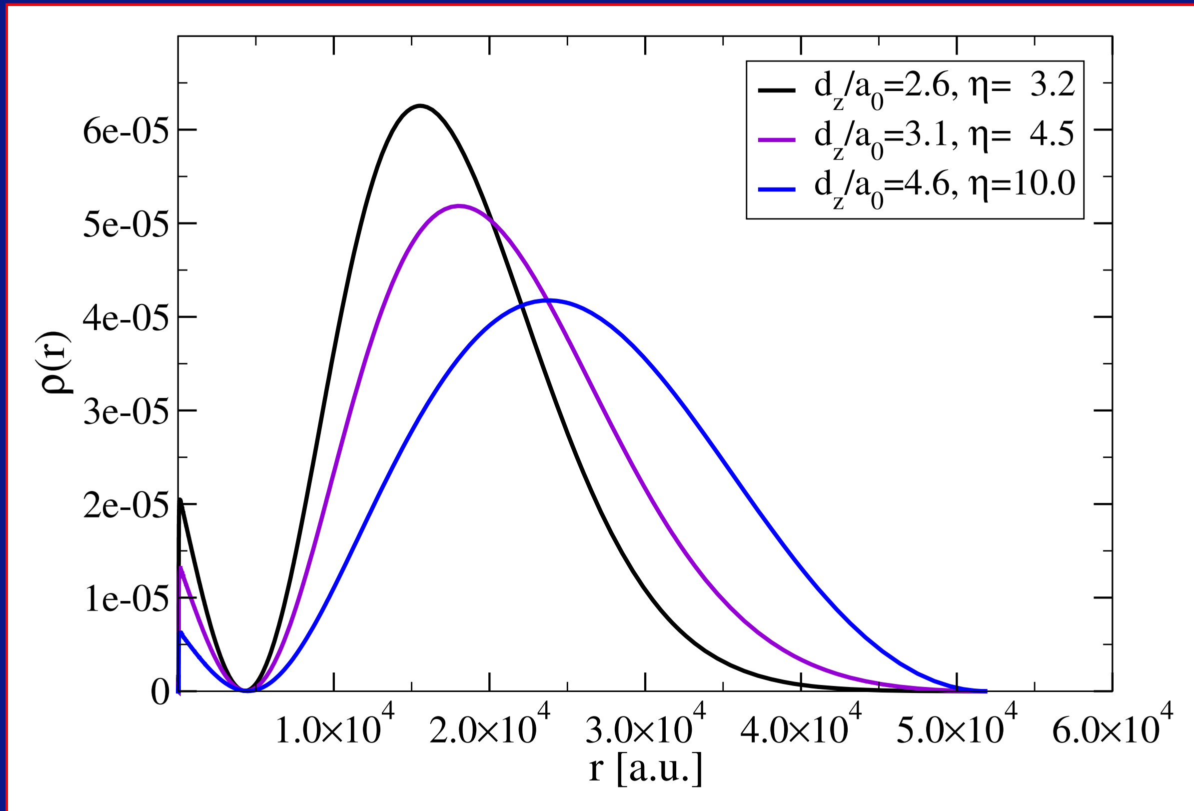
- Introduction of **improved U parameter** by correction of harmonic interaction energy: $U^{\text{corr}} = \mathcal{A} U^{\text{harm}}$ with

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



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.

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

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

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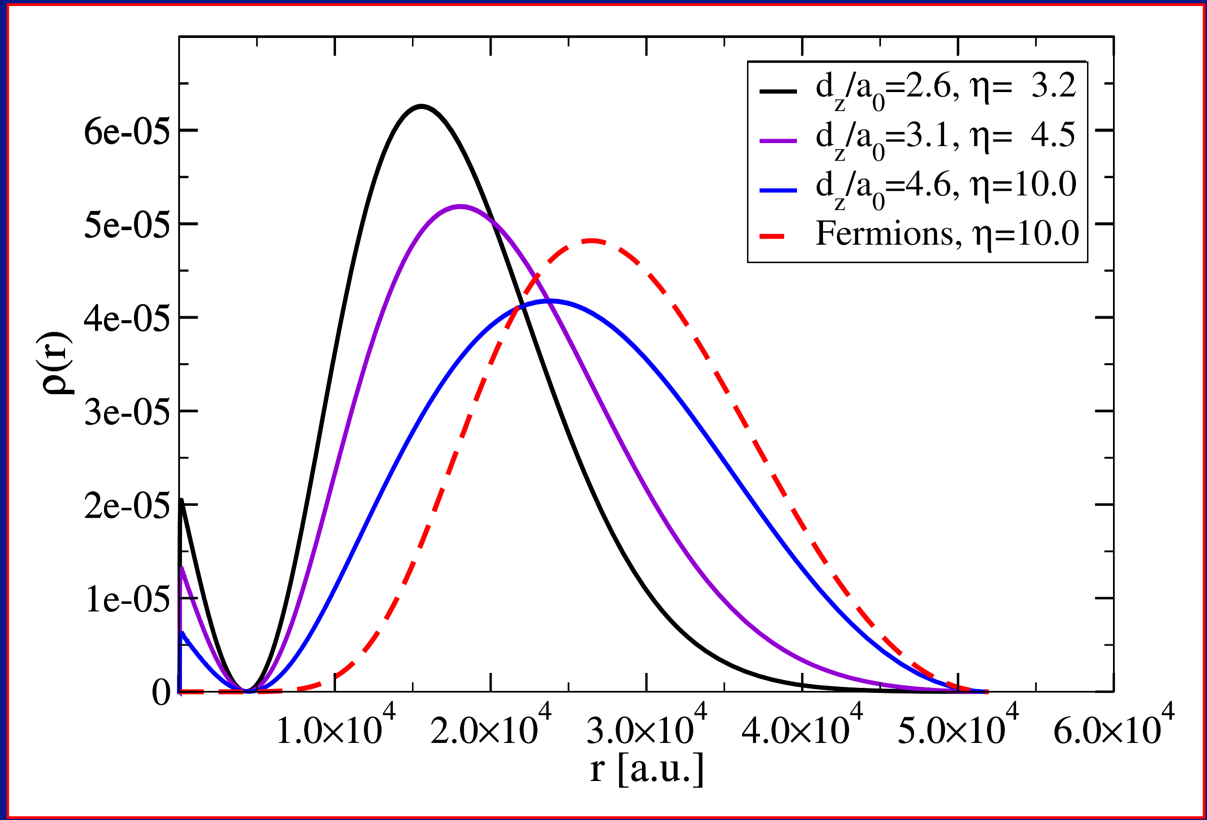

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Confinement-induced resonances (CIR)

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

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

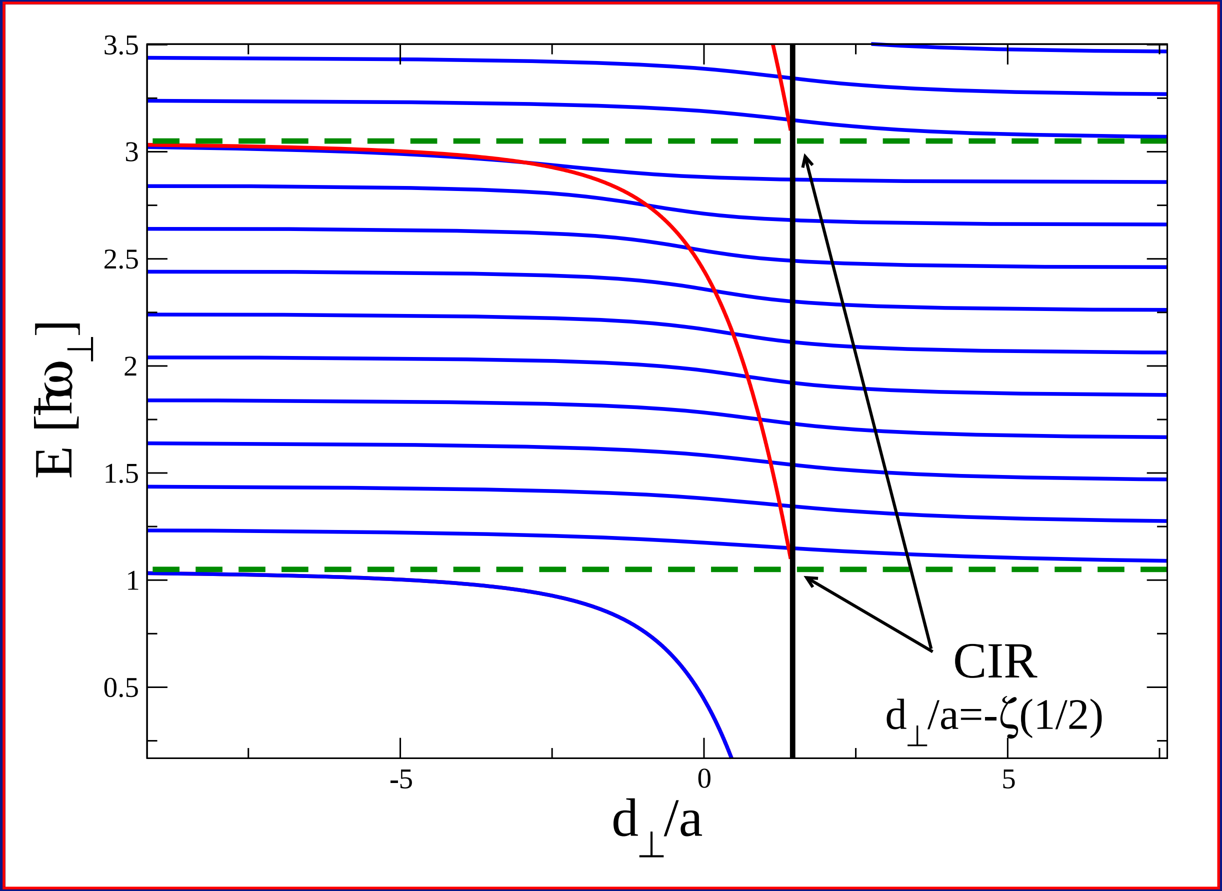
Resonance: $g_{1D} \to \infty$ for $\frac{d_\perp}{a} \;=\; -\zeta(\frac{1}{2}) \;\approx\; 1.46\ldots$

