Resonances in few-body systems

Alejandro Saenz

AG Moderne Optik

Institut für Physik

Humboldt-Universität zu Berlin

(ECT* Trento, Universality in strongly interacting systems, 13.06.2025)

Overview

1. Confined particles (ultracold atoms in optical lattices or tweezers)
   - Influence of the confining potential.
   - Confinement-induced resonances (CIR).
2. Hydrogen-antihydrogen interaction.

Overview

1. Confined particles (ultracold atoms in optical lattices or tweezers)
   - Influence of the confining potential.
   - Confinement-induced resonances (CIR).
2. Hydrogen-antihydrogen interaction.

Acknowledgment:

Simon Sala, Sergey Grishkevich, P.-I. Schneider, Bruno Schulz, Tjark Döscher, Jakob Wulff, Stephen Onyango, Maria Troppenz

Fabio Revuelta (Uni Politecnica de Madrid)

Selim Jochim and his team (U Heidelberg)

Hanns-Christoph Nägerl and his team (U Innsbruck)

Simplified Atom–Atom Interactions

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.

Simplified Atom–Atom Interactions

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.
- Sometimes, the physics is "only" determined by the long-range part (for example valence electrons for (metallic) conduction).

Simplified Atom–Atom Interactions

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.
- Sometimes, the physics is "only" determined by the long-range part (for example valence electrons for (metallic) conduction).
- The short-range of the potential influences, however, the long-range solution (phase shift).

Simplified Atom–Atom Interactions

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.
- Sometimes, the physics is “only” determined by the long-range part (for example valence electrons for (metallic) conduction).
- The short-range of the potential influences, however, the long-range solution (phase shift).
- Substitute the correct potential by a **pseudopotential** that yields the same wavefunction in the outer regime.

Simplified Atom–Atom Interactions

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.
- Sometimes, the physics is "only" determined by the long-range part (for example valence electrons for (metallic) conduction).
- The short-range of the potential influences, however, the long-range solution (phase shift).
- Substitute the correct potential by a **pseudopotential** that yields the same wavefunction in the outer regime.

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

Simplified Atom–Atom Interactions

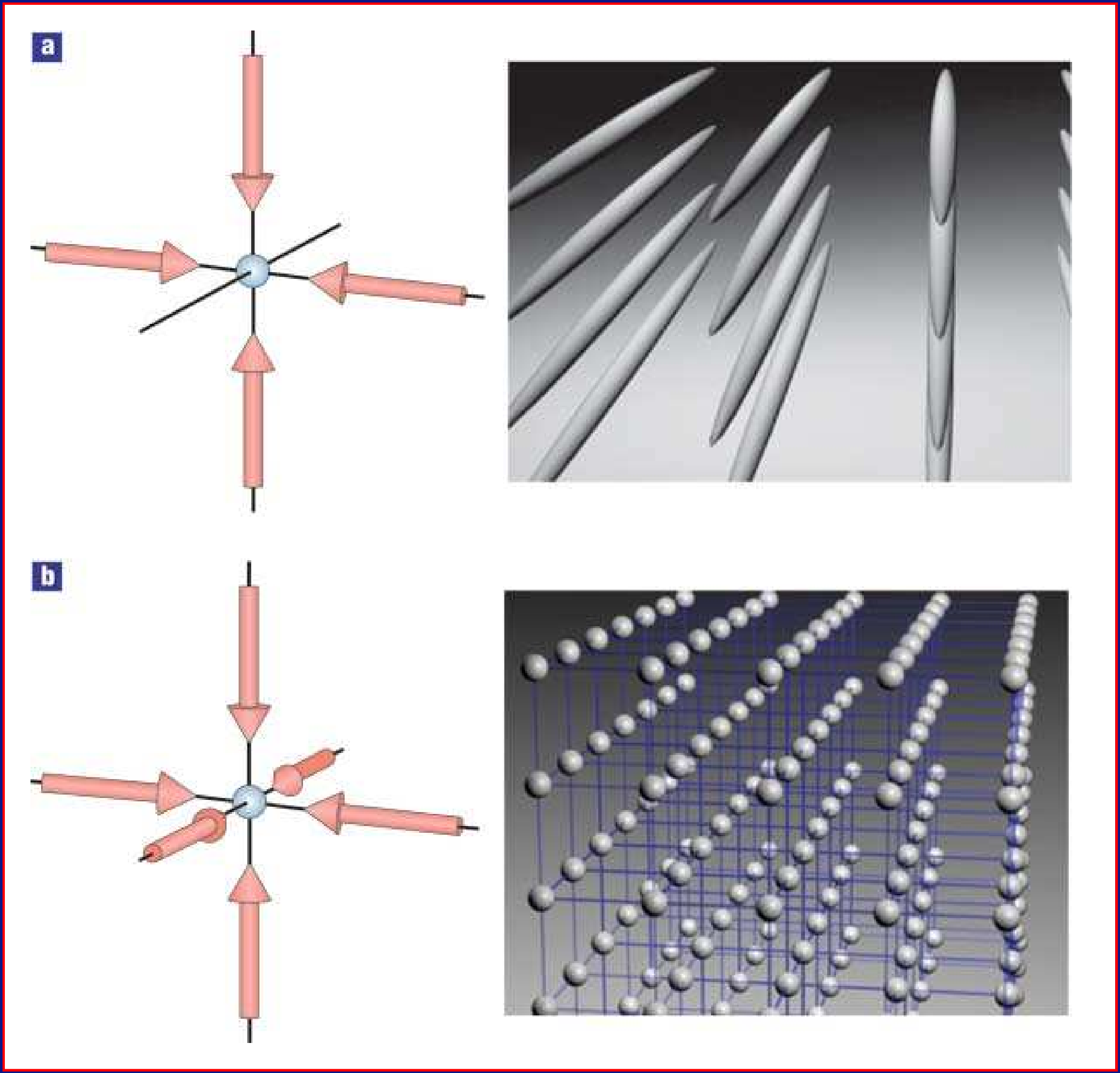
Concept (cf. nuclear or solid-state physics):

- In many cases the wavefunction of a system consists of a complicated short-range and a “simple” long-range part.
- Sometimes, the physics is “only” determined by the long-range part (for example valence electrons for (metallic) conduction).
- The short-range of the potential influences, however, the long-range solution (phase shift).
- Substitute the correct potential by a **pseudopotential** that yields the same wavefunction in the outer regime.

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

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

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

- This relation was derived for $k \rightarrow 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.

External trap potential and interatomic interaction

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

- This relation was derived for $k \to 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.
- However, energy (and length) scales are usually very different.

External trap potential and interatomic interaction

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

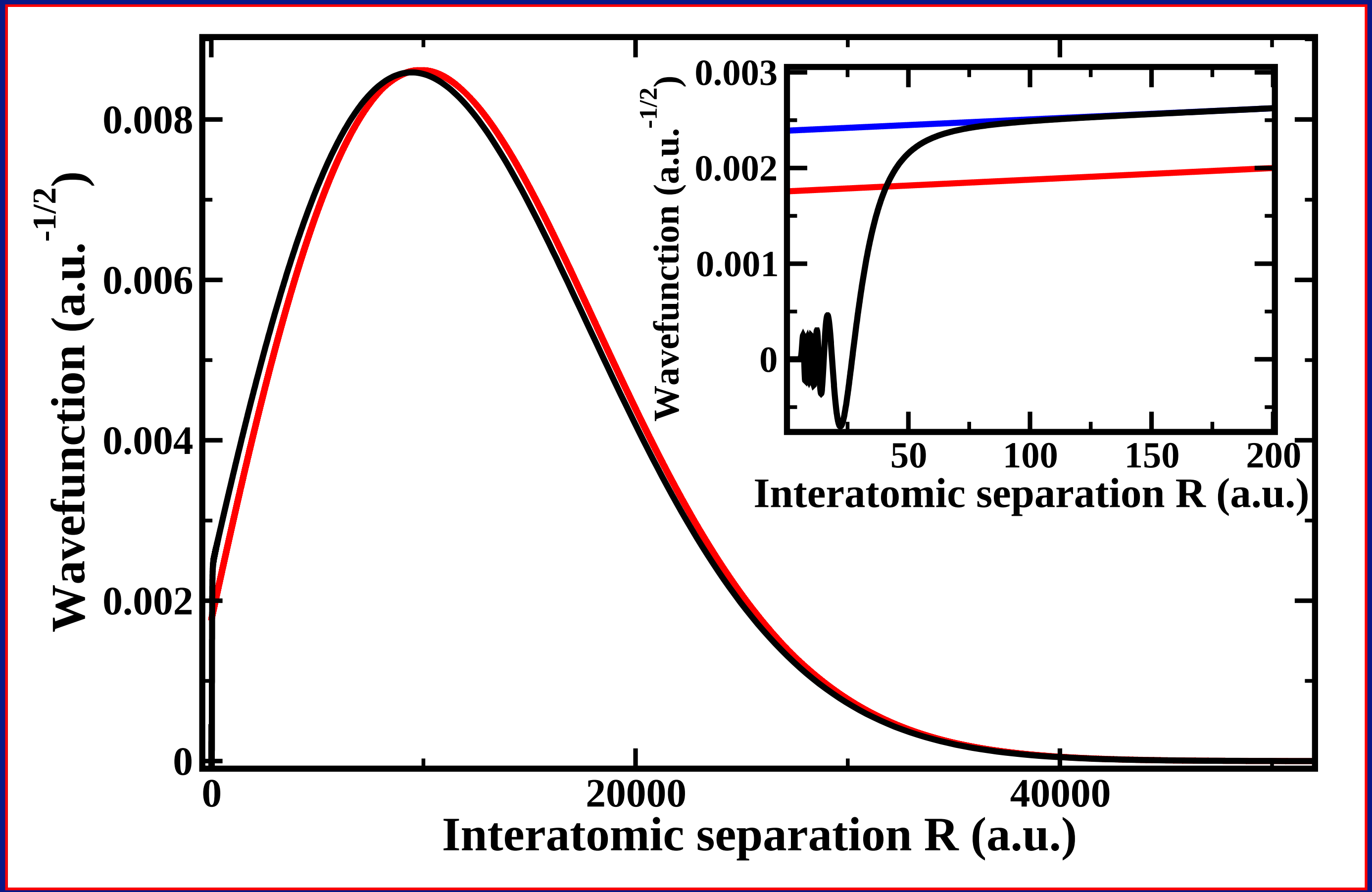
- This relation was derived for $k \rightarrow 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.
- However, energy (and length) scales are usually very different.
- "Usual" molecular bound states: orders of magnitude larger (binding) energies and much more spatially confined than trap states.

External trap potential and interatomic interaction

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 (noticeably) quantized: zero-point motion.
- However, energy (and length) scales are usually very different.
- "Usual" molecular bound states: orders of magnitude larger (binding) energies and much more spatially confined than trap states.
- 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.

External trap potential and interatomic interaction

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 (noticeably) quantized: zero-point motion.

External trap potential and interatomic interaction

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

- This relation was derived for $k \to 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.
- Intercept of ψ on R axis does not agree with $a_{\rm sc}$.
  Example ^{6}Li (state a $^3\Sigma_u$) in 10 kHz trap:
  Deviation for ψ small, intercept at -2023 for $a_{\rm sc} = -2030\,a_0$.
  This is not true for $\psi_{\rm pseudo}$: intercept at -1447 for $a_{\rm sc} = -2030\,a_0$.

External trap potential and interatomic interaction

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

- This relation was derived for $k \to 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.
- 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 $a_{\mathrm{sc}} = -2030\,a_0$.
  This is not true for ψ_{pseudo}: intercept at -1447 for $a_{\mathrm{sc}} = -2030\,a_0$.
- Introduce an energy-dependent $a_{\mathrm{sc}}(E)$ that inserted in $V_{\mathrm{pseudo}}(R)$ matches (for $E = \frac{3}{2}\,\hbar\omega_{\mathrm{trap}}$) the correct ψ (at $R \to \infty$).

External trap potential and interatomic interaction

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

- This relation was derived for $k \rightarrow 0$ (limit of zero-collision energy).
- In a (tight) trap energy is (noticeably) quantized: zero-point motion.
- 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 $a_{\mathrm{sc}} = -2030\,a_0$.

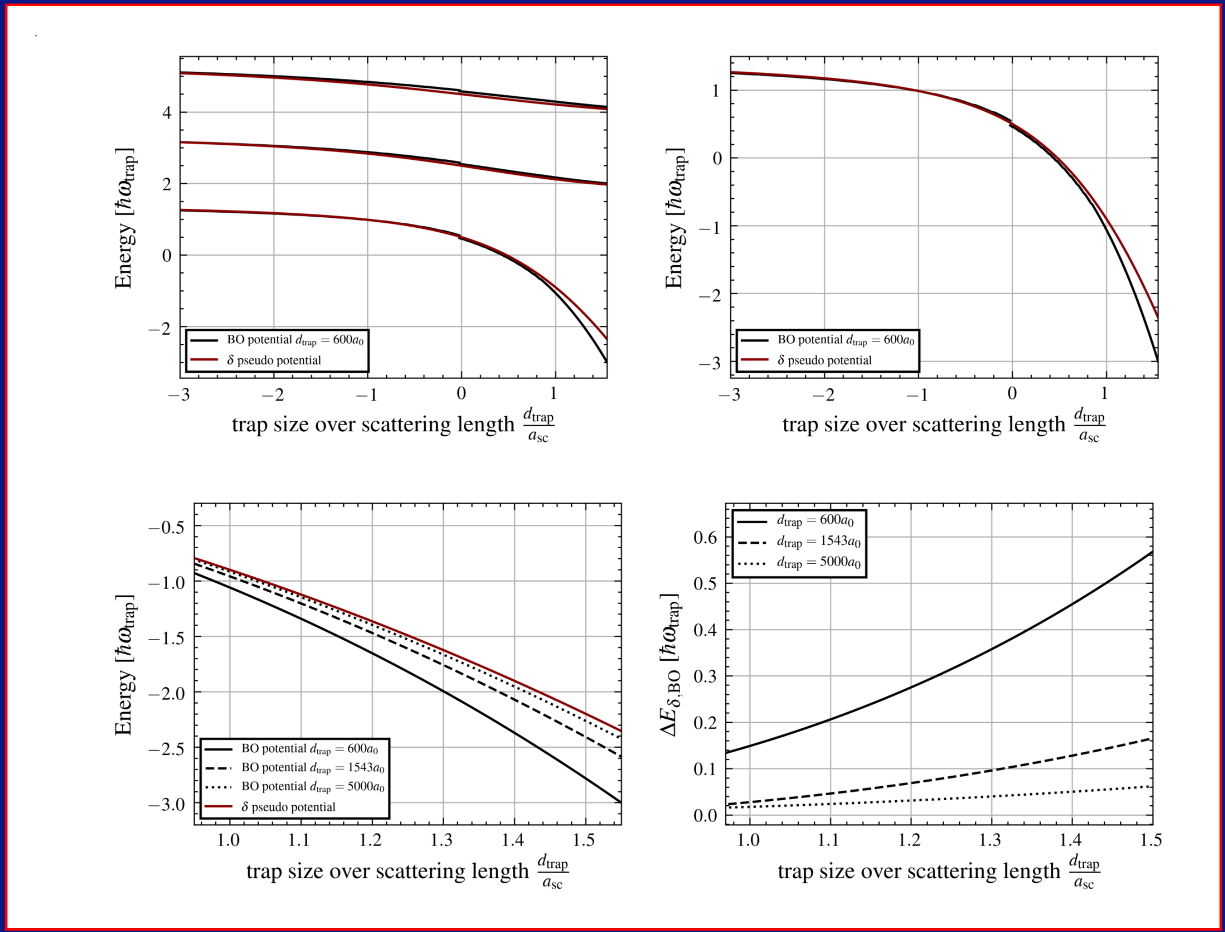
  This is not true for ψ_{pseudo}: intercept at -1447 for $a_{\mathrm{sc}} = -2030\,a_0$.
- Introduce an energy-dependent $a_{\mathrm{sc}}(E)$ that inserted in $V_{\mathrm{pseudo}}(R)$ matches (for $E = \frac{3}{2}\,\hbar\omega_{\mathrm{trap}}$) the correct ψ (at $R \rightarrow \infty$).

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

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

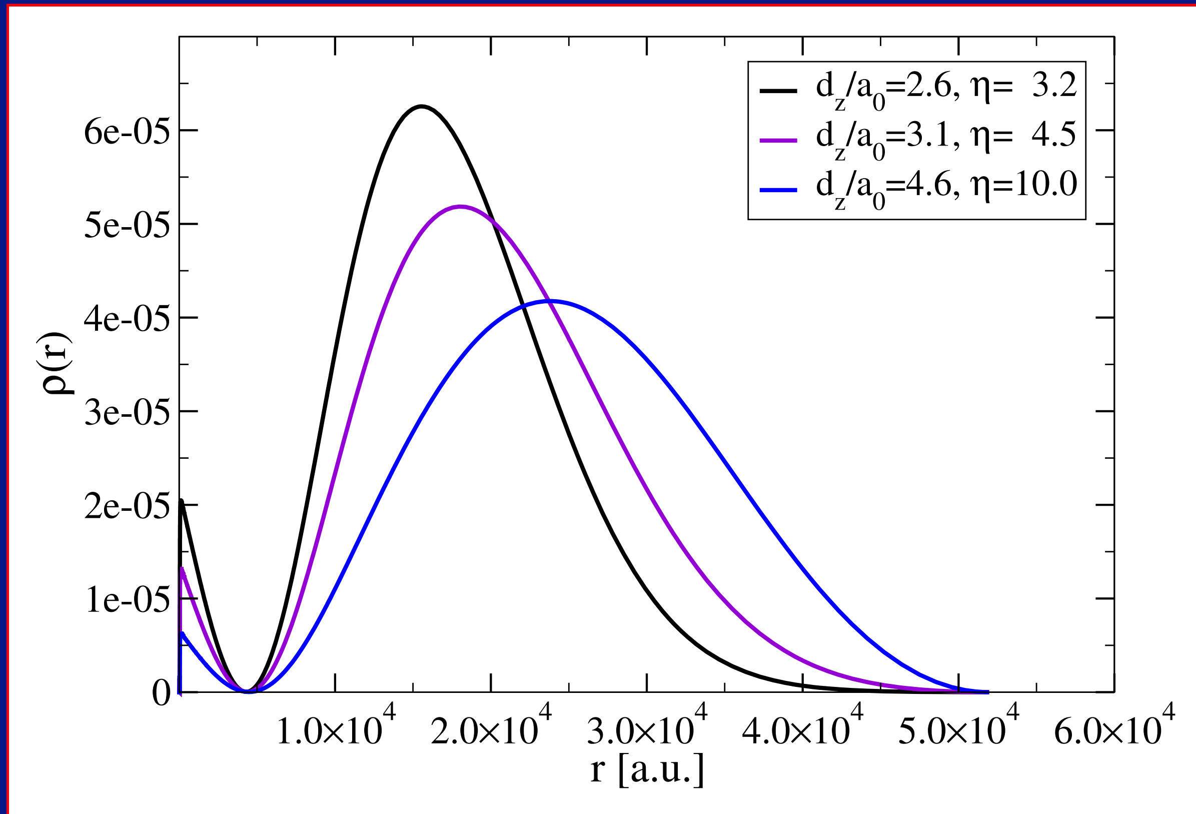
Trap size (in)dependence

Analytical solution for two identical particles with δ interaction in harmonic trap
$\longrightarrow$ energies depend only on the ratio scattering length a_s to trap length $d_{\rm ho}$.



Trap-length independence is not valid for realistic interaction potential!

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



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

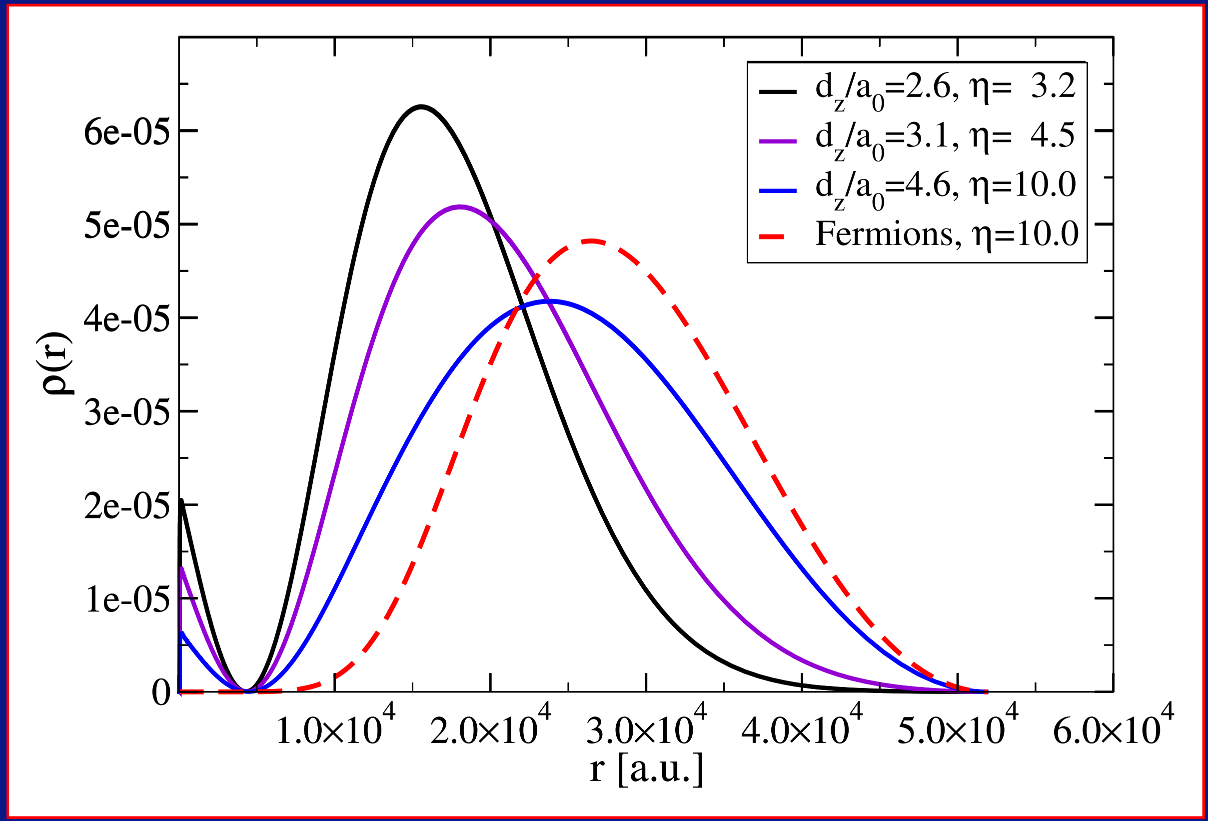
– scattering length $a_0 = 5624$ a.u.

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

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

– full Born-Oppenheimer potential.

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



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

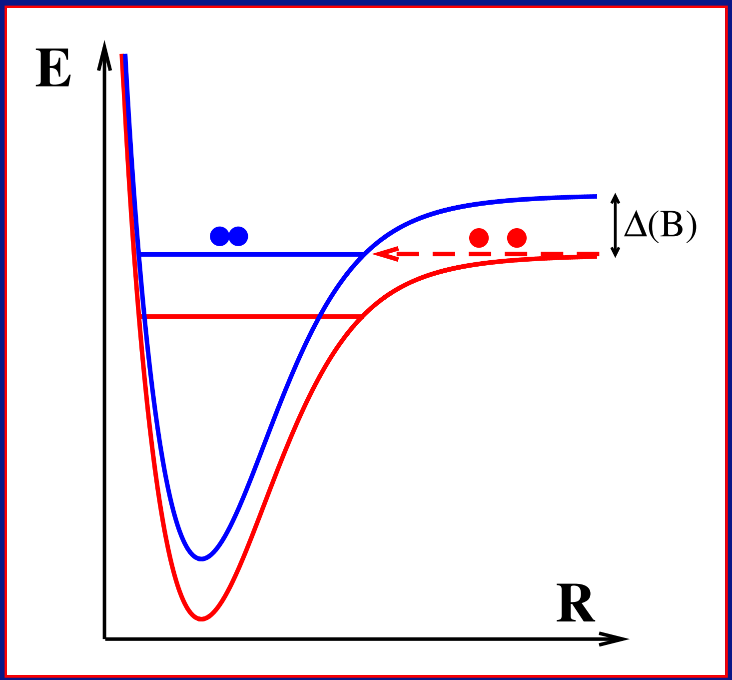
– scattering length $a_0 = 5624$ a.u.

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

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

– full Born-Oppenheimer potential.

Tunable interaction: magnetic Feshbach resonances



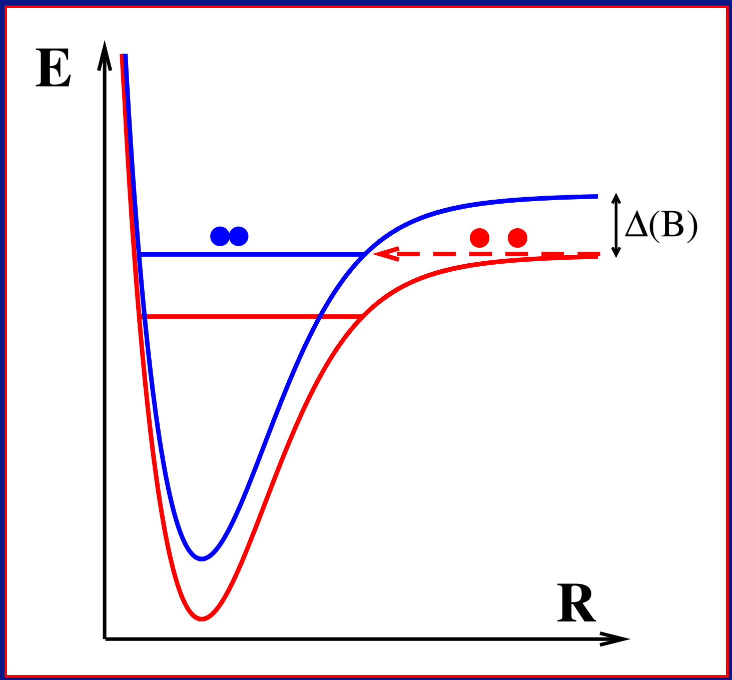
Simple picture:

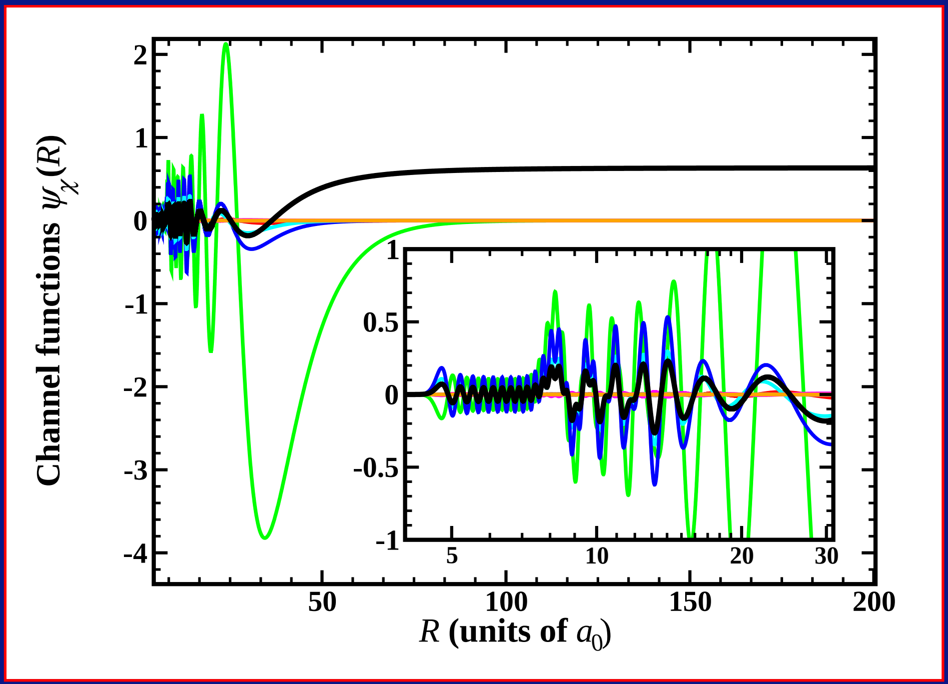
Only **2 channels**:

– open (continuum) channel,

– closed (bound) channel.

Tunable interaction: magnetic Feshbach resonances





Simple picture:

Only **2 channels**:

– open (continuum) channel,

– closed (bound) channel.

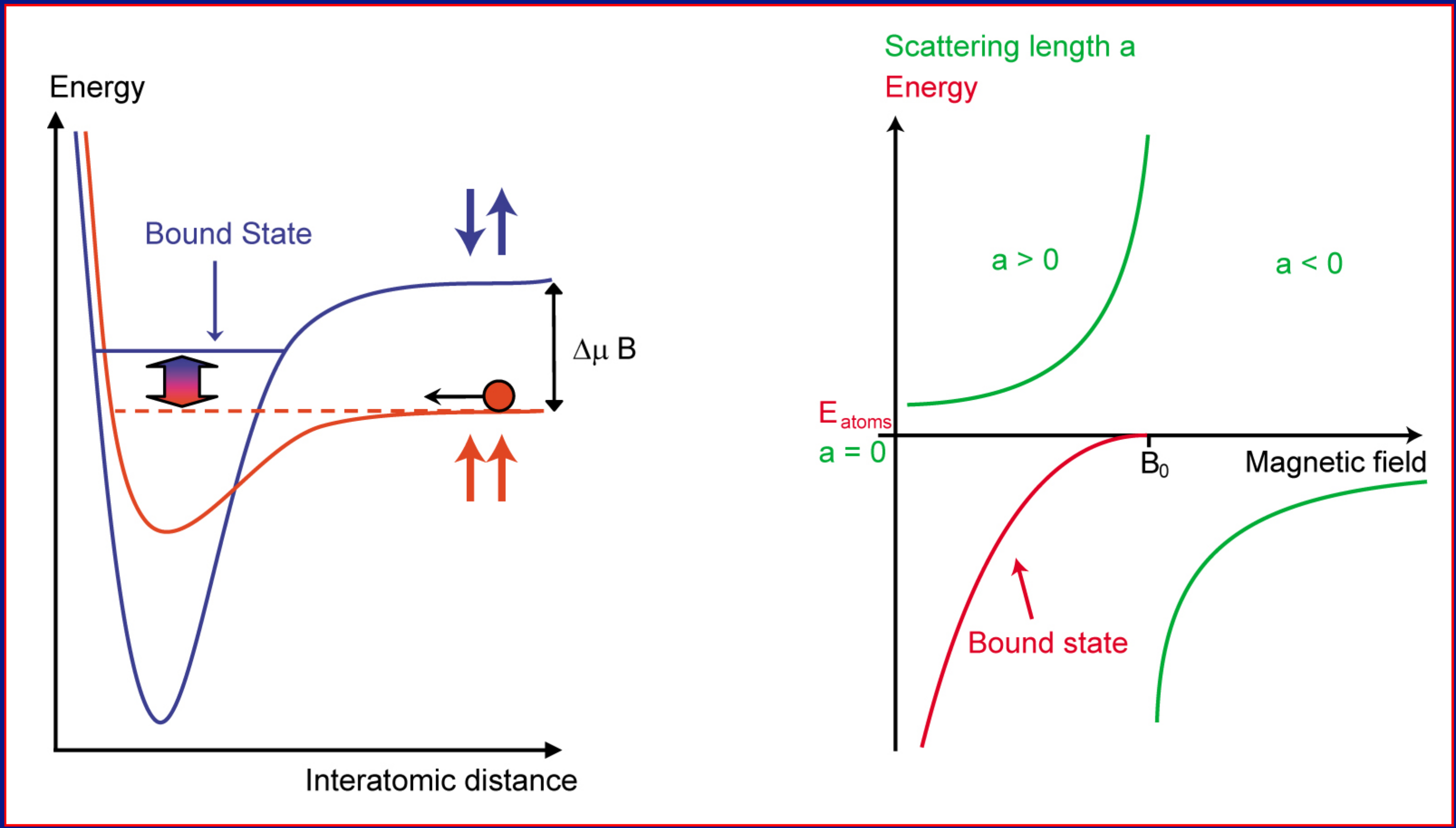
Multichannel reality:

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)].