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:

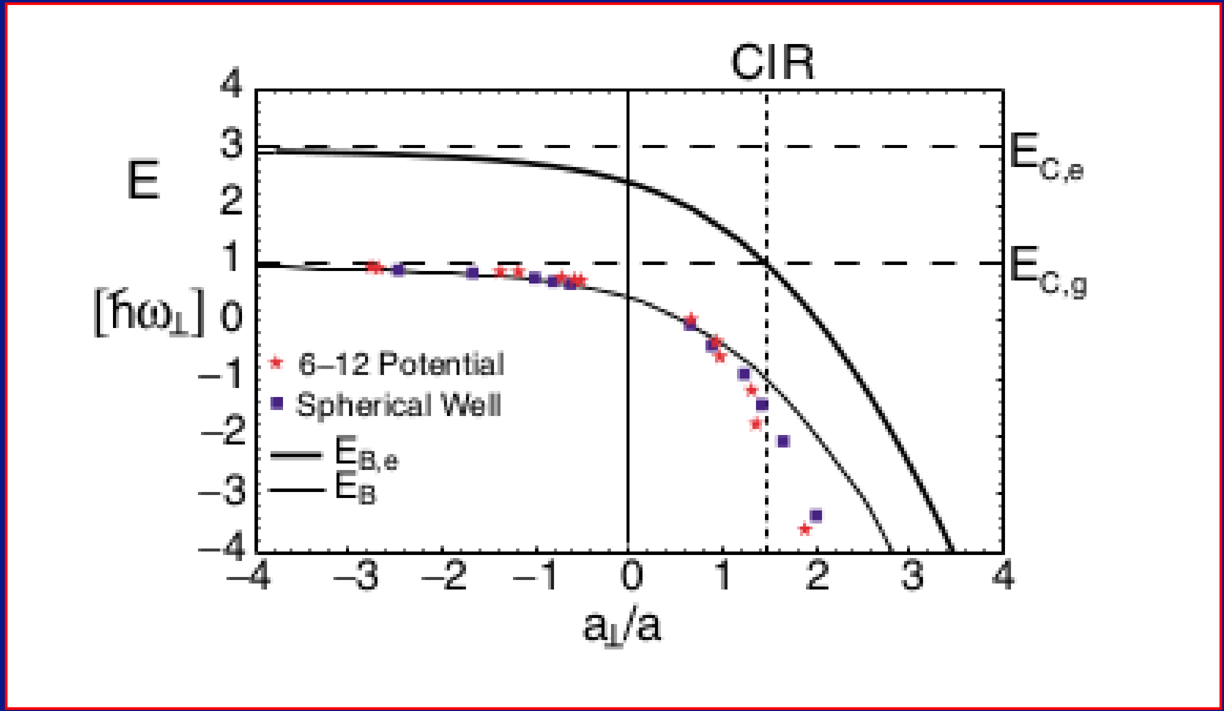


Blue: quasi 1D spectrum

Red: artificially(!) excited bound state

Green: quasi continuum threshold

Olshanii's model (II)



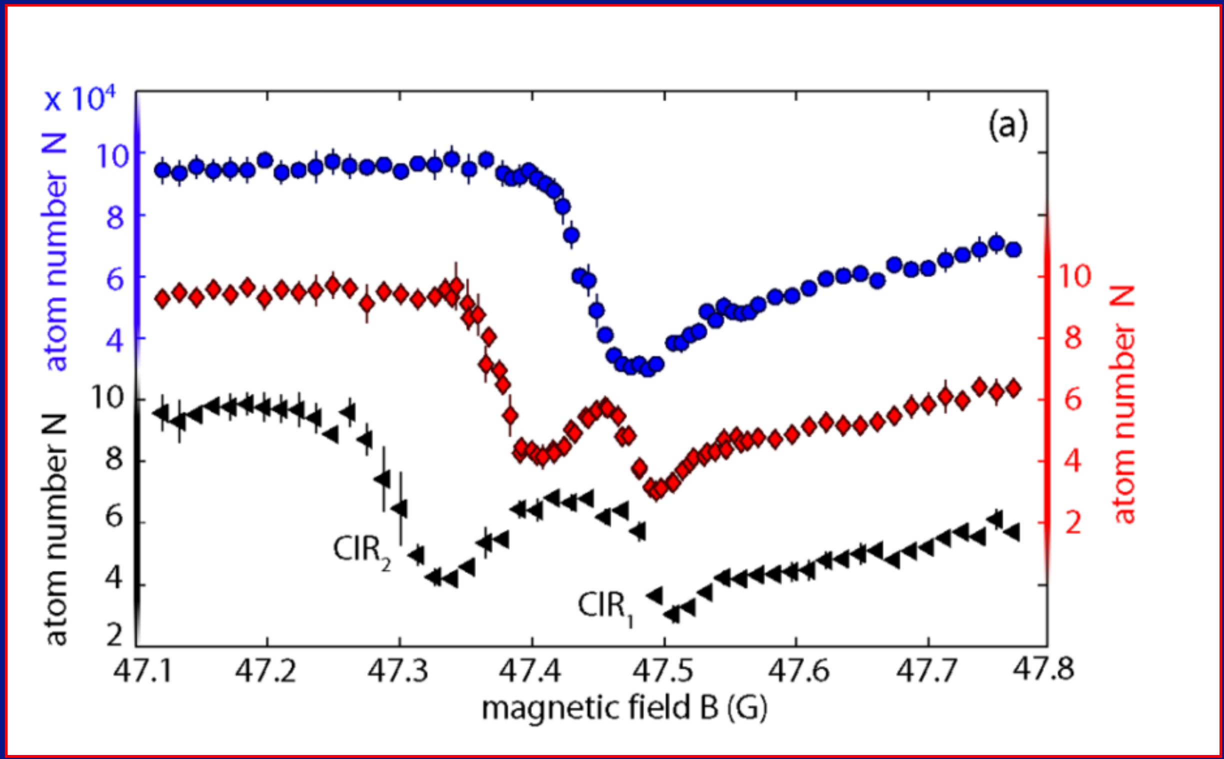
T. Bergeman et al., PRL **91**, 163201 (2003)

Result:

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

Note: No data points on shifted state!

Innsbruck experiment (Cs atoms)

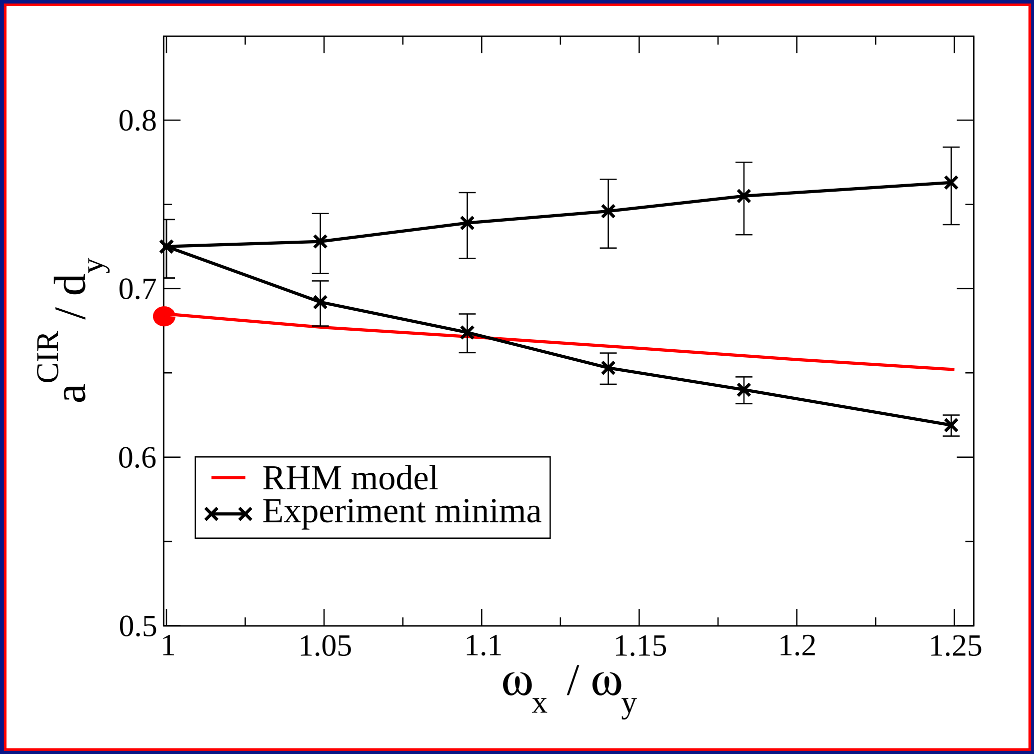


Blue curve: Atom losses for $\omega_x = \omega_y \gg \omega_z$ (anisotropy fixed, a varied).