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)].
- **Theory for magnetic Feshbach resonances derived for free space**.

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)].
- **Theory for magnetic Feshbach resonances derived for free space**.

Influence of lattice (confinement) on magnetic Feshbach resonances?

Magnetic Feshbach resonances (MFRs) in a harmonic trap

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

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.)

With this one can

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.)

With this one can

1. recover the known energy relation in the trap
   ($a_{\mathrm{ho}} = \sqrt{\hbar/m\omega}$)

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

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.)

With this one can

1. recover the known energy relation in the trap
   ($a_{\mathrm{ho}} = \sqrt{\hbar/m\omega}$)

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

2. derive the energy-dependent scattering length

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

   in contrast to a previously suggested form

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

Magnetic Feshbach resonances (MFRs) in a harmonic trap

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

With this one can

1. recover the known energy relation in the trap ($a_{\text{ho}} = \sqrt{\hbar/m\omega}$)

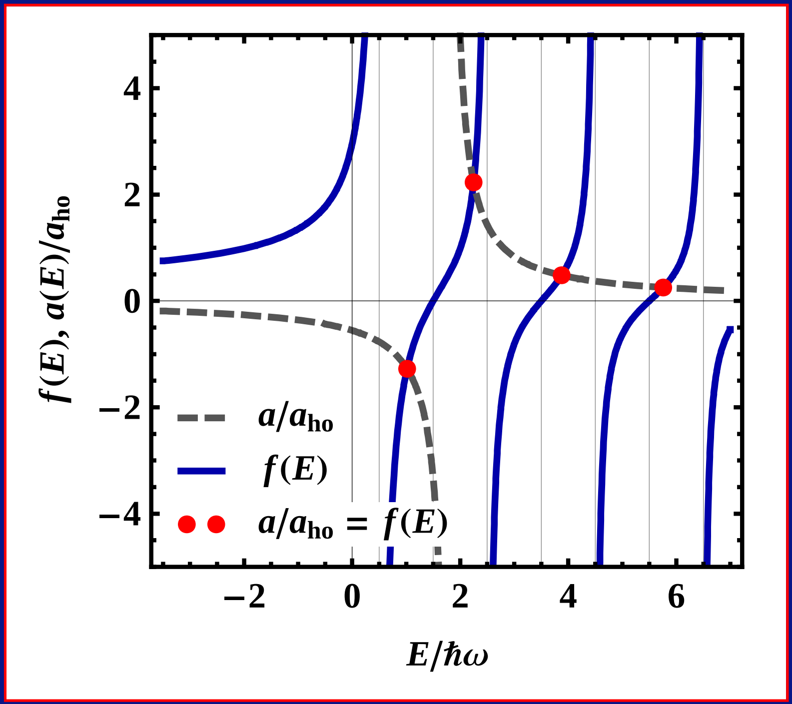
$$\frac{a}{a_{\text{ho}}} = f(E) \equiv \frac{\Gamma\left(1/4 - E/2\hbar\omega\right)}{\Gamma\left(3/4 - E/2\hbar\omega\right)}$$

2. derive the energy-dependent scattering length

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

in contrast to a previously suggested form

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



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

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.)

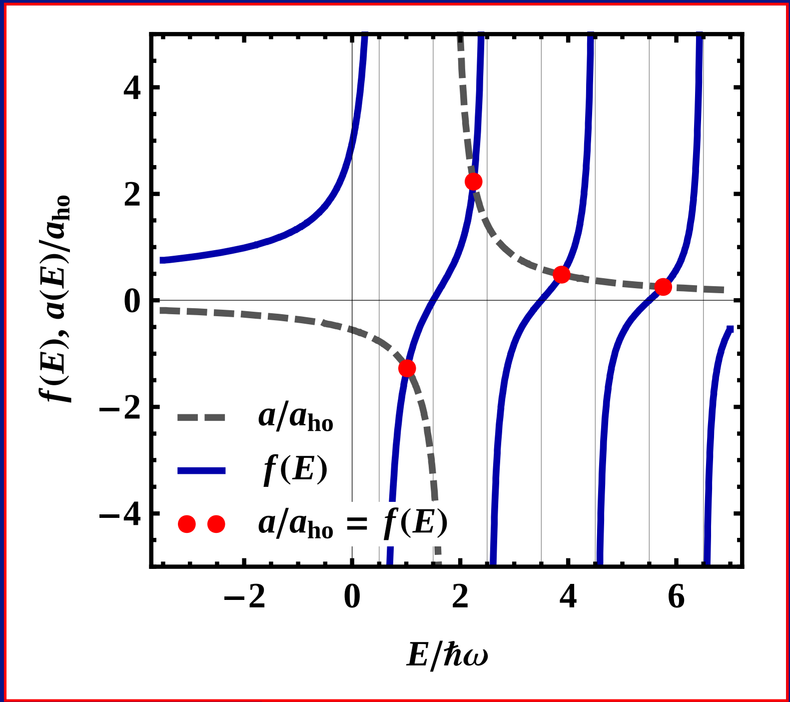
With this one can

1. recover the known energy relation in the trap ($a_{\mathrm{ho}} = \sqrt{\hbar/m\omega}$)

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

2. derive the energy-dependent scattering length

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



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

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.)

With this one can

1. recover the known energy relation in the trap ($a_{\rm ho} = \sqrt{\hbar/m\omega}$)

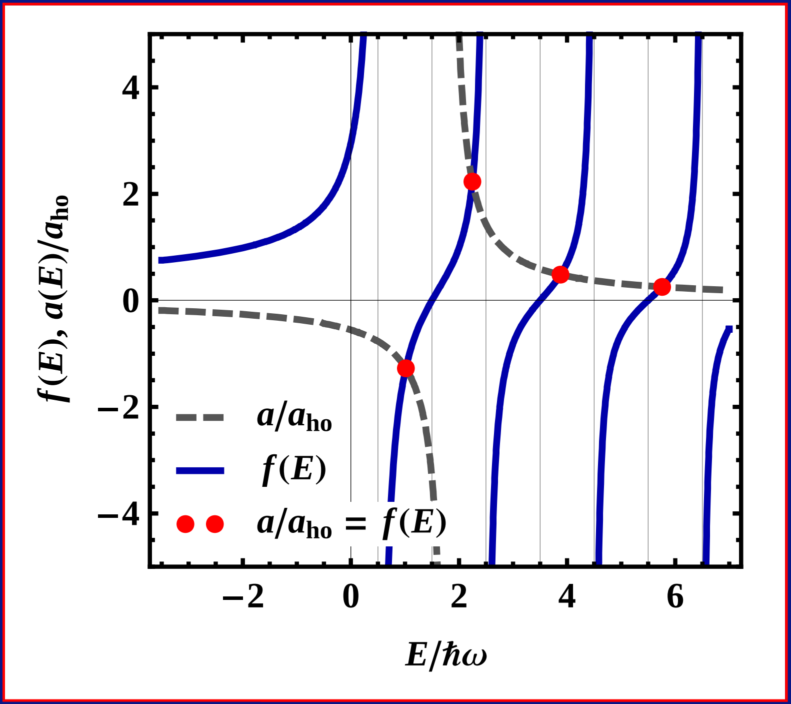
$$\frac{a}{a_{\rm ho}} = f(E) \equiv \frac{\Gamma\left(1/4 - E/2\hbar\omega\right)}{\Gamma\left(3/4 - E/2\hbar\omega\right)}$$

2. derive the energy-dependent scattering length

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

3. derive the admixture of the closed channel

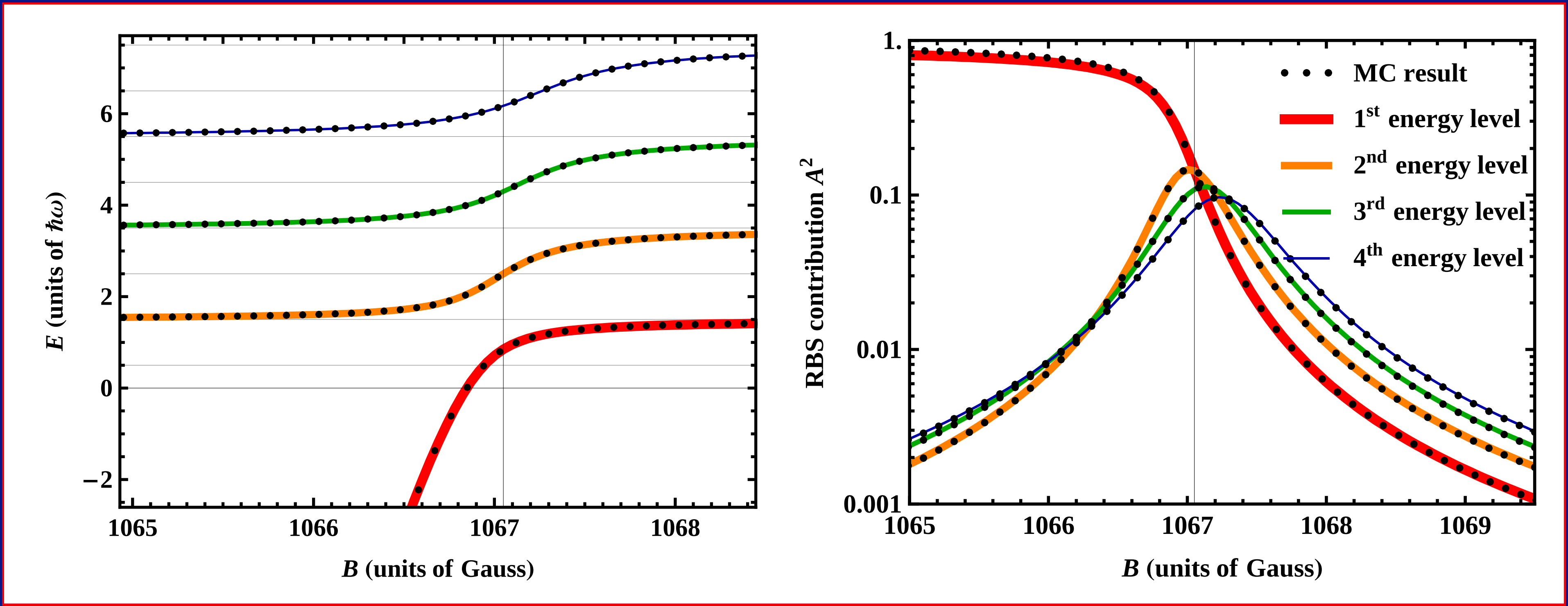
$$\frac{A}{C} \propto \frac{f(E) - a_{\rm bg}/a_{\rm ho}}{\sqrt{f'(E)}}$$



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

How good is the model?

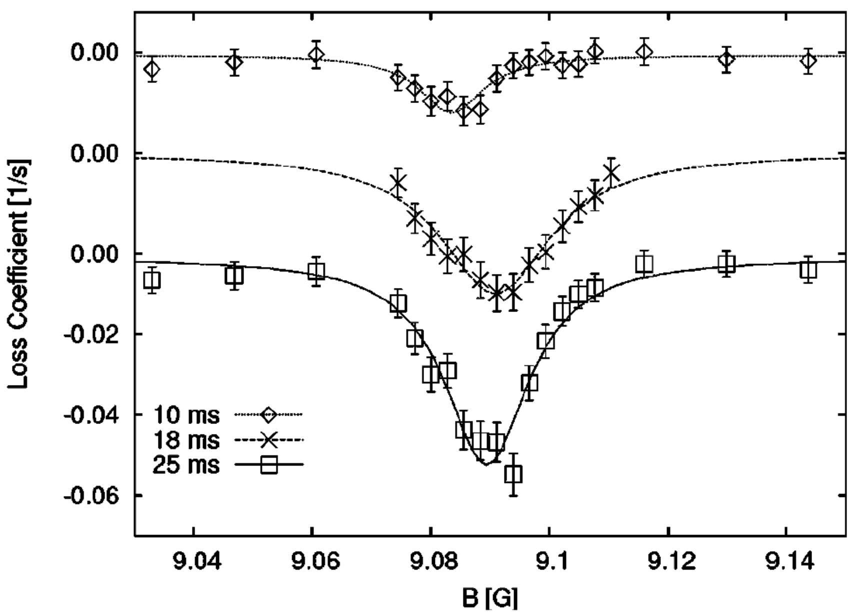
Comparison with full coupled-channel calculations for ^{6}Li-^{87}Rb in a 200 kHz trap:

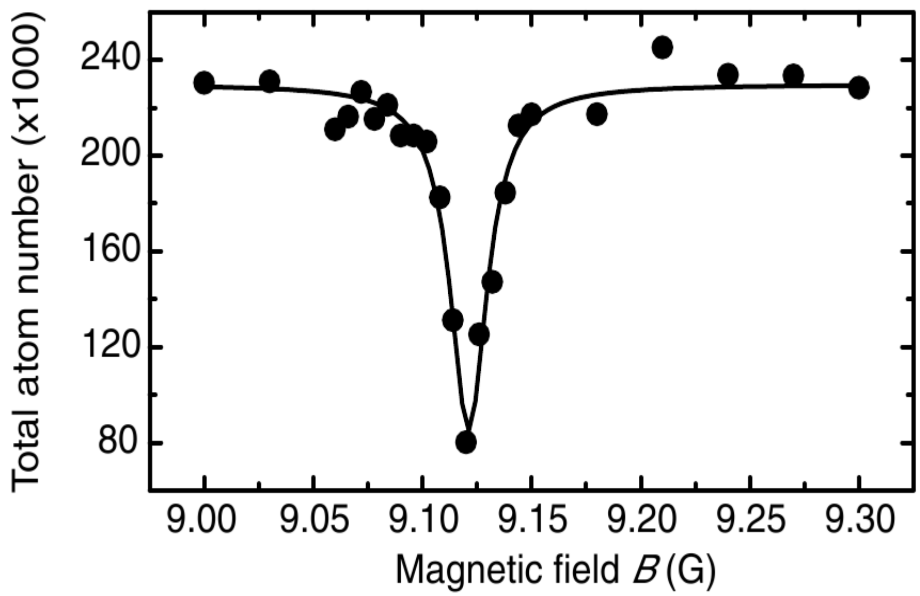


- **Energy deviation** $< 0.003\,\hbar\omega$.
- **Closed-channel admixture deviation** $< 0.1\%$.

Explaining a puzzling 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}),
- the harmonic approximation is adopted for the lattice potential, and
- both atoms “feel” the same lattice potential.

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}),
- the harmonic approximation is adopted for the lattice potential, and
- both atoms "feel" the same lattice potential.

However, coupling of center-of-mass (COM) and relative (REL) motion

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

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).