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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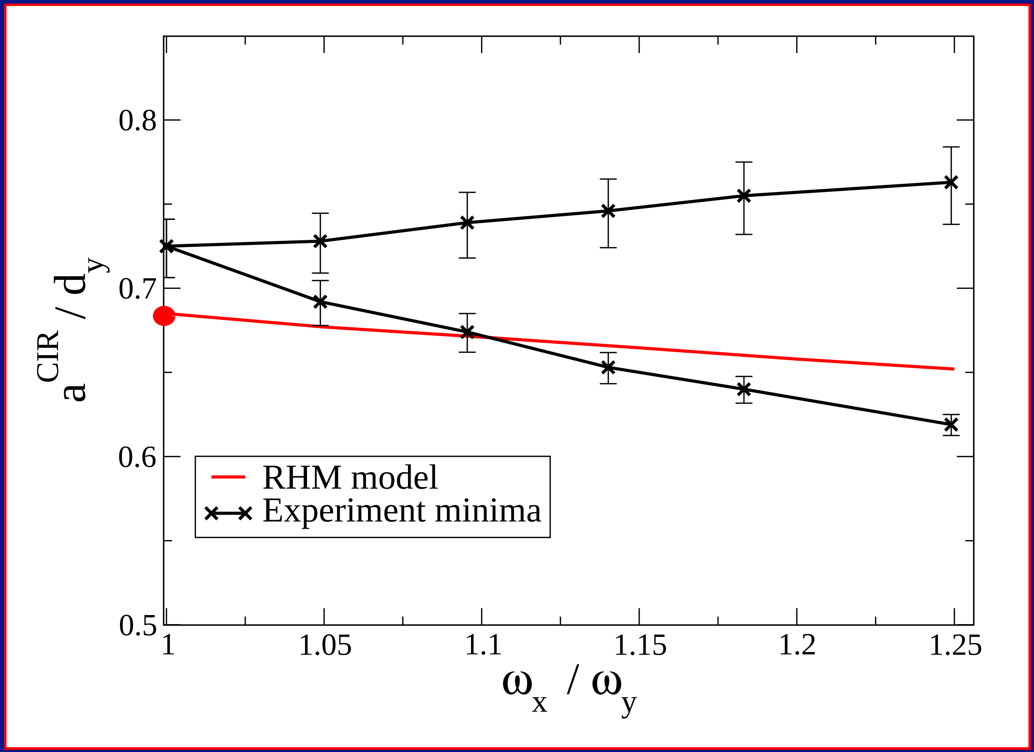

E. Haller et al., PRL, **104**, 153203 (2010)

⇒ 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.):

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

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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.

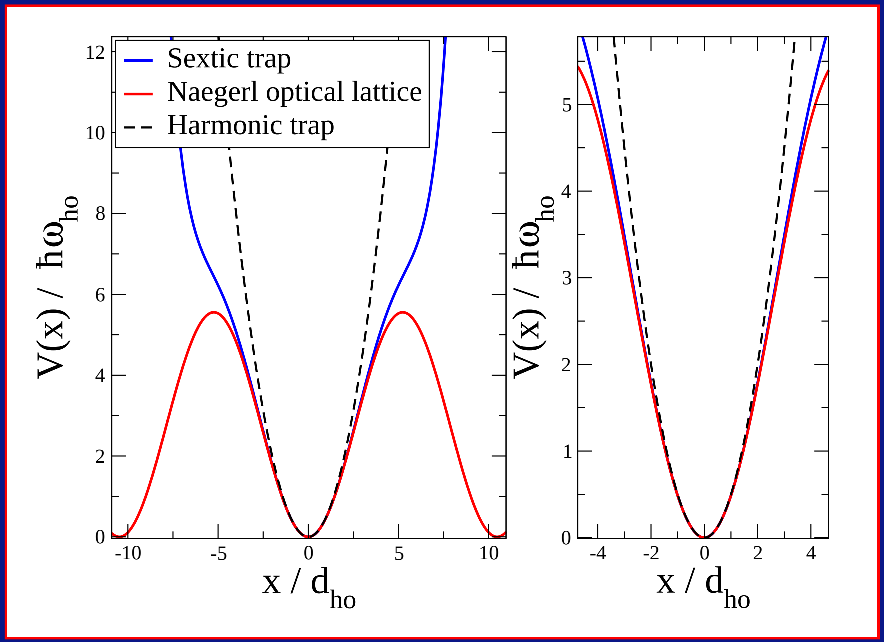
Full treatment of two atoms in quasi-1D trap:

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

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

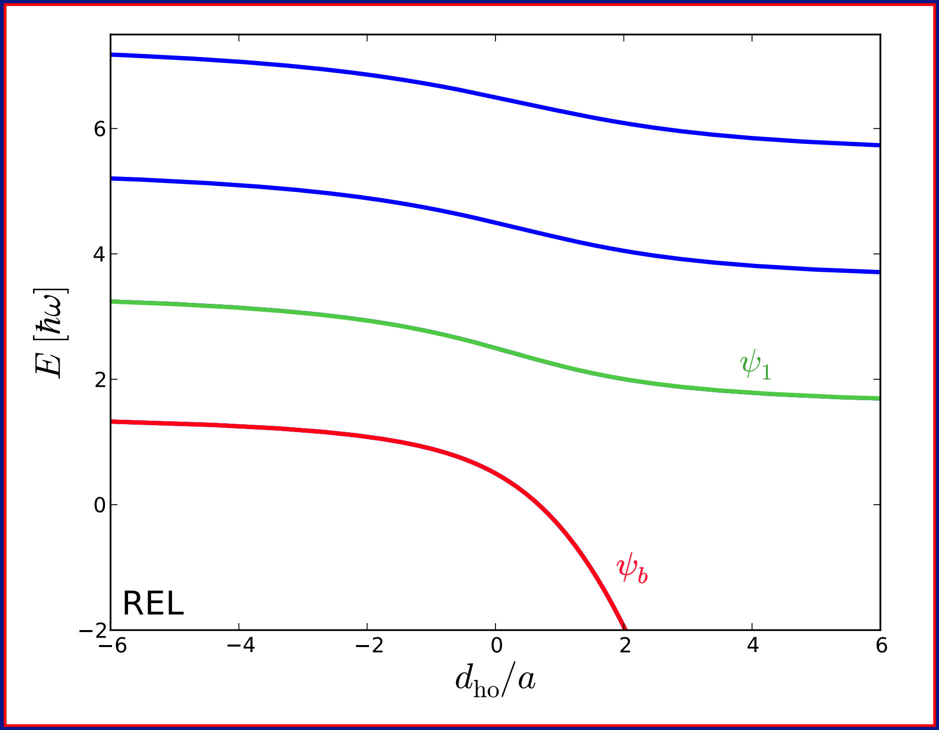
Note:

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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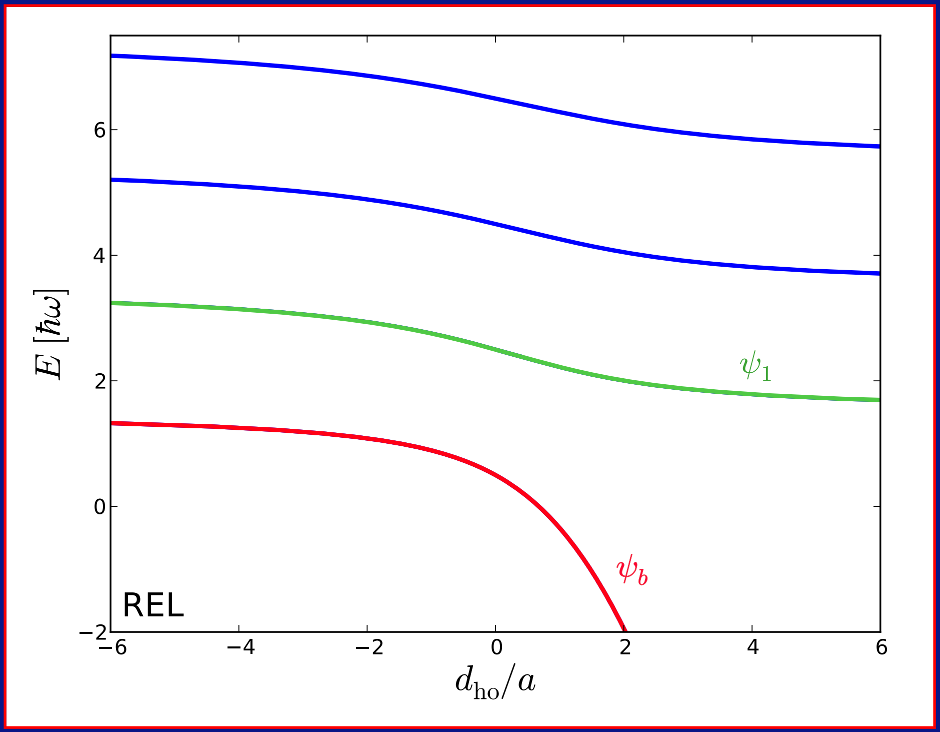