Elastic confinement-induced resonances (ECIR)

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

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

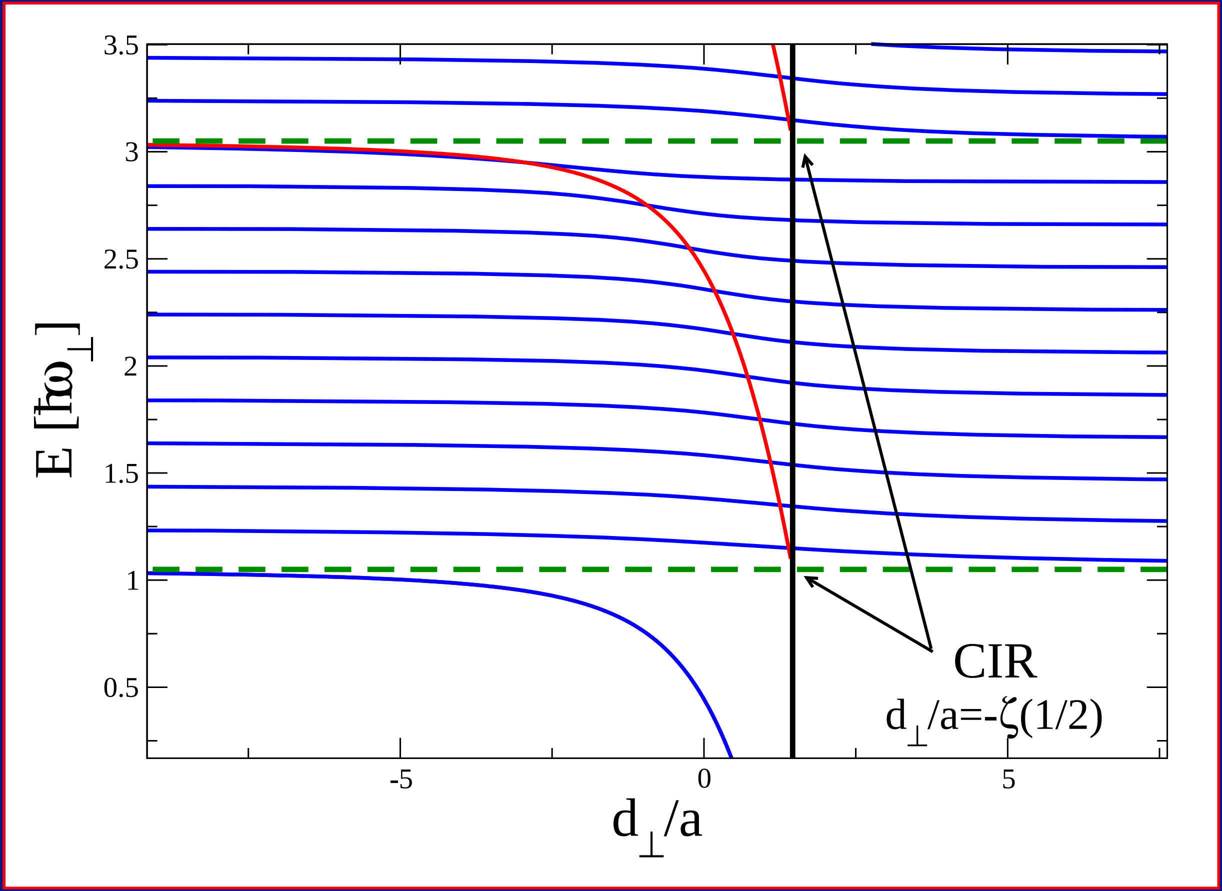
Resonance: $g_{1D} \to \infty$ for $\frac{d_\perp}{a} \;=\; -\zeta(\frac{1}{2}) \;\approx\; 1.46\ldots$

Analogously: confinement-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:

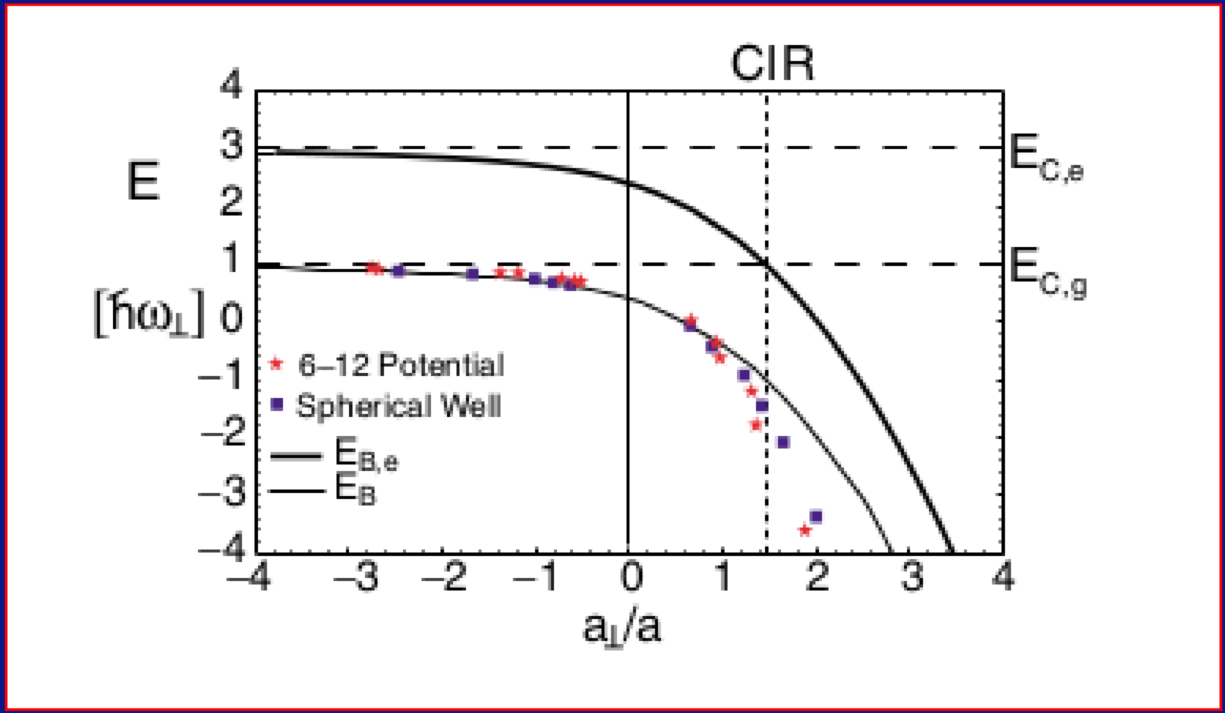


Blue: quasi 1D spectrum

Red: artificially(!) excited bound state

Green: quasi continuum threshold

Olshanii's model (II)



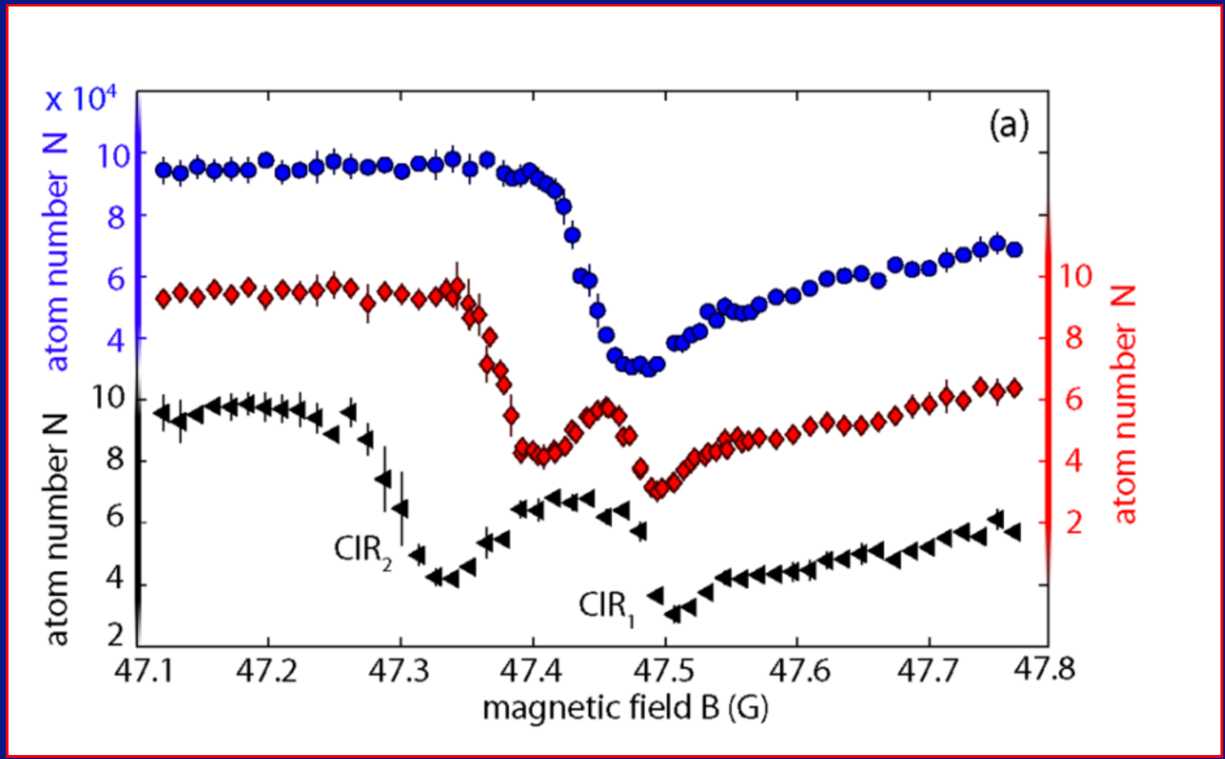
T. Bergeman et al., PRL **91**, 163201 (2003)

Result:

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

Note: No data points on shifted state!

Innsbruck experiment (Cs atoms)

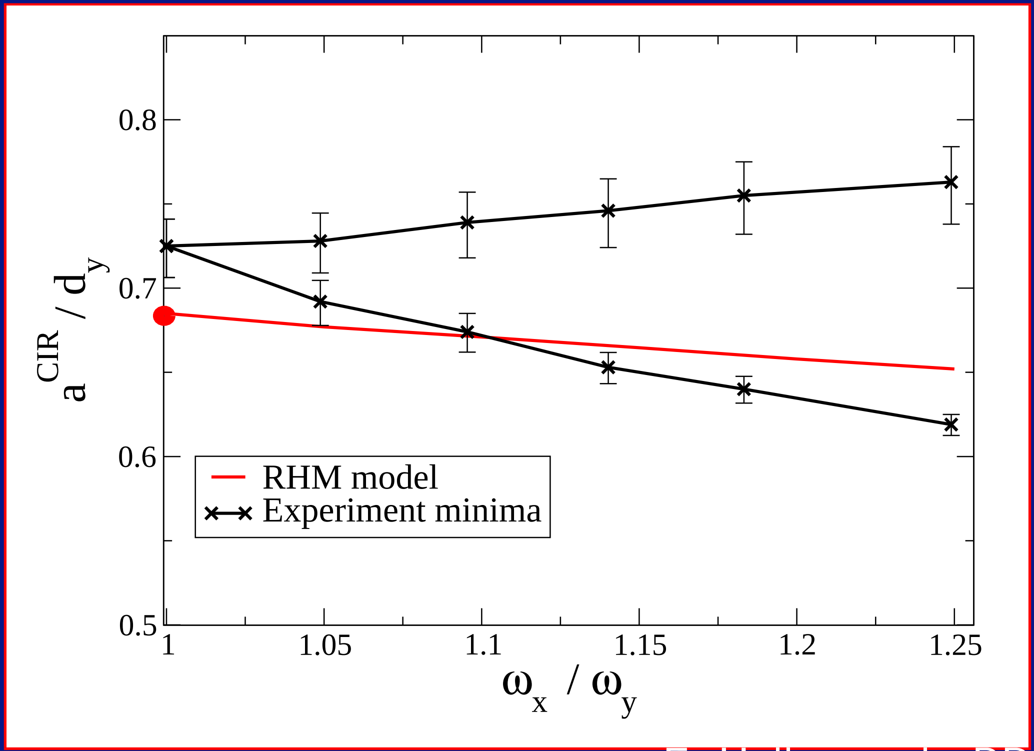


Blue curve: Atom losses for $\omega_x = \omega_y \gg \omega_z$ (anisotropy fixed, a varied).

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

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

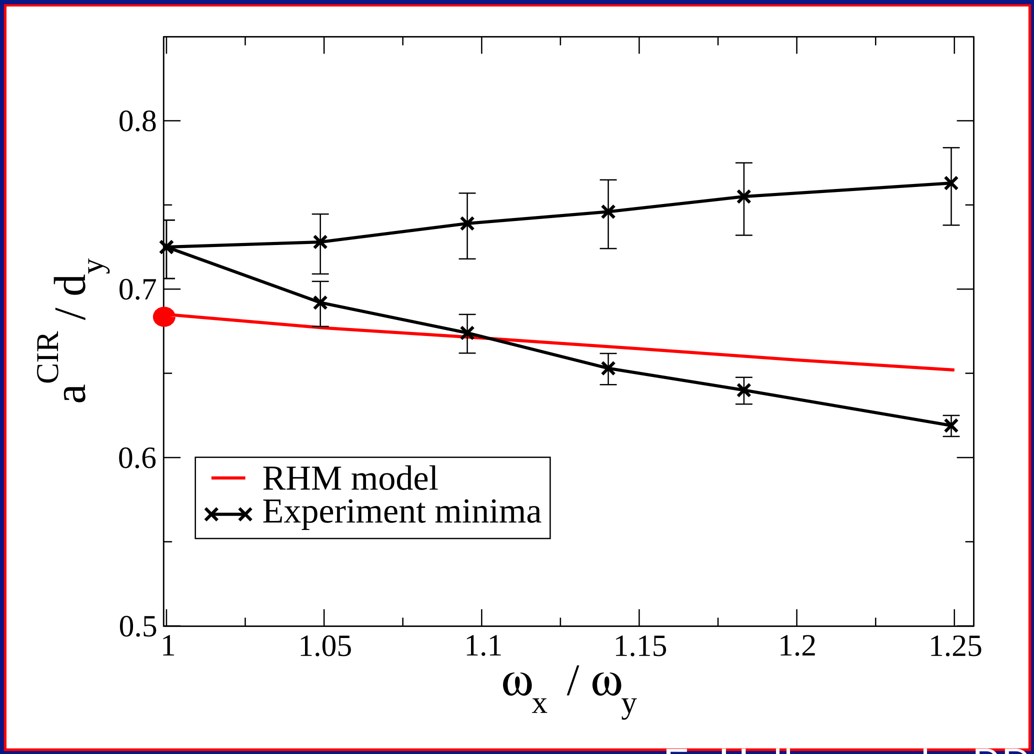
Problem: agreement and conflict with theory



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

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

Problem: agreement and conflict with theory



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 $\omega_x = \omega_y$.

Complete confusion:

Innsbruck loss experiment (Haller et al.):

- **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.

Complete confusion:

Innsbruck loss experiment (Haller et al.):

- **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.

Complete confusion:

Innsbruck loss experiment (Haller et al.):

- **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.

Complete confusion:

Innsbruck loss experiment (Haller et al.):

- **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: direct measurement of the binding energies.

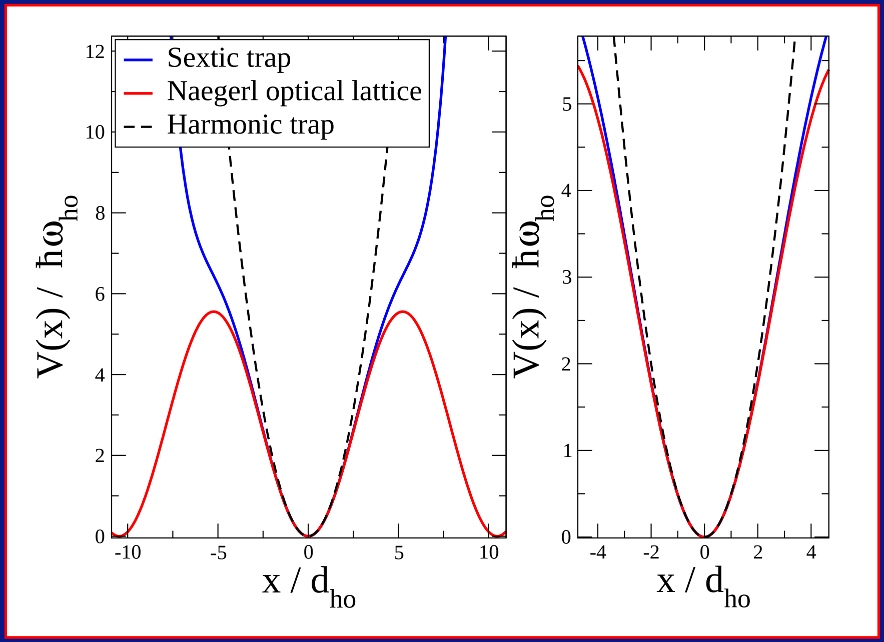
Full treatment of two atoms in quasi-1D trap:

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

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

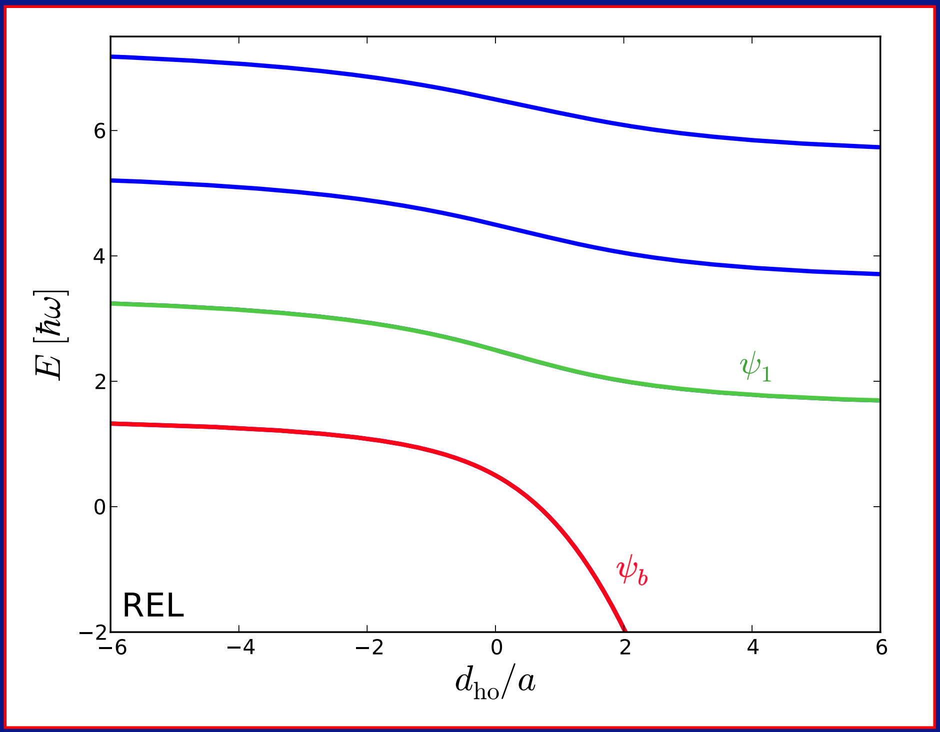
Note:

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



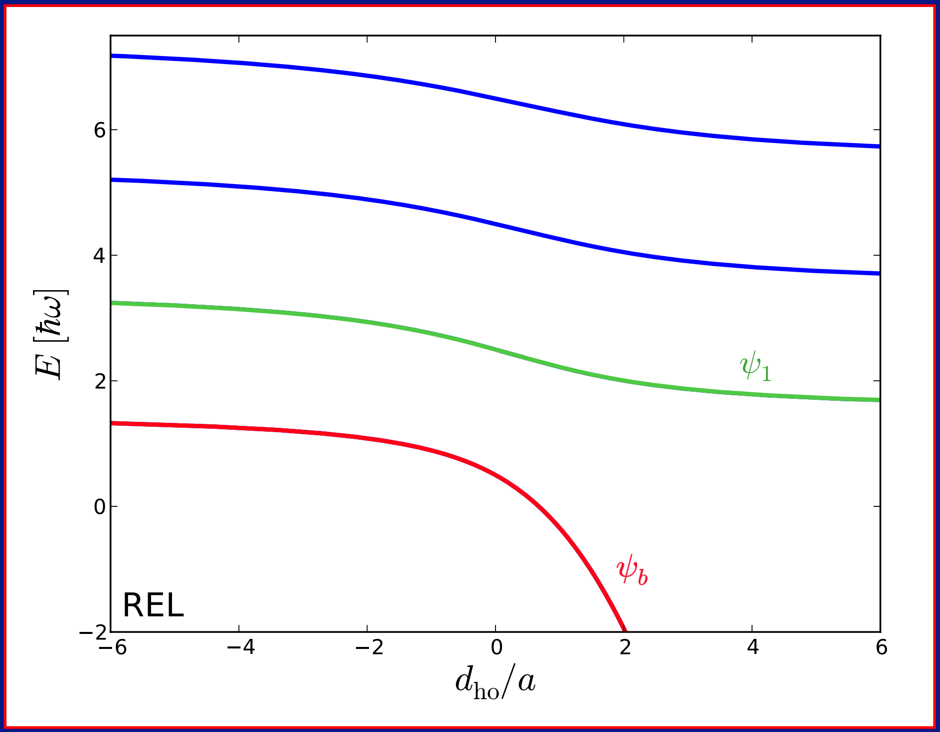
Relative motion only

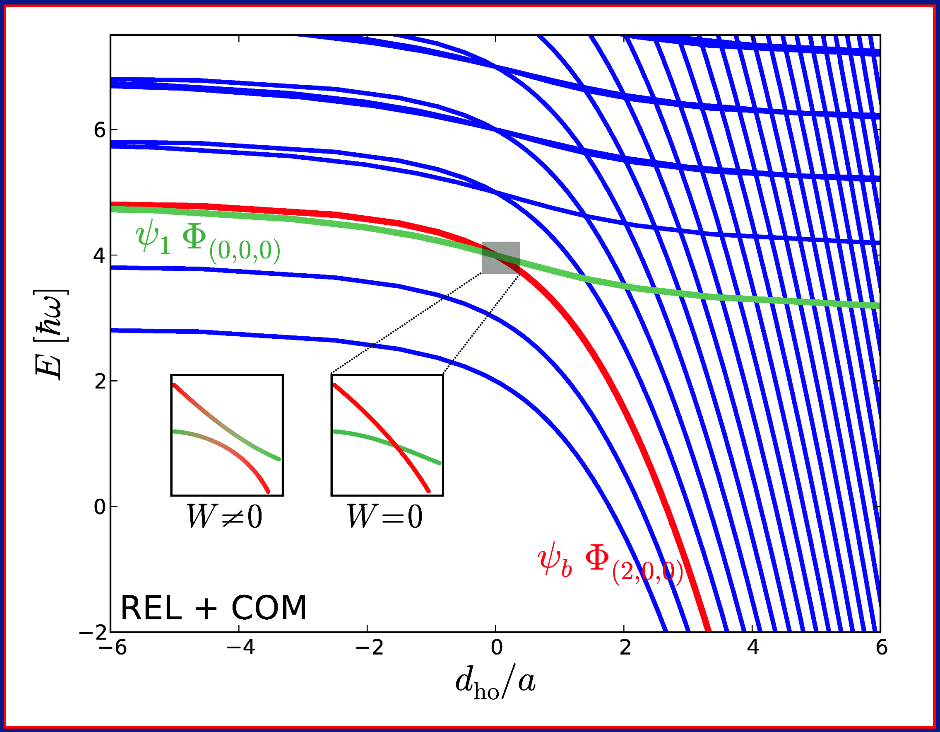
ψ_b: (molecular) bound state

ψ_1: lowest-lying trap state

Energy spectra (cartoon)

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





Relative motion only

ψ_b: (molecular) bound state

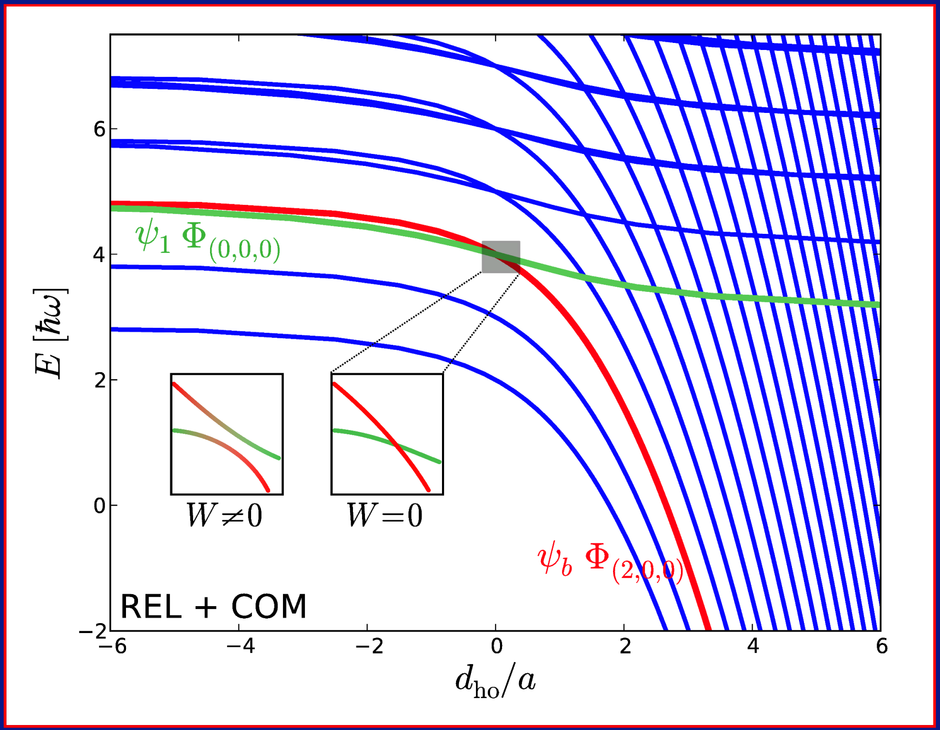
ψ_1: lowest-lying trap state

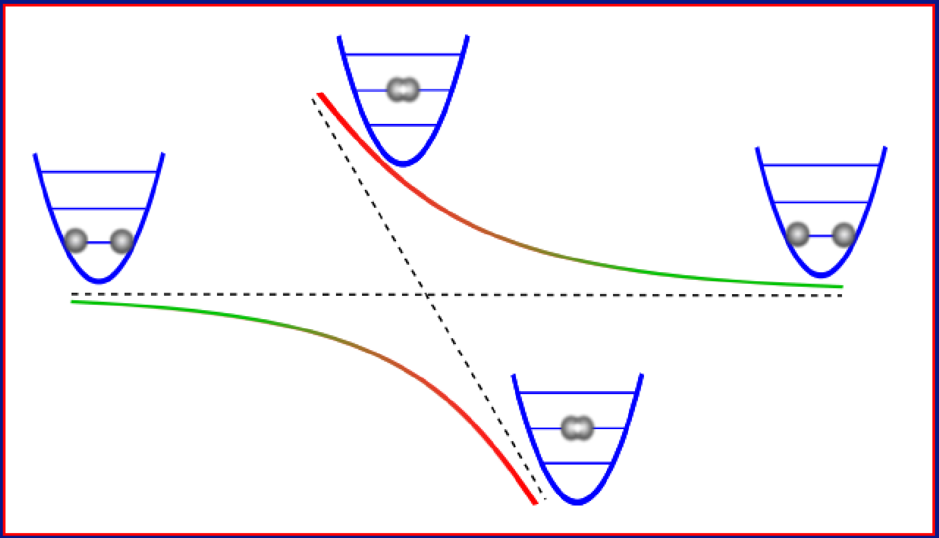
Full spectrum

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

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

Molecule formation due to confinement





Full spectrum

Avoided crossing

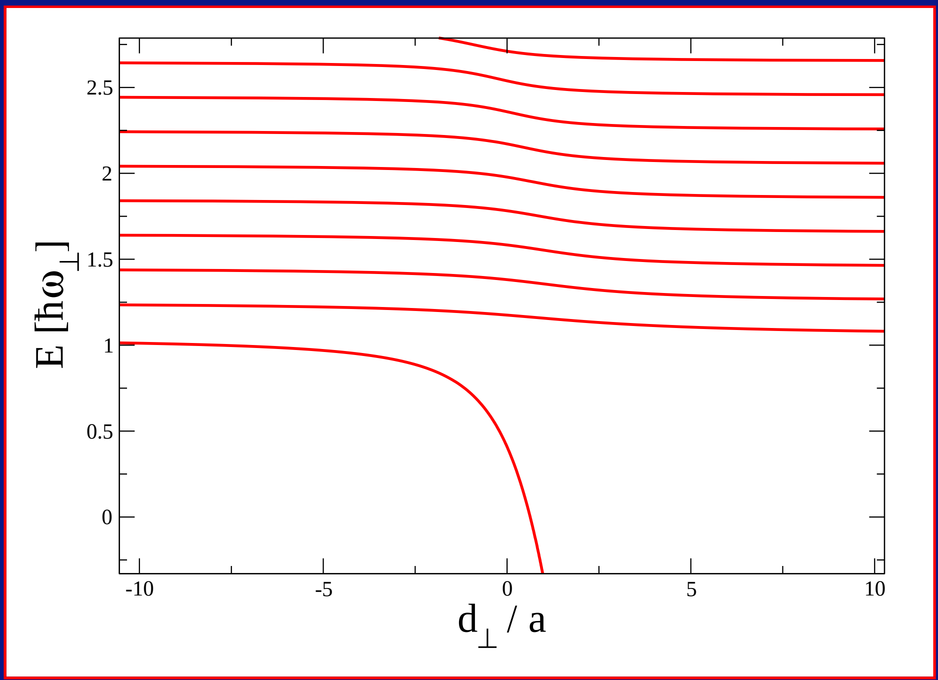
Coupling of center-of-mass (com) and relative (rel) motion ($W \neq 0$):

$\longrightarrow$ avoided crossing

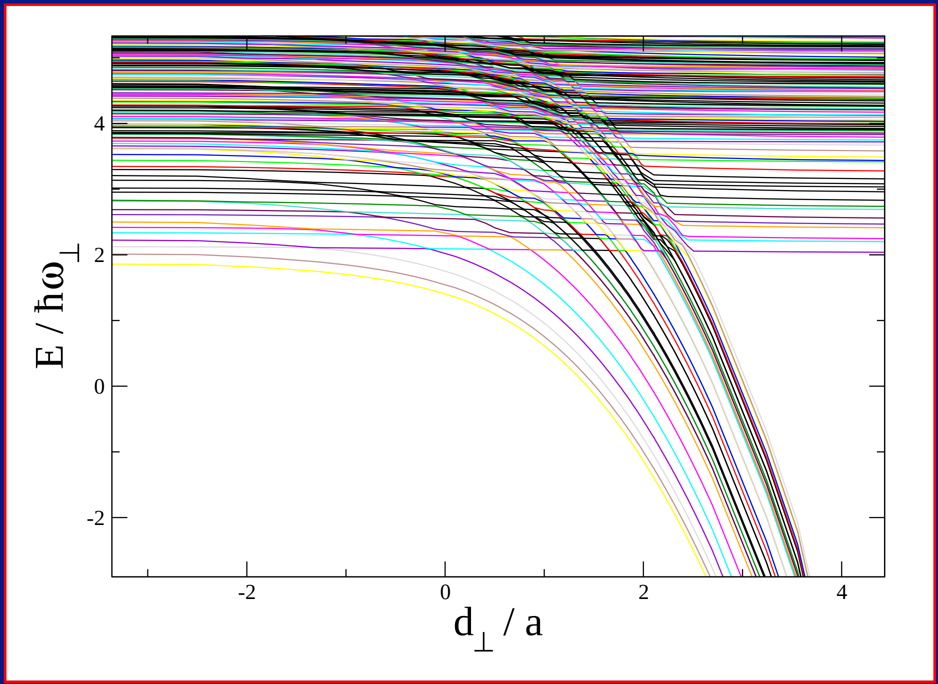
$\longrightarrow$ **molecule formation possible!**

Energy spectra (ab initio results)