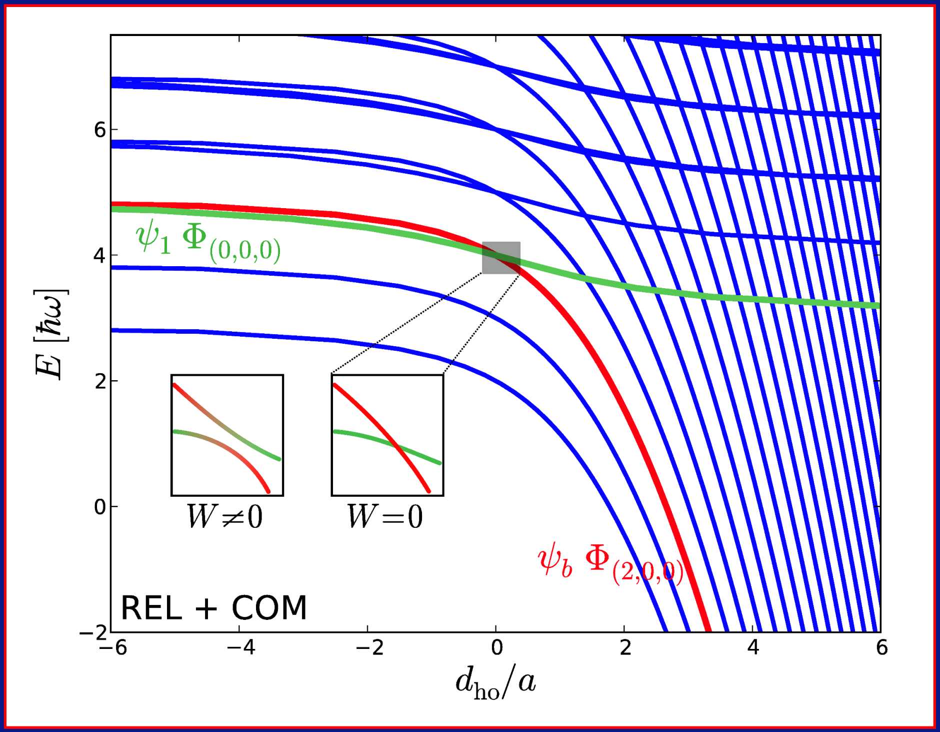

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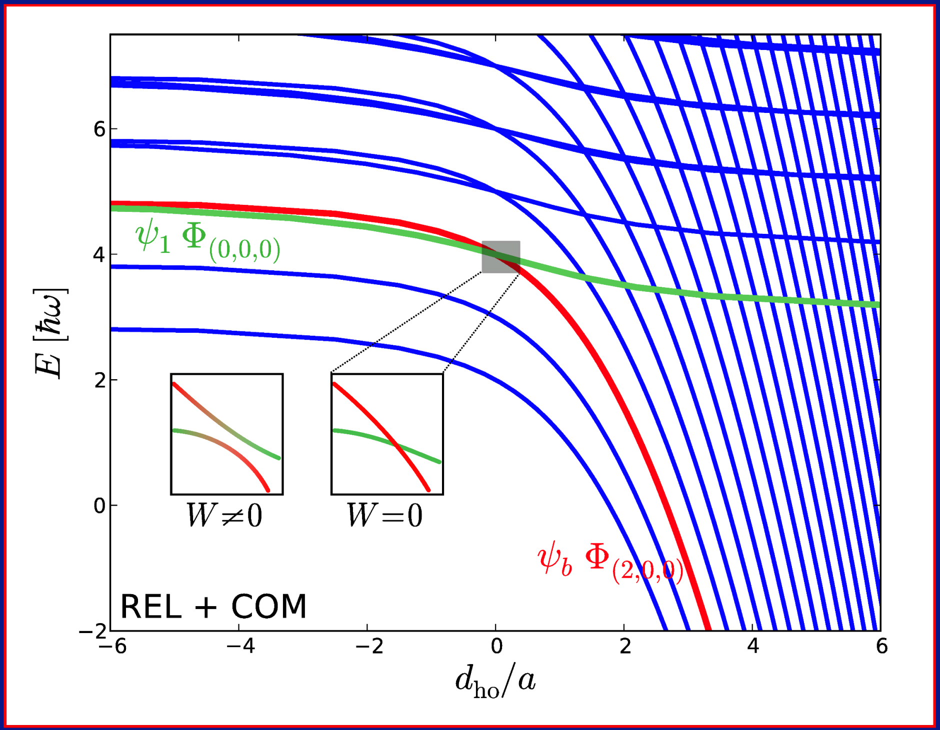
Full spectrum

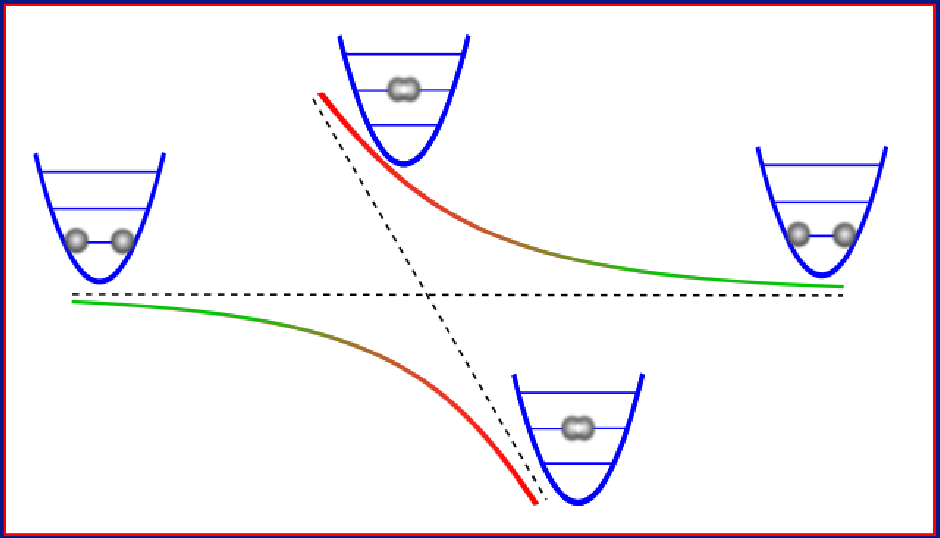
$\Phi_{(0,0,0)}$: ground com state

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

Molecule formation due to confinement



Full spectrum



Avoided crossing

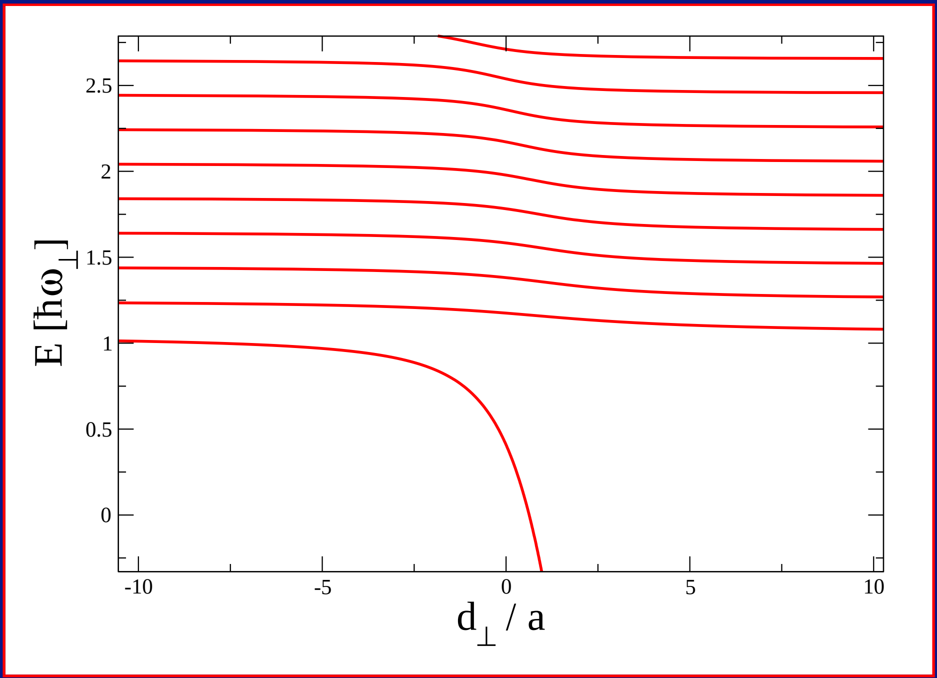
Coupling of center-of-mass (com) and relative (rel) motion ($W \neq 0$):

$\longrightarrow$ avoided crossing

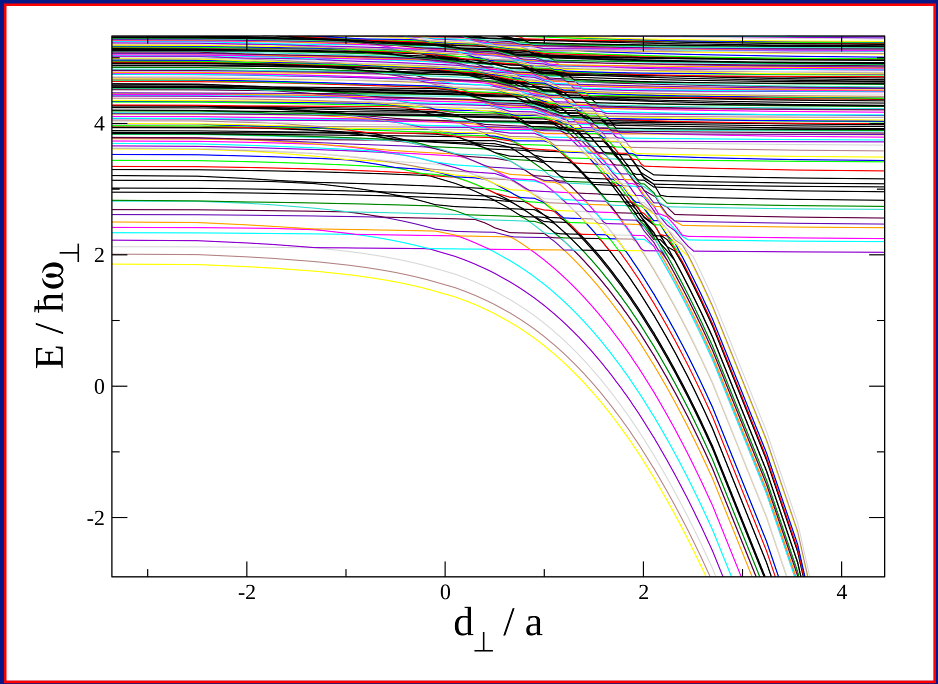
$\longrightarrow$ **molecule formation possible!**