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



REL

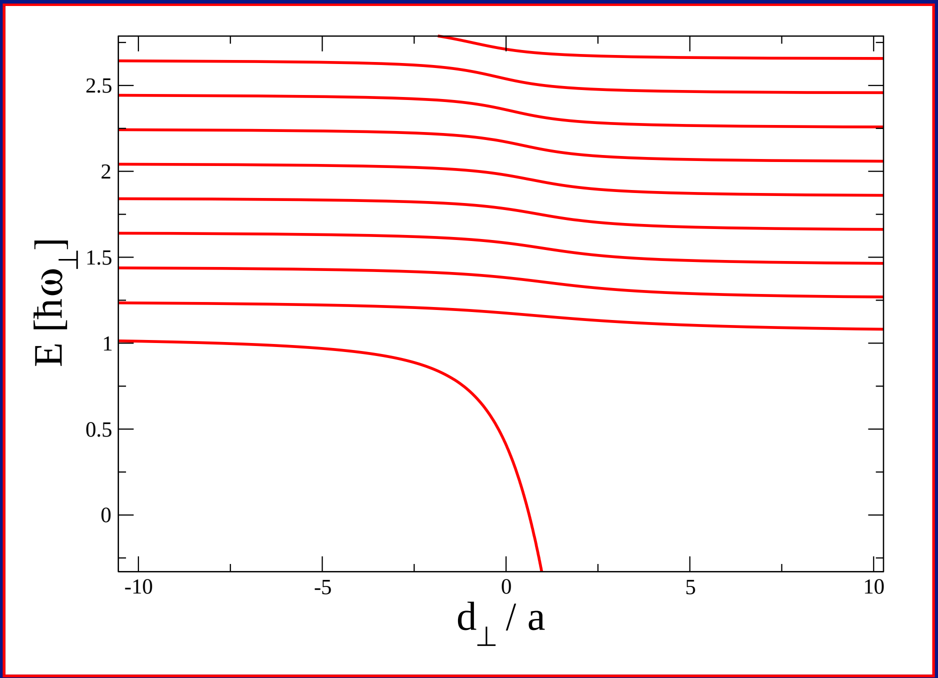


REL + COM + COUPLING

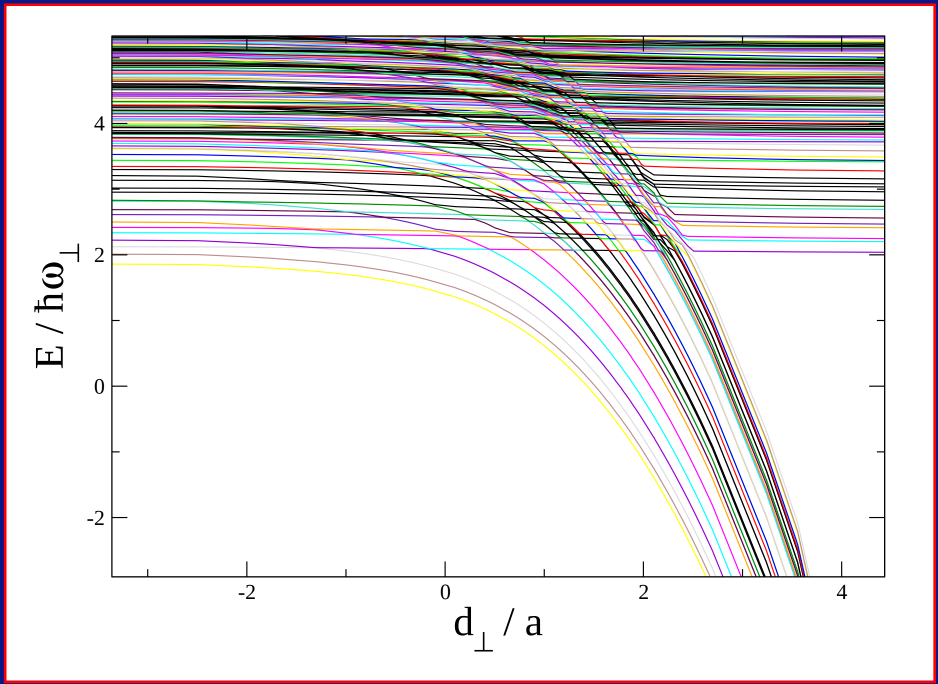
Many crossings are found in the coupled model,

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

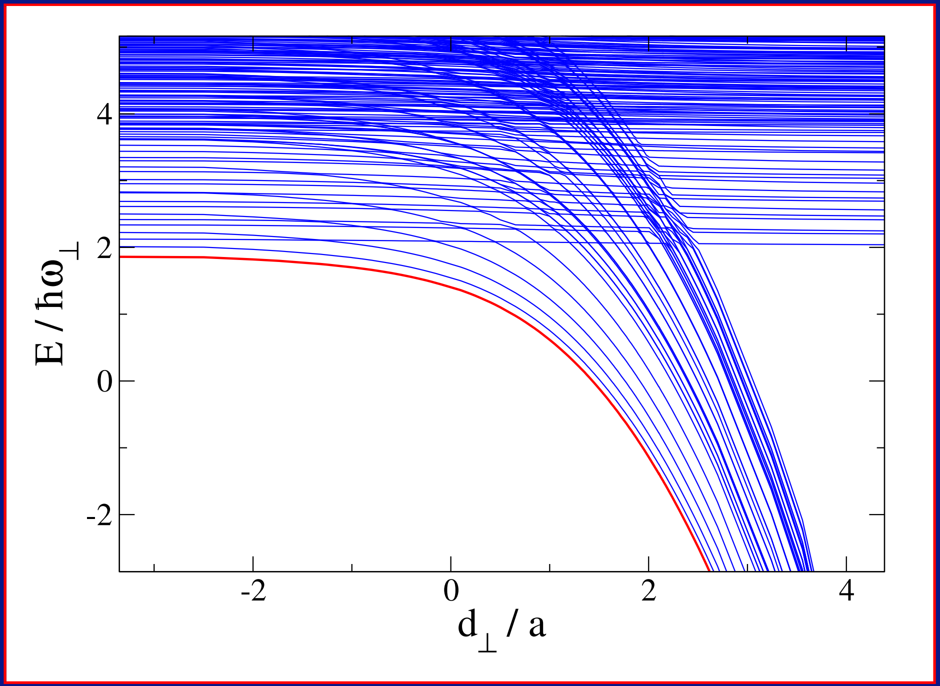
Ultracold: only ground trap state populated $\Longrightarrow m = k = 0$.

Resonances:

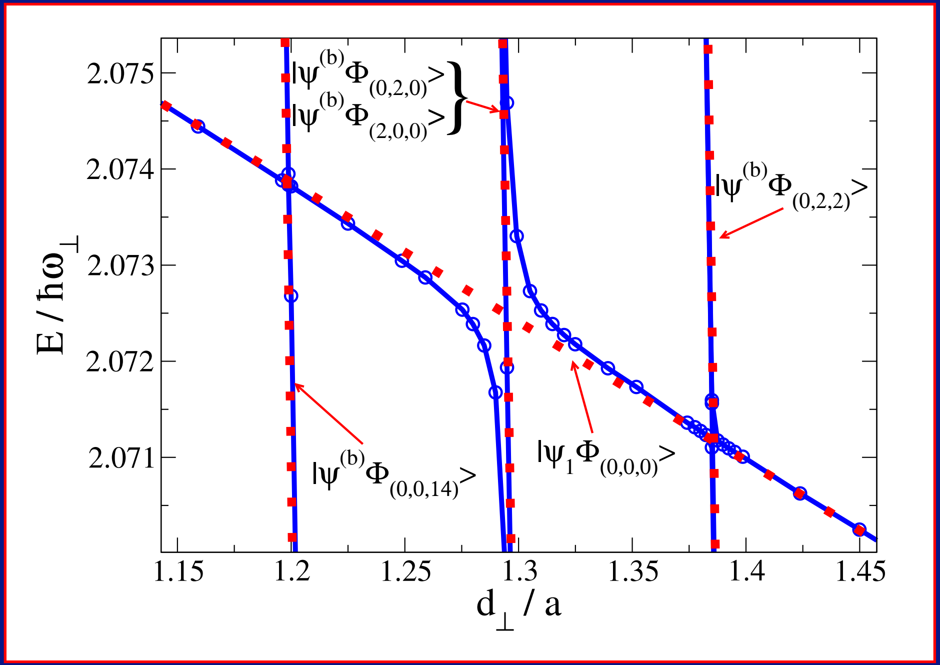
Crossing of transversally COM excited REL bound state with ground (COM and REL) trap state.

Avoided Crossings (I)

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



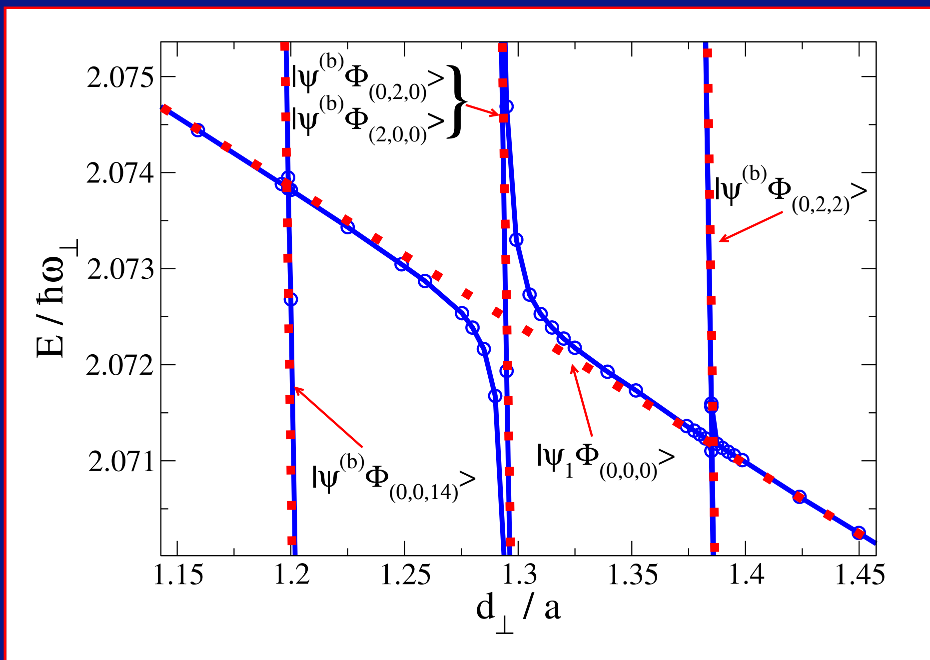
Large part of spectrum



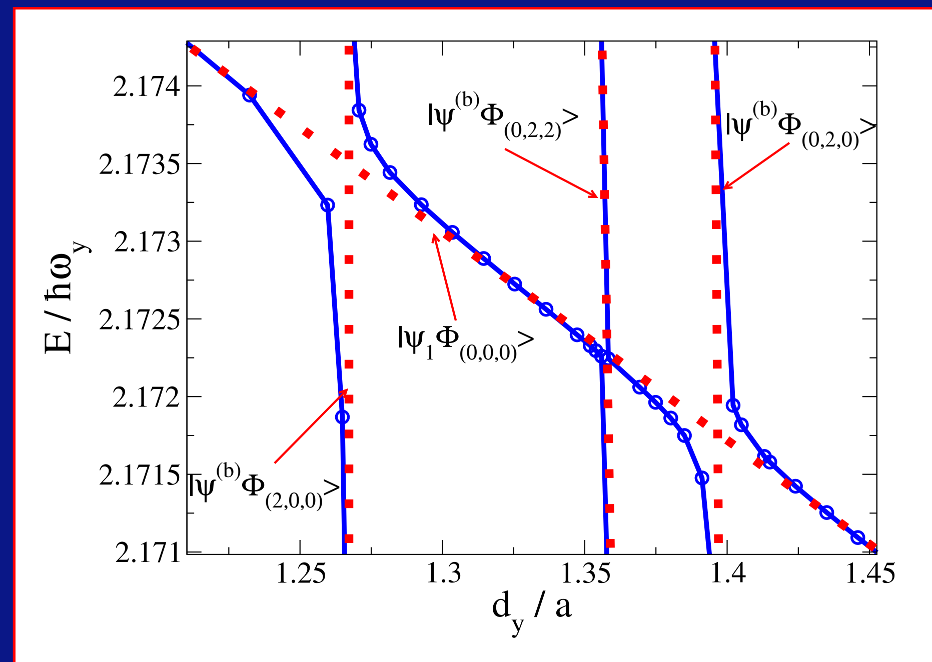
Zoom-in in spectrum.

Avoided Crossings (II)

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



$\omega_x = \omega_y \gg \omega_z$



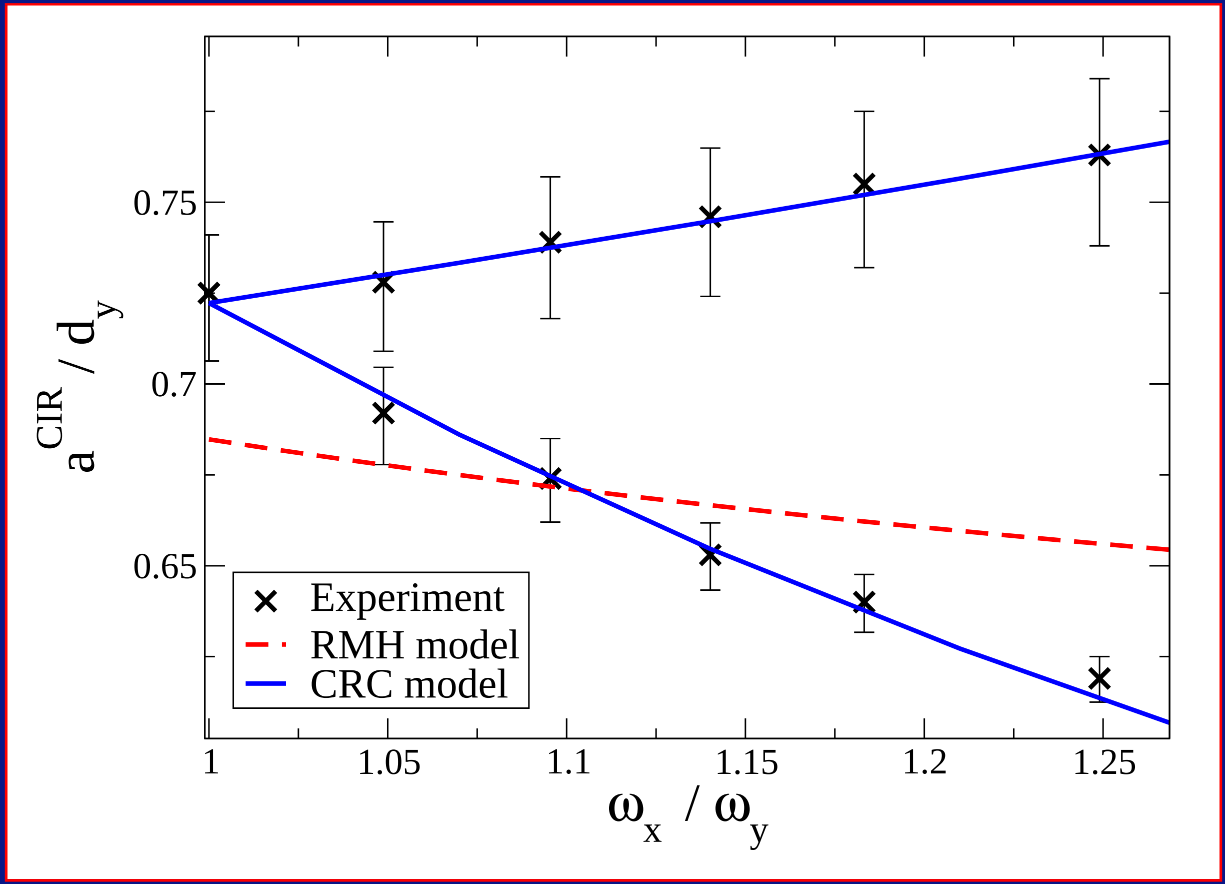
$\omega_x \neq \omega_y \gg \omega_z$

$\Rightarrow$ 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)]

Elastic vs. inelastic CIRs

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).
- **Inelastic CIR:** molecule formation, thus atom loss.