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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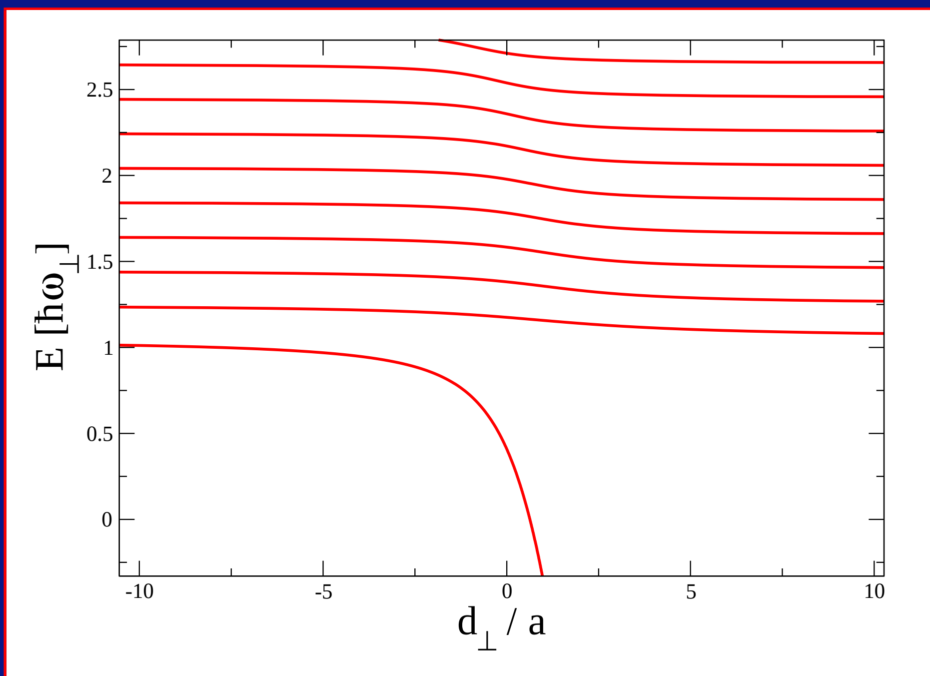
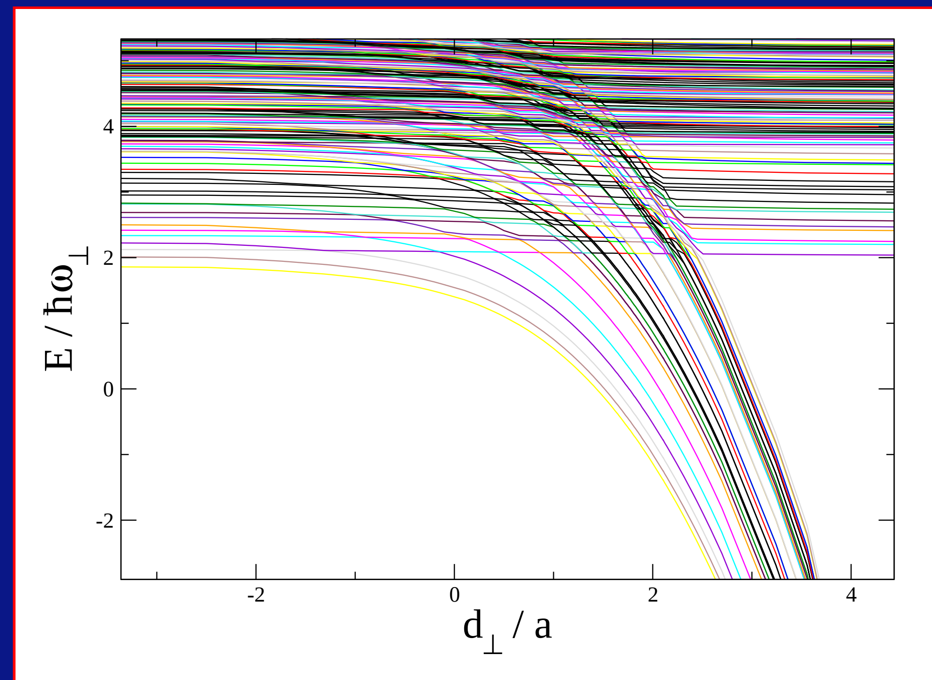


REL



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

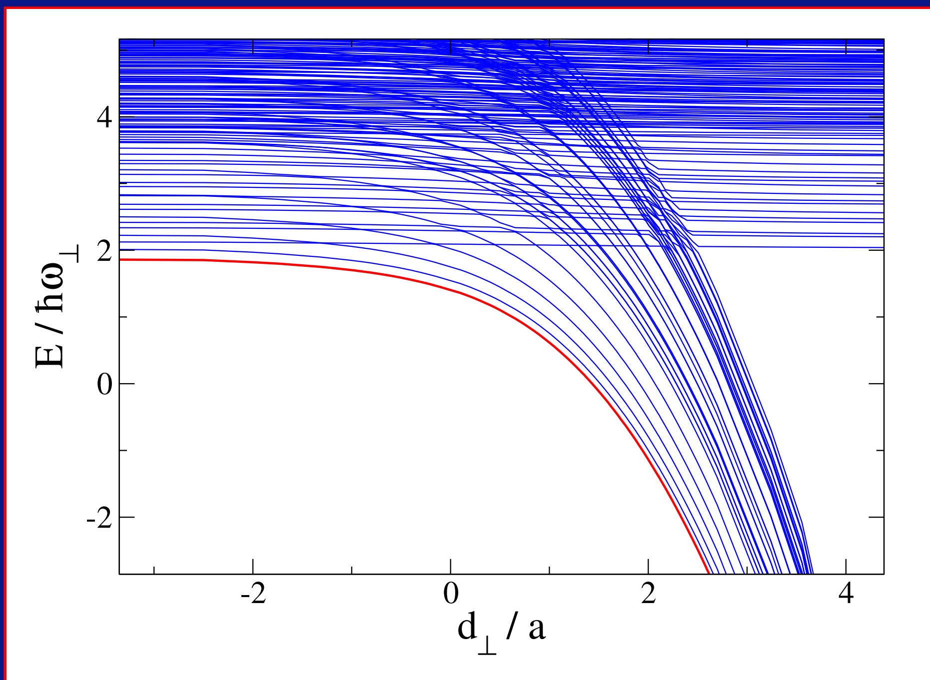
Ultracold: only ground trap state populated $\Longrightarrow m = k = 0$.

Resonances:

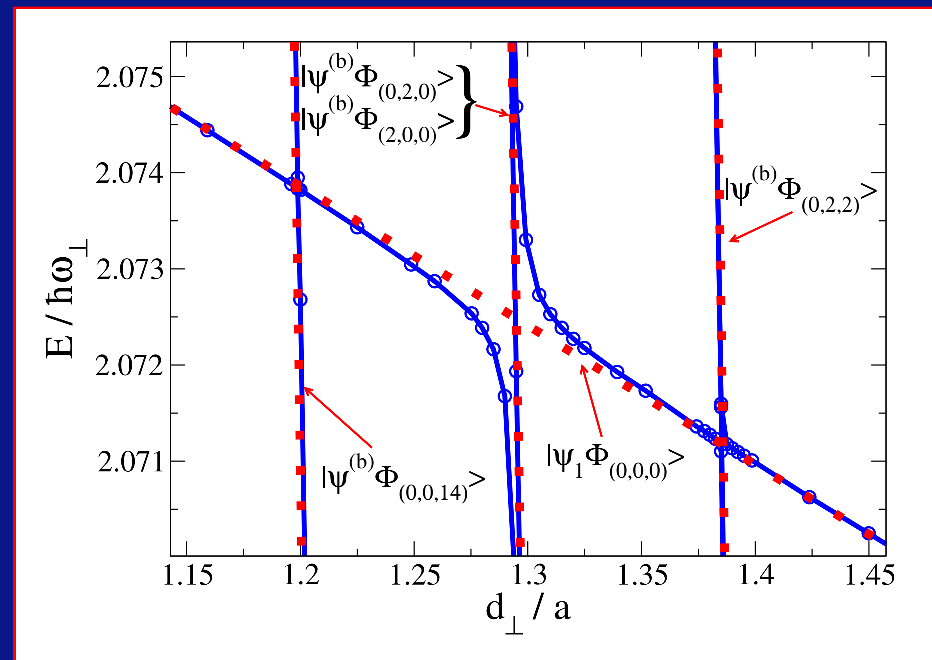
Crossing of transversally COM excited REL bound state with ground (COM and REL) trap state.

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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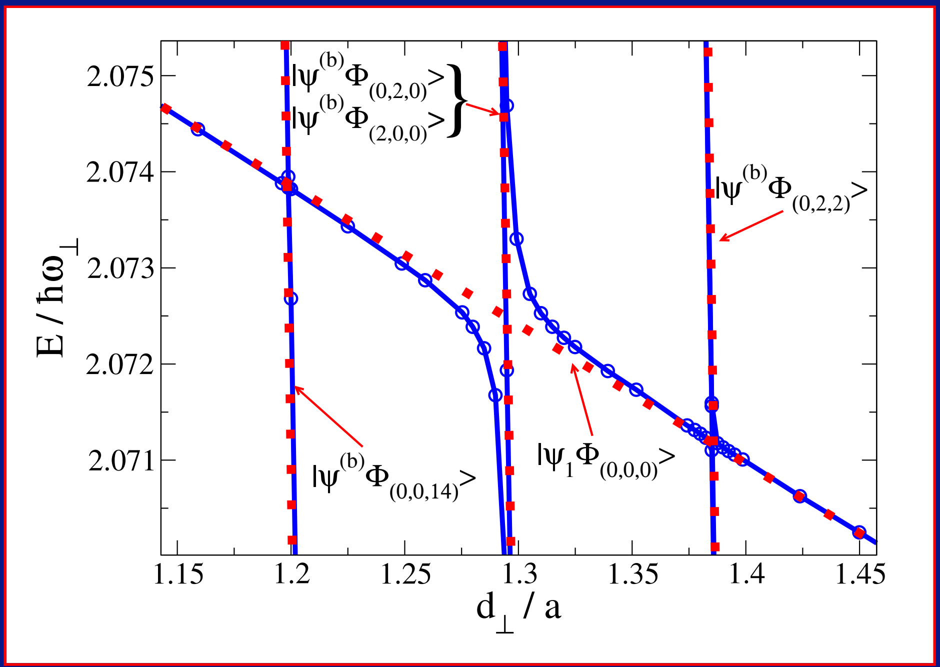
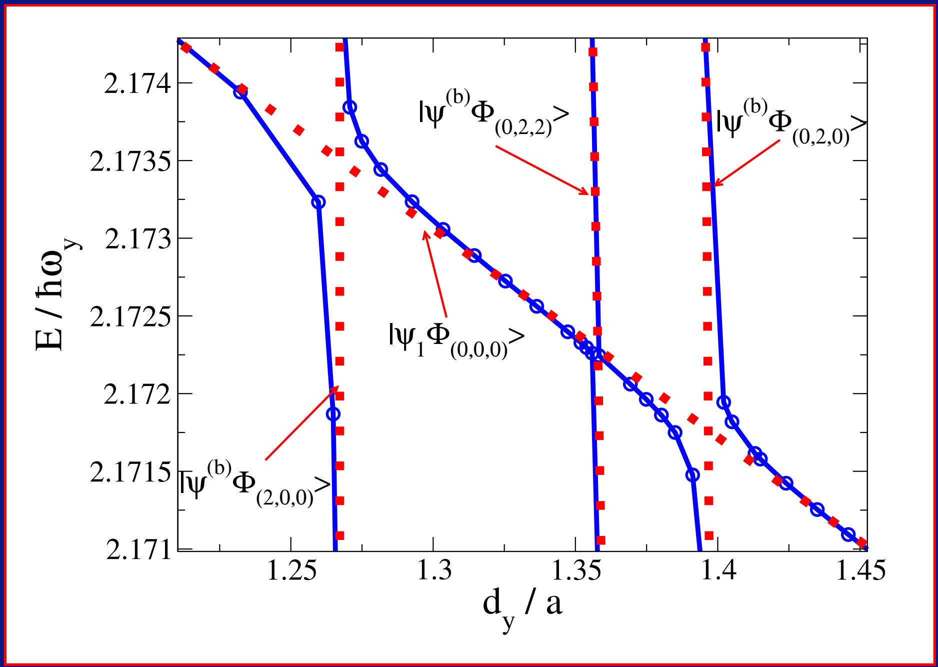


$\omega_x = \omega_y \gg \omega_z$



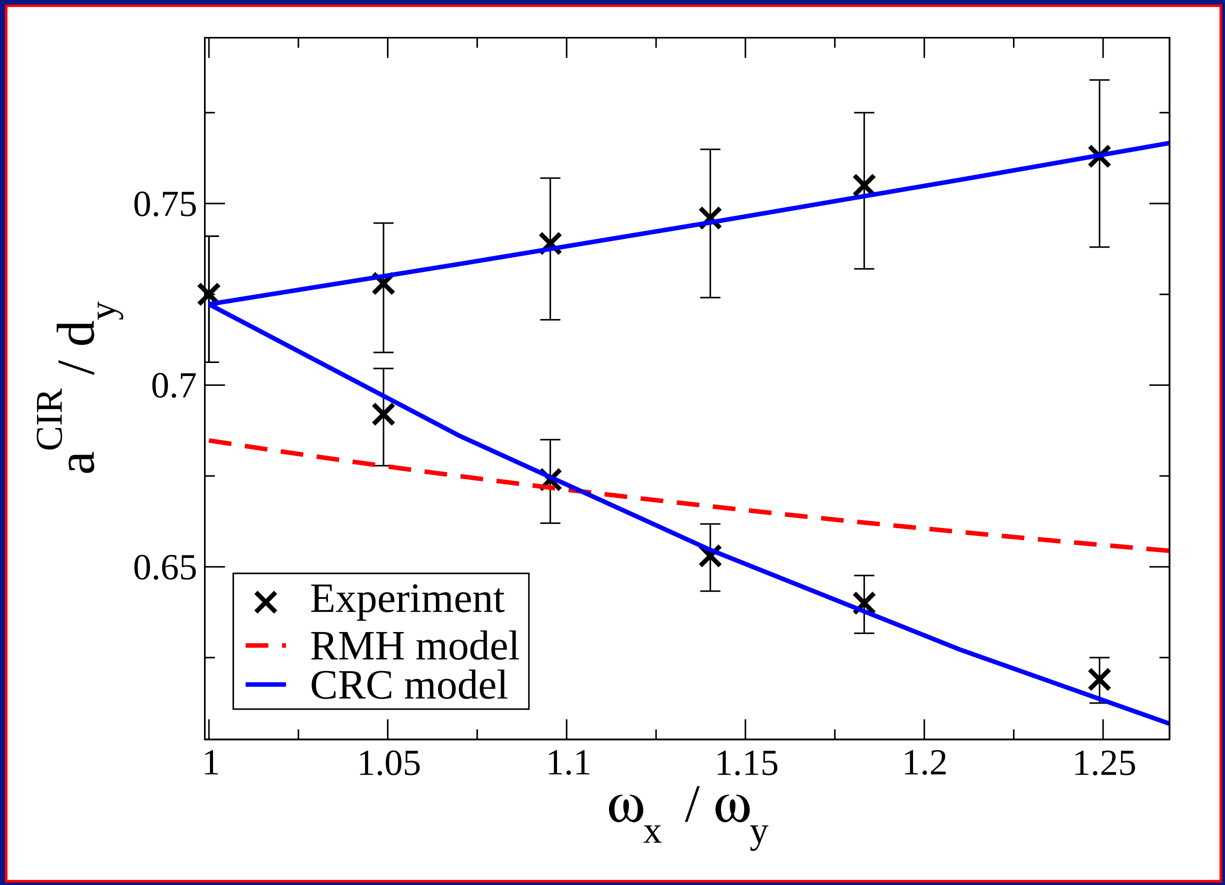
$\omega_x \neq \omega_y \gg \omega_z$

$\Rightarrow$ 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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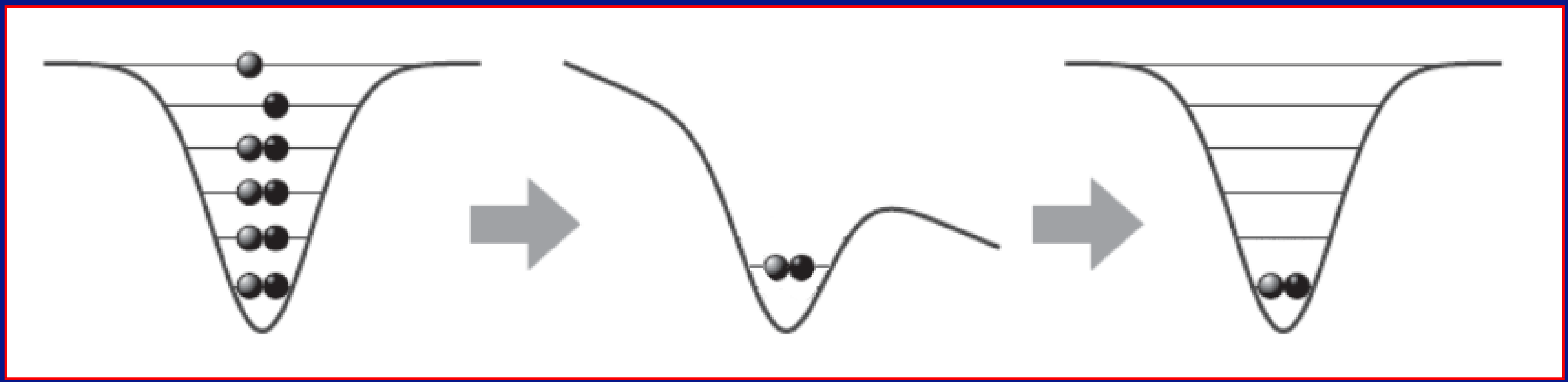
- Losses in a many-body system (Innsbruck experiment) are very unspecific, in contrast to Cambridge rf experiment.
- “See KITP recording: Gora Shlyapnikov said that there is no problem in 2D.”