Elastic vs. inelastic CIRs

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).
- **Inelastic CIR:** molecule formation, thus atom loss.
- **Quasi 1D:** accidentally at similar positions (in fact overlapping), but widths differs by about one order of magnitude (elastic: broader).
- **Quasi 2D:** positions differ even by sign of a.

Elastic vs. inelastic CIRs

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).
- **Inelastic CIR:** molecule formation, thus atom loss.
- **Quasi 1D:** accidentally at similar positions (in fact overlapping), but widths differs by about one order of magnitude (elastic: broader).
- **Quasi 2D:** positions differ even by sign of a.

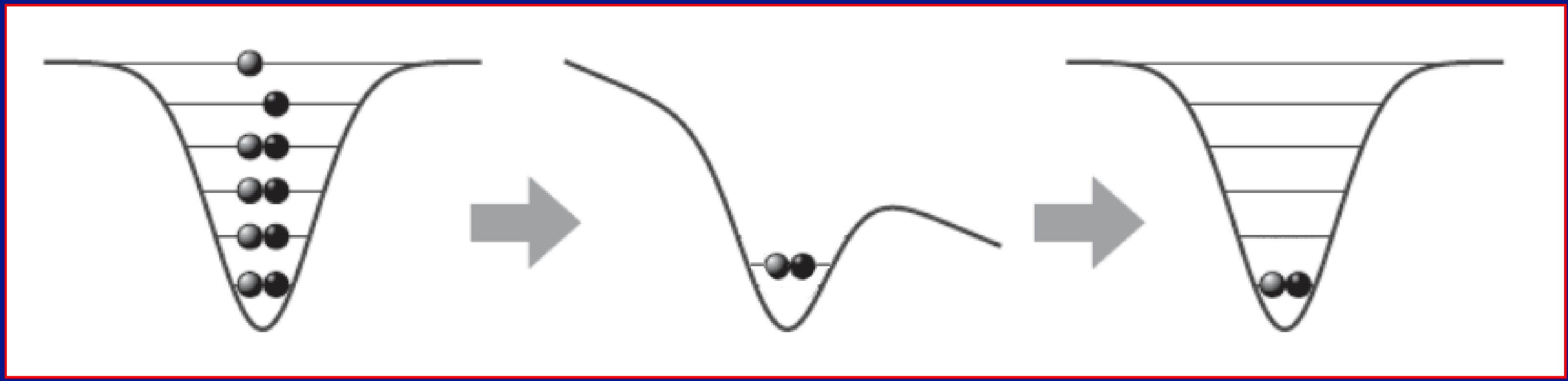
Note: The possibility to create molecules due to anharmonicity had earlier been suggested: Bolda, Tiesinga, Julienne [PRA **71**, 033404 (2005)]; Schneider, Grishkevich, A.S, [*Phys. Rev. A* **80**, 013404 (2009)]; Kestner, Duan [*N. J. Phys.* **12**, 053016 (2010)].

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)]

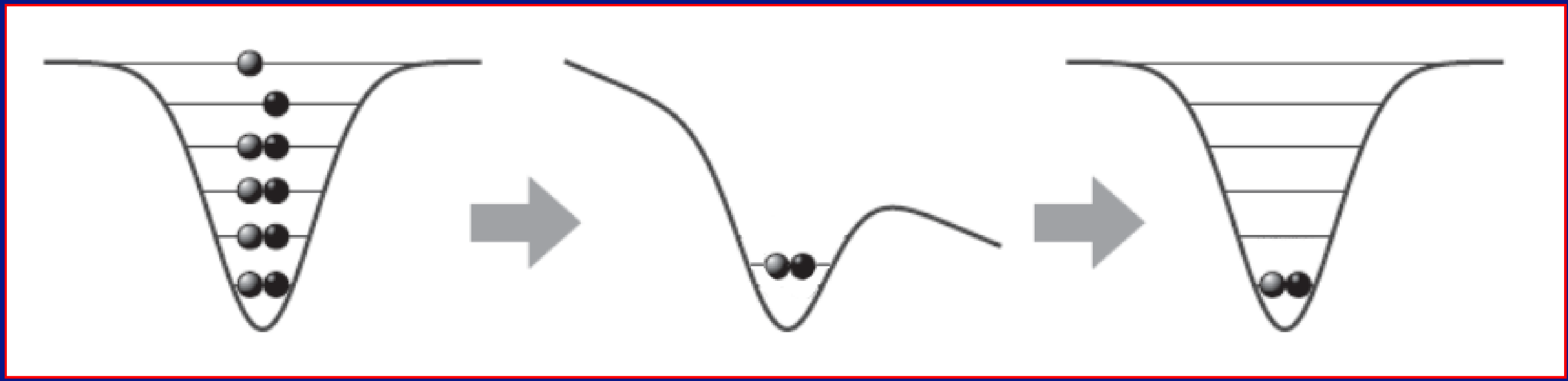


Experimental test (with group of S. Jochim)

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)]



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

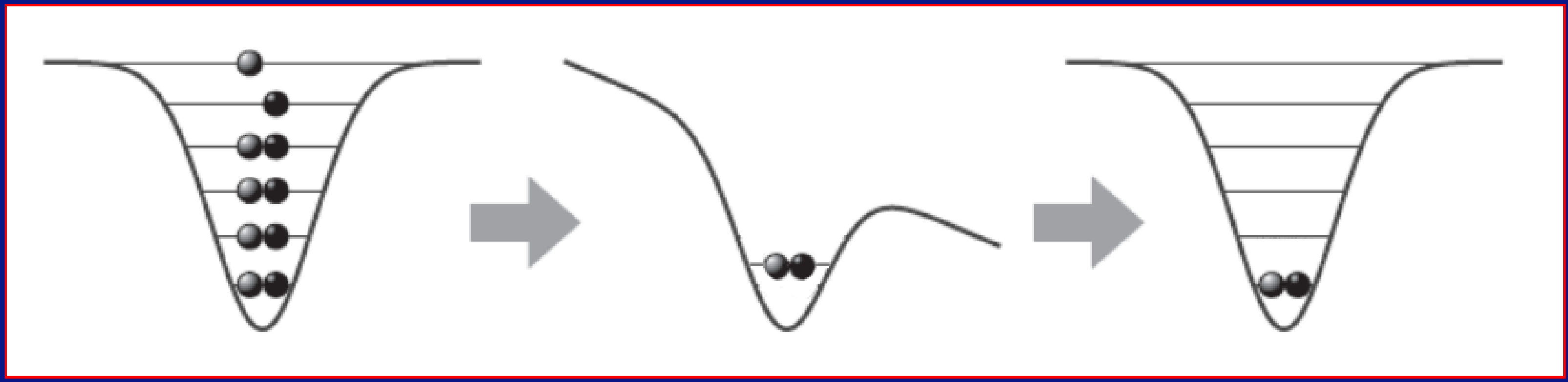
Interaction energy shifts two-atom ground state $\Rightarrow$ modified **atomic** tunnel rate.

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)]



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

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 (due to doubled mass).

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

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

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.

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

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.

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

[M. Troppenz, S. Sala, P.-I. Schneider, and A.S., arXiv:1509.01159]

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

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.

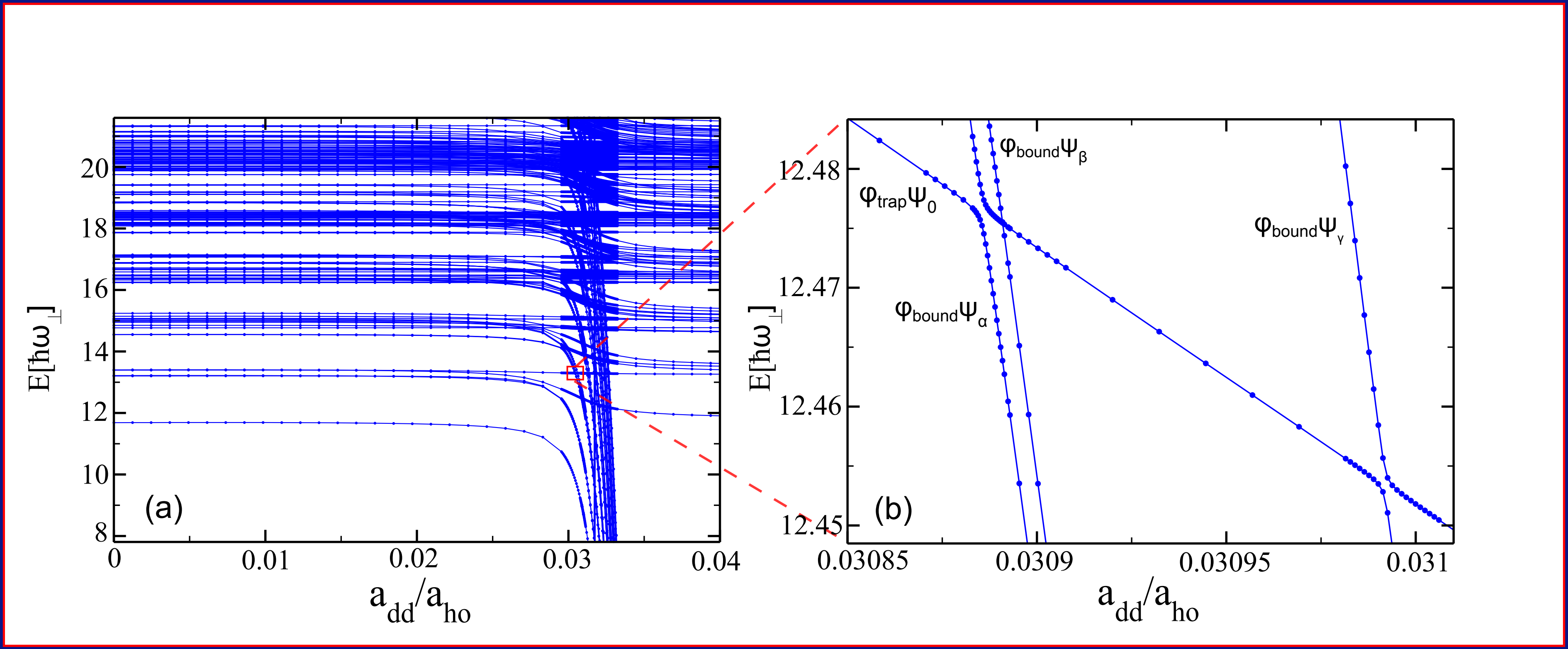
For excitons (electron-hole pairs) larger change of density.

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

[M. Troppenz, S. Sala, P.-I. Schneider, and A.S., arXiv:1509.01159]

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

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)]

Inelastic CIRs / Lattice-induced resonances

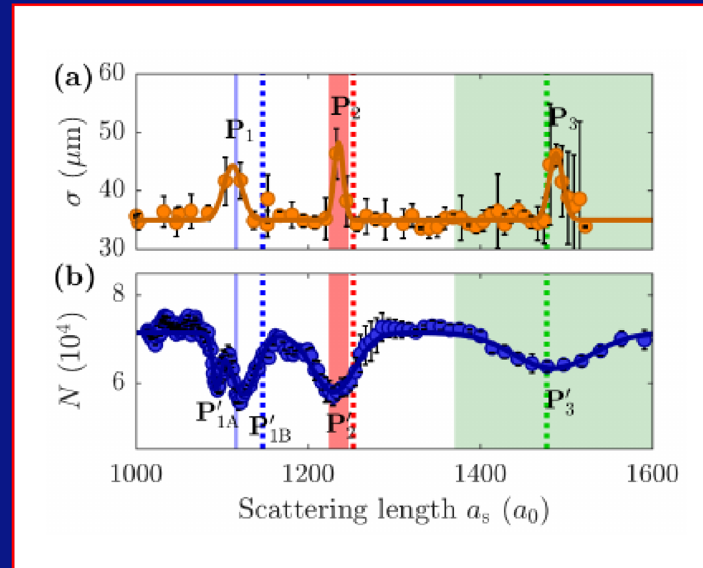
PHYSICAL REVIEW LETTERS **131,** 213002 (2023)

Observation of Confinement-Induced Resonances in a 3D Lattice

Deborah Capecchi,[1] Camilo Cantillano,[1] Manfred J. Mark,[1,2] Florian Meinert,[3] Andreas Schindewolf,[4,5] Manuele Landini,[1] Alejandro Saenz,[6] Fabio Revuelta,[7] and Hanns-Christoph Nägerl[1]
[1]*Institut für Experimentalphysik und Zentrum für Quantenphysik, Universität Innsbruck, 6020 Innsbruck, Austria*
[2]*Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria*
[3]*5.Physikalisches Institut and Center for Integrated Quantum Science and Technology, Universität Stuttgart, 70569 Stuttgart, Germany*
[4]*Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany*
[5]*Munich Center for Quantum Science and Technology, 80799 München, Germany*
[6]*Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany*
[7]*Grupo de Sistemas Complejos, Escuela Técnica Superior de Ingeniería Agronómica, Alimentaria y de Biosistemas, Universidad Politécnica de Madrid, 28040 Madrid, Spain*

(Received 6 October 2022; accepted 25 August 2023; published 21 November 2023)

We report on the observation of confinement-induced resonances for strong three-dimensional (3D) confinement in a lattice potential. Starting from a Mott-insulator state with predominantly single-site occupancy, we detect loss and heating features at specific values for the confinement length and the 3D scattering length. Two independent models, based on the coupling between the center-of-mass and the relative motion of the particles as mediated by the lattice, predict the resonance positions to a good approximation, suggesting a universal behavior. Our results extend confinement-induced resonances to any dimensionality and open up an alternative method for interaction tuning and controlled molecule formation under strong 3D confinement.



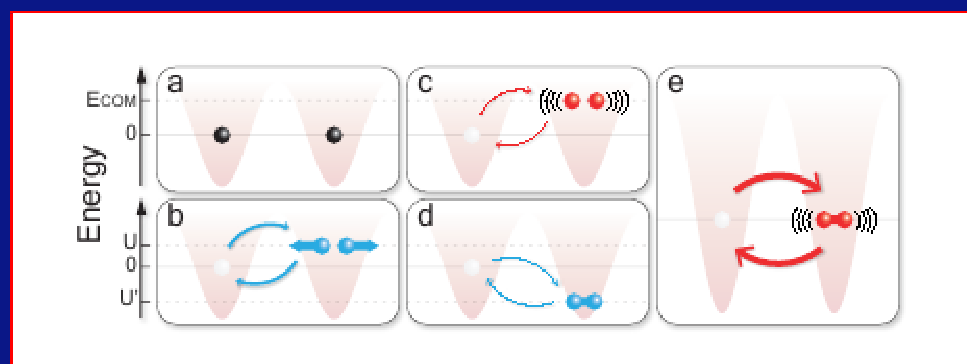
PHYSICAL REVIEW LETTERS **131,** 213001 (2023)

Spin Dynamics Dominated by Resonant Tunneling into Molecular States

Yoo Kyung Lee,[*,†] Hanzhen Lin (林翰桢),[†] and Wolfgang Ketterle
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA;
Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA;
and MIT-Harvard Center for Ultracold Atoms, Cambridge, 02139 Massachusetts, USA

(Received 11 August 2022; accepted 29 June 2023; published 21 November 2023)

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 be explained only 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.