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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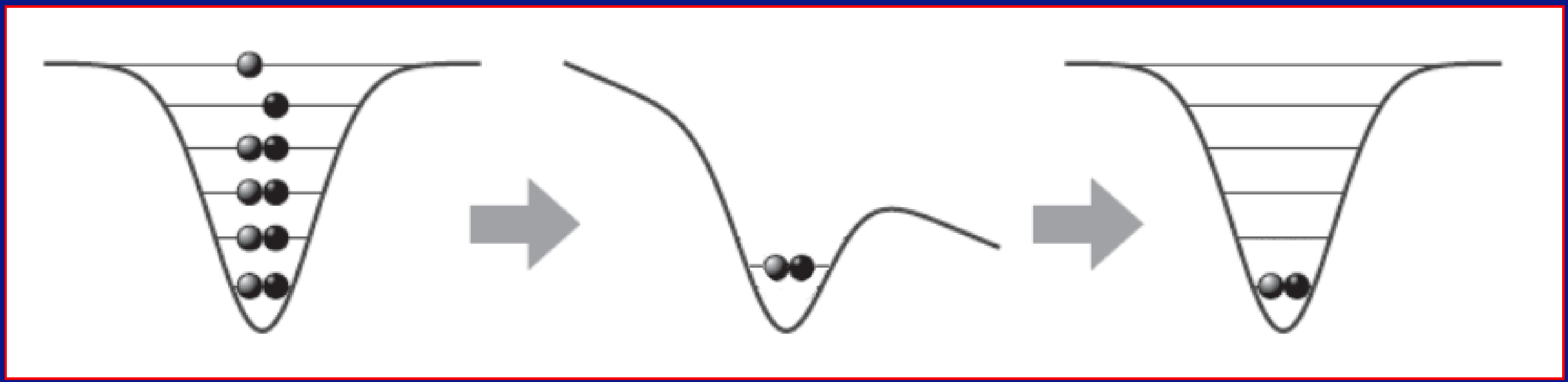

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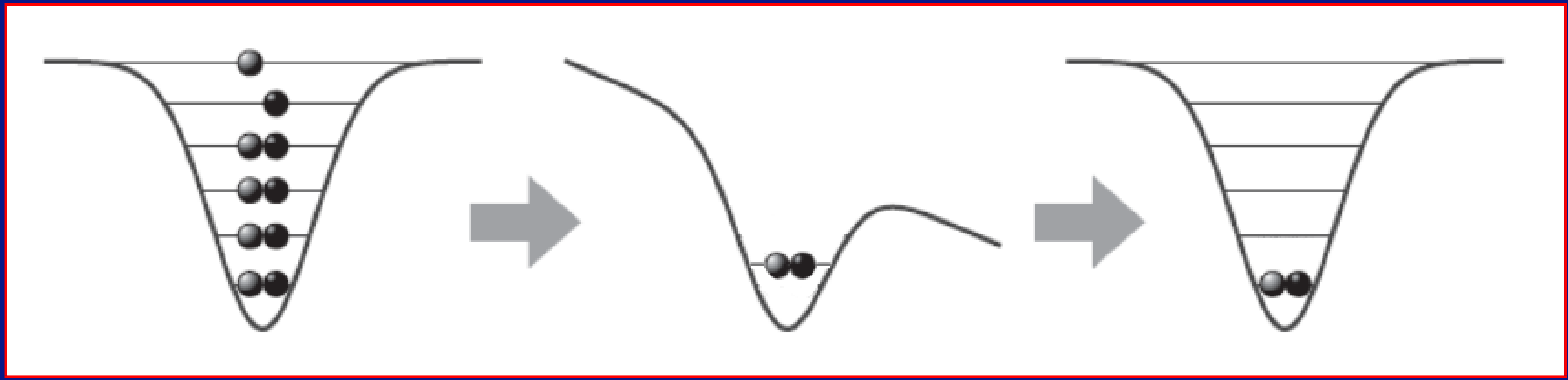

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2. Detection of molecules: measurement of tunneling atoms at a B field where deeply bound molecules do not tunnel.

Comparison ab initio result to experiment

COM	Position [G]		FWHM[G]		Ω_0[Hz]/ 2π	
excitation	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!

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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, A.S., *in preparation*]

Outlook: beyond two particles

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- Renormalization of δ function needed
  $\longrightarrow$ easy universal scheme available?
- Other model potentials, for example Gaussians
  $\longrightarrow$ universal way / recipe how to choose it?

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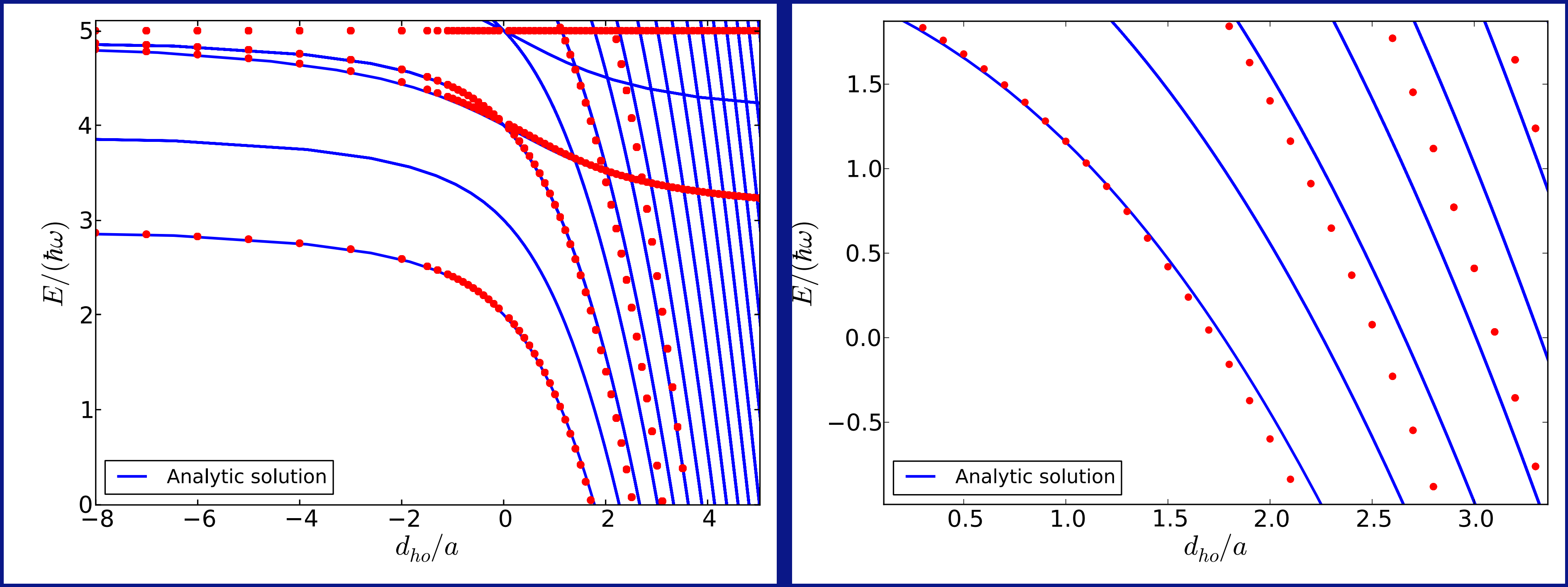
Configuration interaction (exact diagonalization): CI singles (CIS) and full CI.

Comparison: δ pseudopotential vs. Born-Oppenheimer

For going beyond two particles, the adopted two-body interaction must be validated.

Our two-body code may serve as reference (here using a ^{7}Li–^{7}Li Born-Oppenheimer potential curve.

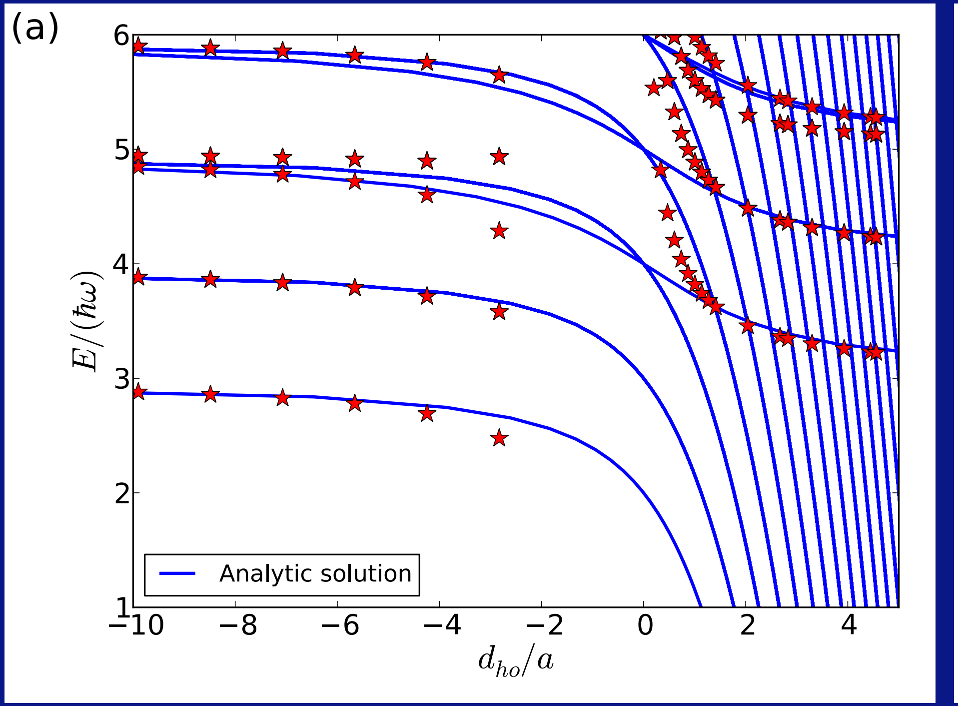
Analytical result: result for δ pseudopotential in harmonic trap.



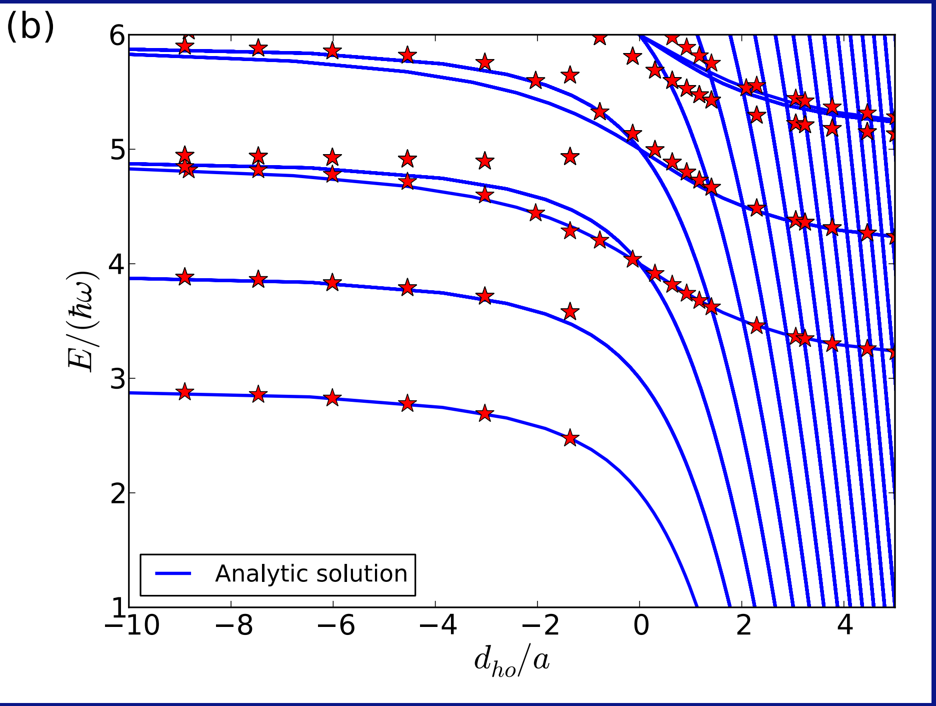
Configuration interaction (singles) with δ function

The **δ-function pseudopotential** requires **renormalization** when used in configuration-interaction / exact-diagonalization approaches for **2D or 3D systems**.

Most basic check of renormalization procedure: compare 2-body calculation with analytical result.



no renormalization

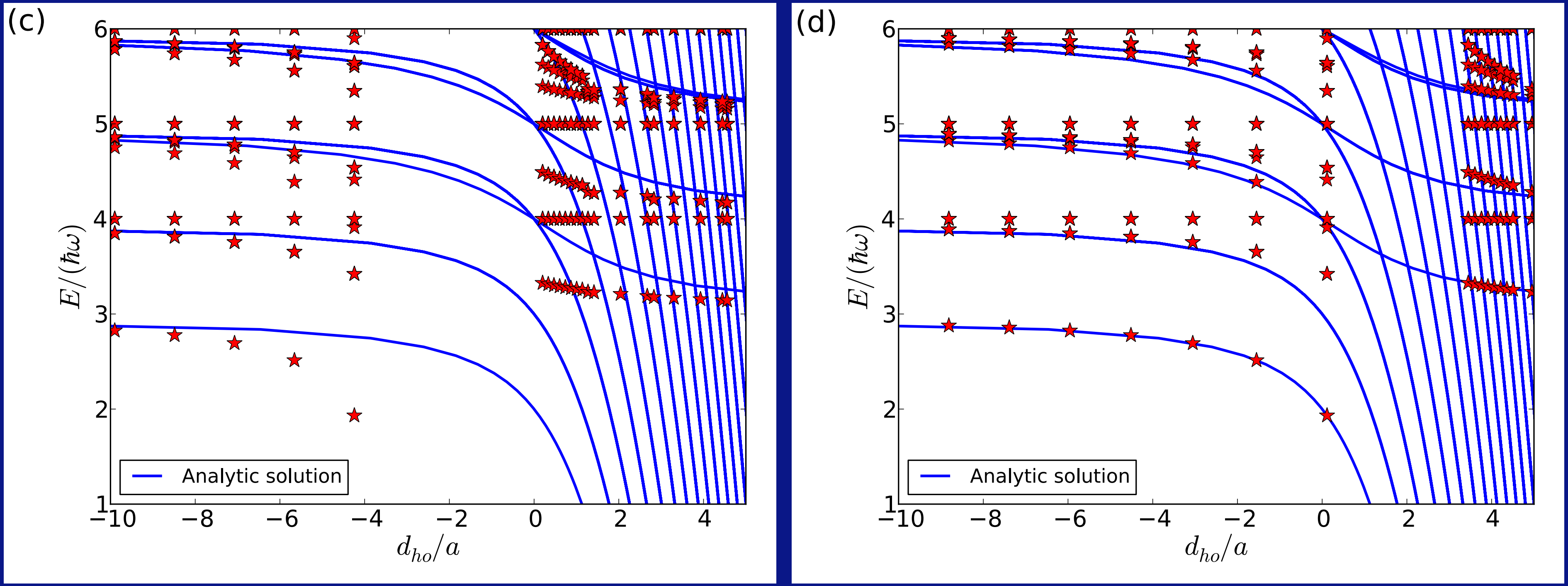


with renormalization

Configuration interaction (full) with δ function

The **δ-function pseudopotential** requires **renormalization** when used in configuration-interaction / exact-diagonalization approaches for **2D or 3D systems**.

Most basic check of renormalization procedure: compare 2-body calculation with analytical result.



no renormalization

with renormalization

Configuration interaction (full vs. singles)

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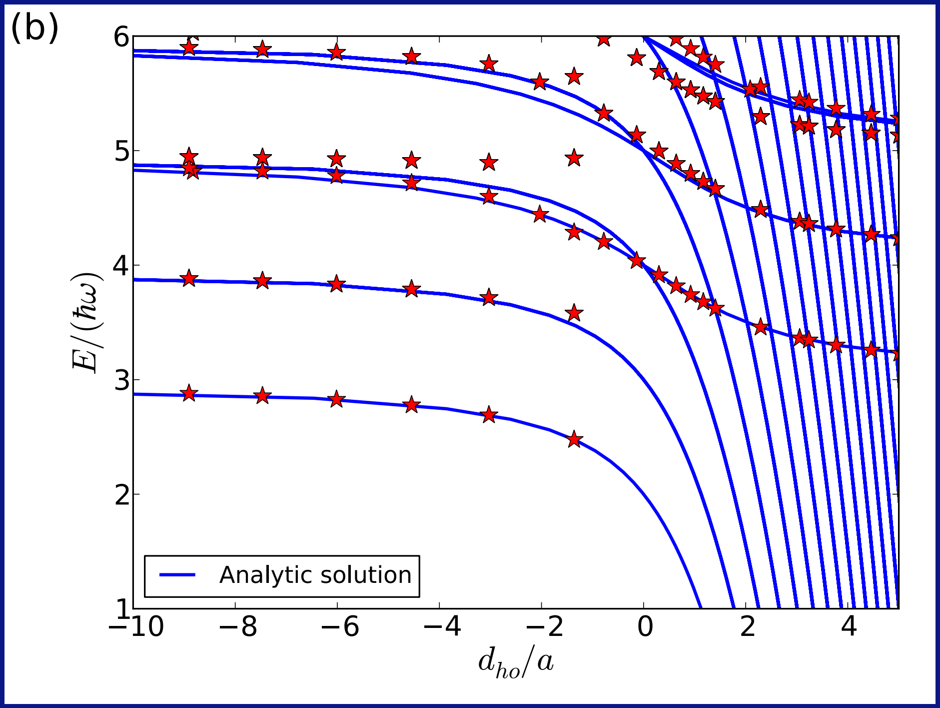
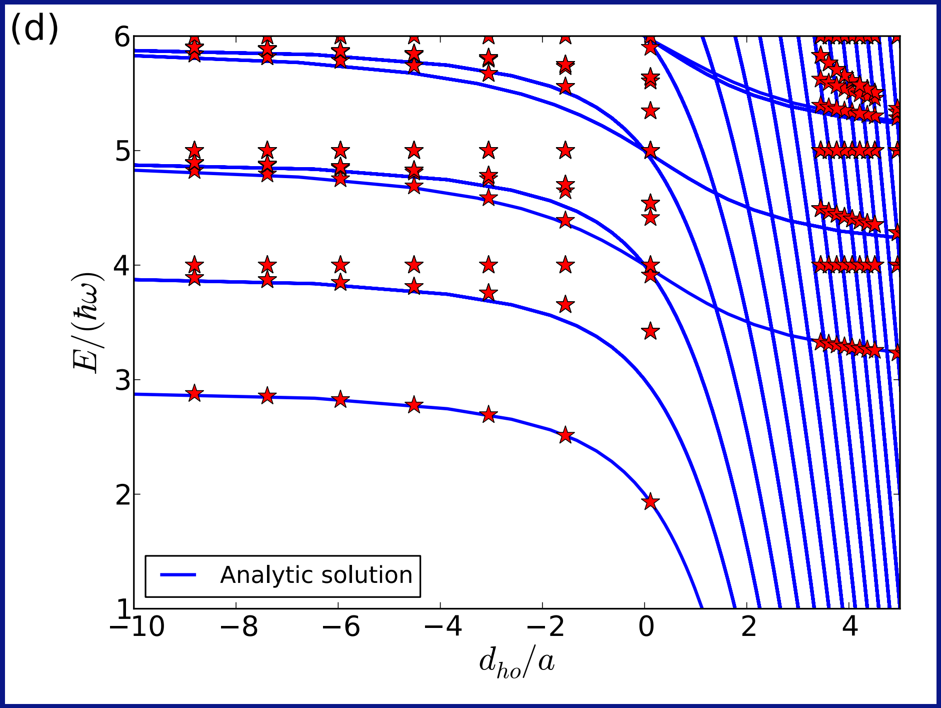
Most basic check of renormalization procedure: compare 2-body calculation with analytical result.



CI (singles only)



full CI

Configuration interaction with Gaussian interaction

Instead of a δ pseudopotential, a **model Gaussian interaction** potential may be used. (Here: Gaussian exponent equal to 5 d_{ho}^{-2}.)