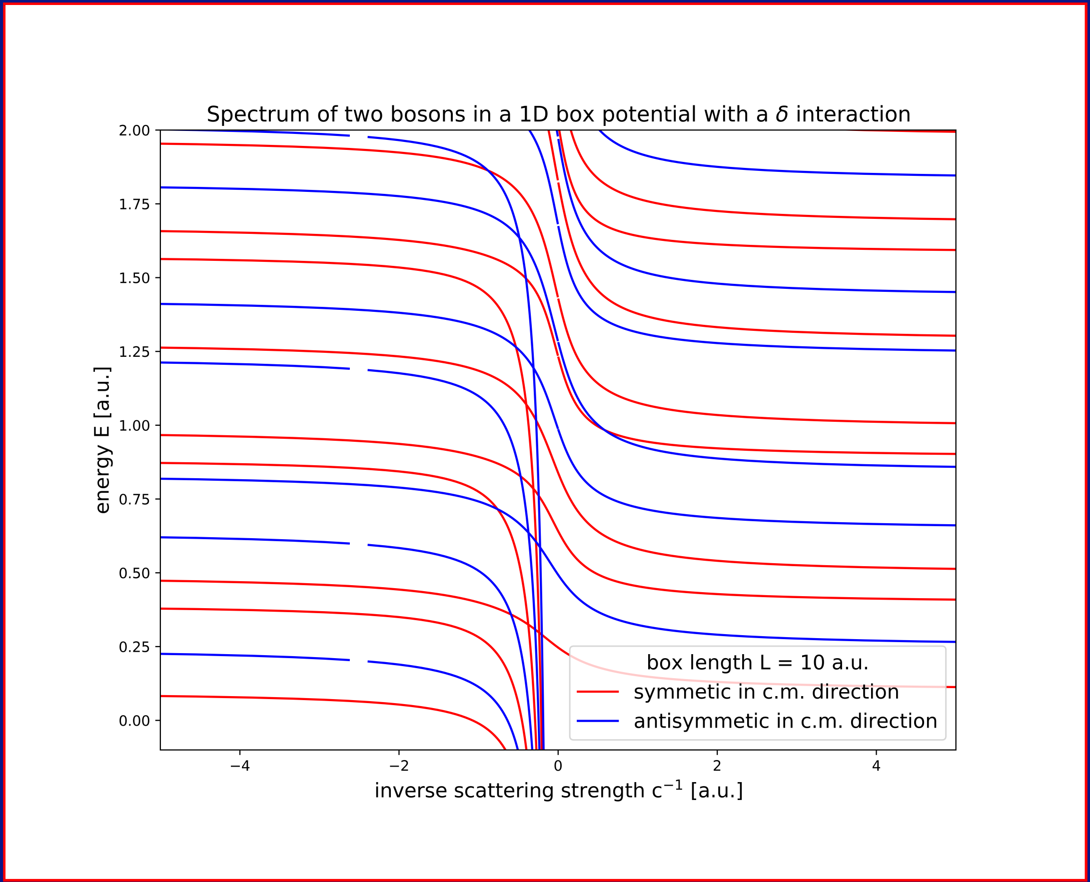


ICIR in square-well potential?

Analytical solution for two particles with δ interaction in square-well potential exists:

Bethe ansatz in absolute(!) coordinates.

Center-of-mass and relative motions seem to be coupled, but:



no coupling due to symmetry!

Overview

1. Confined particles (ultracold atoms in optical lattices or tweezers).
   - Influence of the confining potential.
   - Confinement-induced resonances (CIR).

2. Hydrogen-antihydrogen interaction.

Acknowledgment:

Lyding Brumm (HU Berlin), Piotr Froelich (U Uppsala), Svante Jonsell (U Stockholm), Alex Dalgarno [Harvard], Bernard Zygelman (U Las Vegas)

Historical motivation for $\mathrm{H\bar{H}}$

- Hydrogen-antihydrogen ($\mathrm{H\bar{H}}$) is the most fundamental neutral system of compund matter and antimatter particles.

Historical motivation for $H\bar{H}$

- Hydrogen-antihydrogen ($H\bar{H}$) is the most fundamental neutral system of compund matter and antimatter particles.

- Check of the proposal to cool antihydrogen with ultracold hydrogen.
  - ⋆ So far, only hot antihydrogen atoms are produced (ATHENA and ATRAP at CERN),
    but precision spectroscopy requires cold ones.
  - ⋆ Can hydrogen BEC be used for cooling?

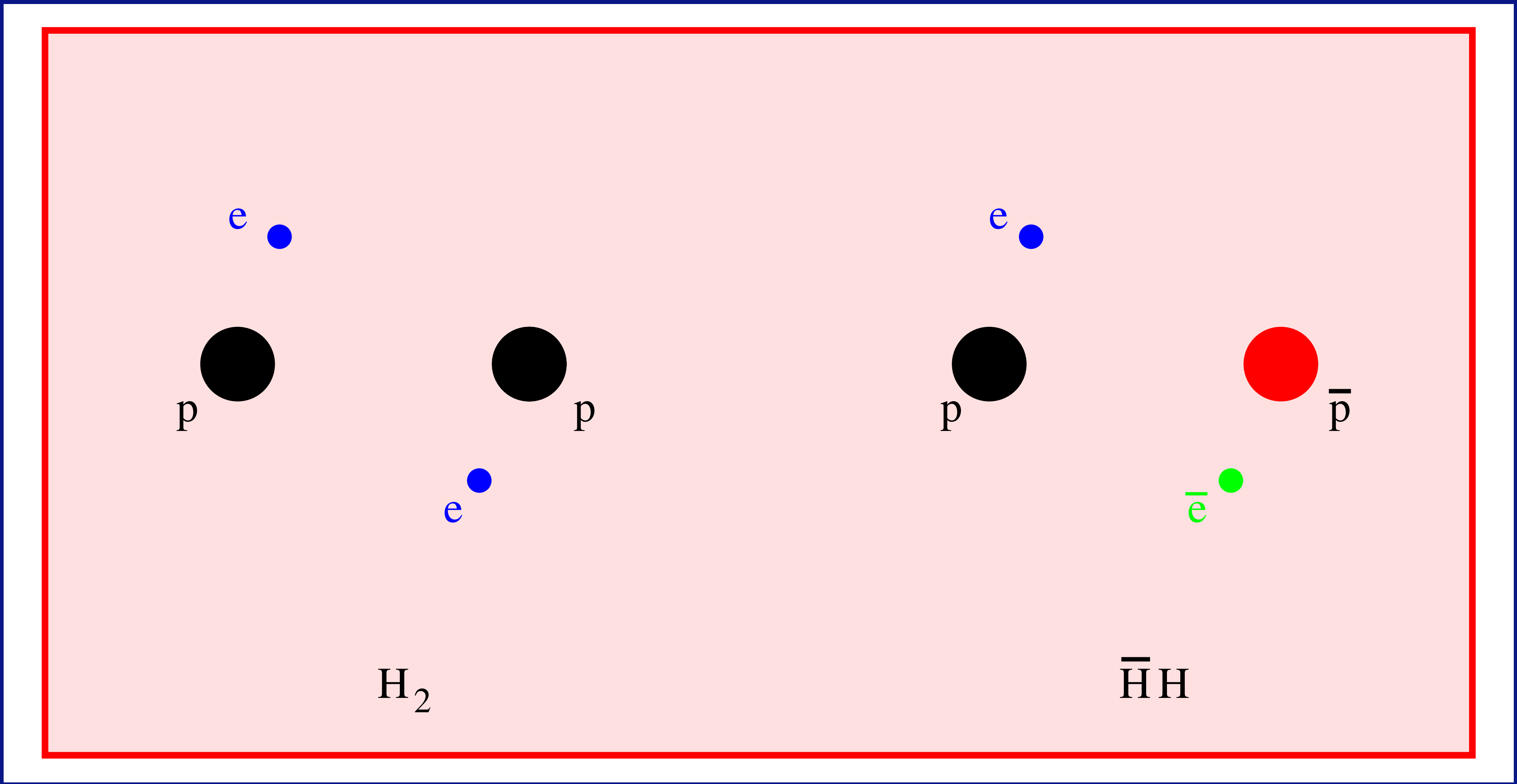
Historical motivation for $H\bar{H}$

- Hydrogen-antihydrogen ($H\bar{H}$) is the most fundamental neutral system of compund matter and antimatter particles.

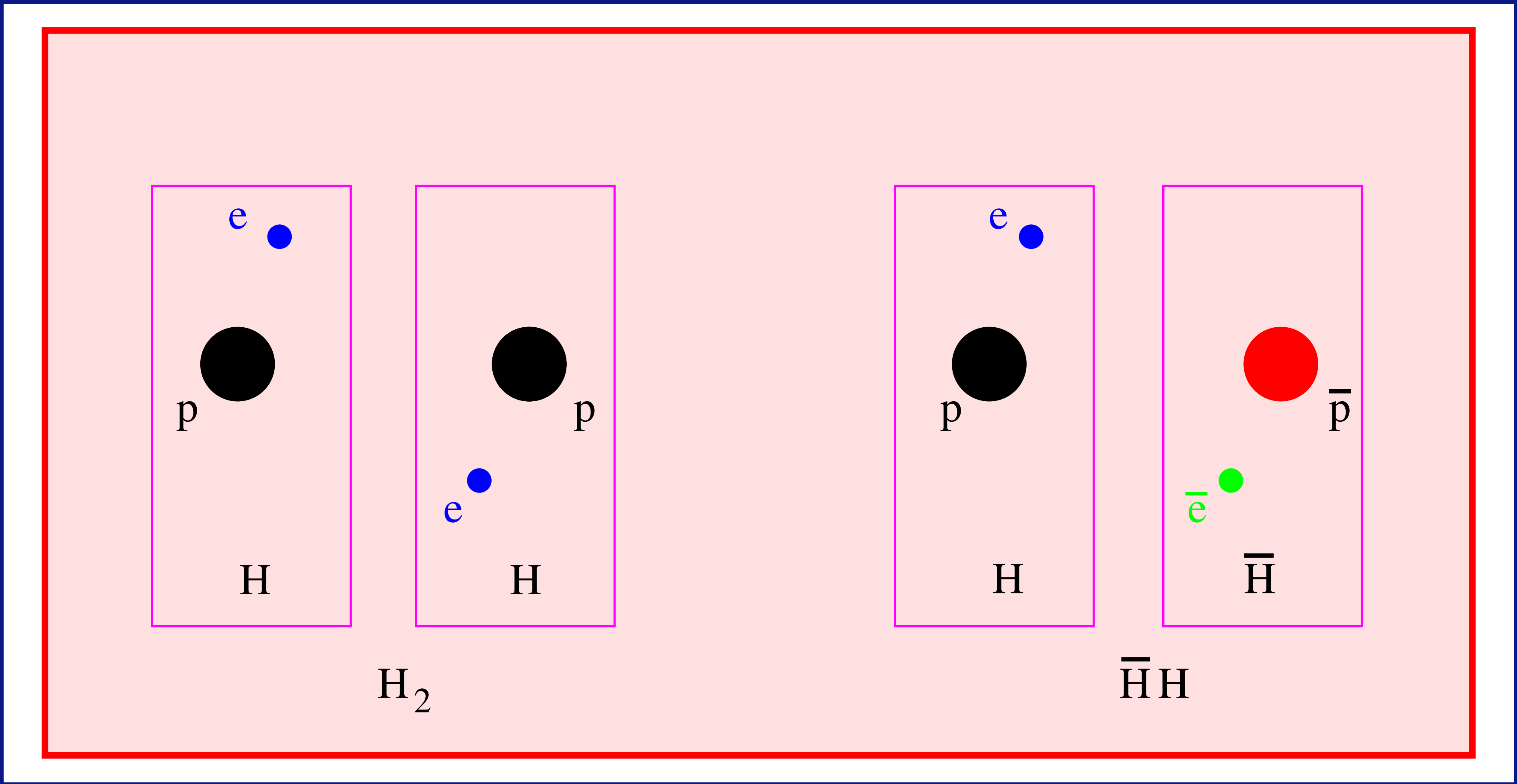
- Check of the proposal to cool antihydrogen with ultracold hydrogen.
  - ⋆ So far, only hot antihydrogen atoms are produced (ATHENA and ATRAP at CERN),
    but precision spectroscopy requires cold ones.
  - ⋆ Can hydrogen BEC be used for cooling?

- Deexcitation of excited $\bar{H}$ atoms using ground state H atoms.
  - ⋆ So far, highly excited antihydrogen atoms are produced,
    but precision spectroscopy requires ground-state atoms.
  - ⋆ Can ground-state hydrogen atoms be used for deexcitation?

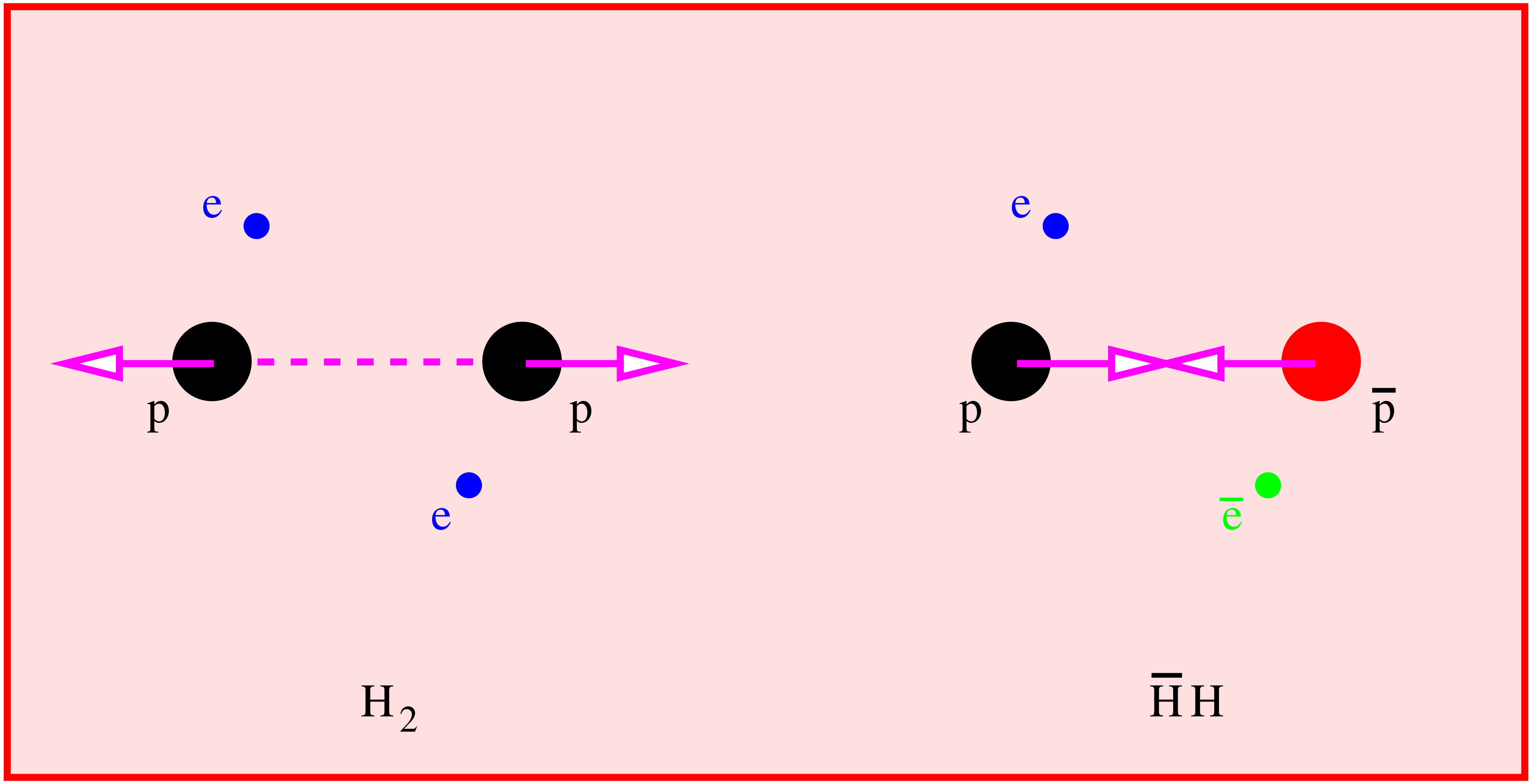
Comparison of $H\bar{H}$ and H_2



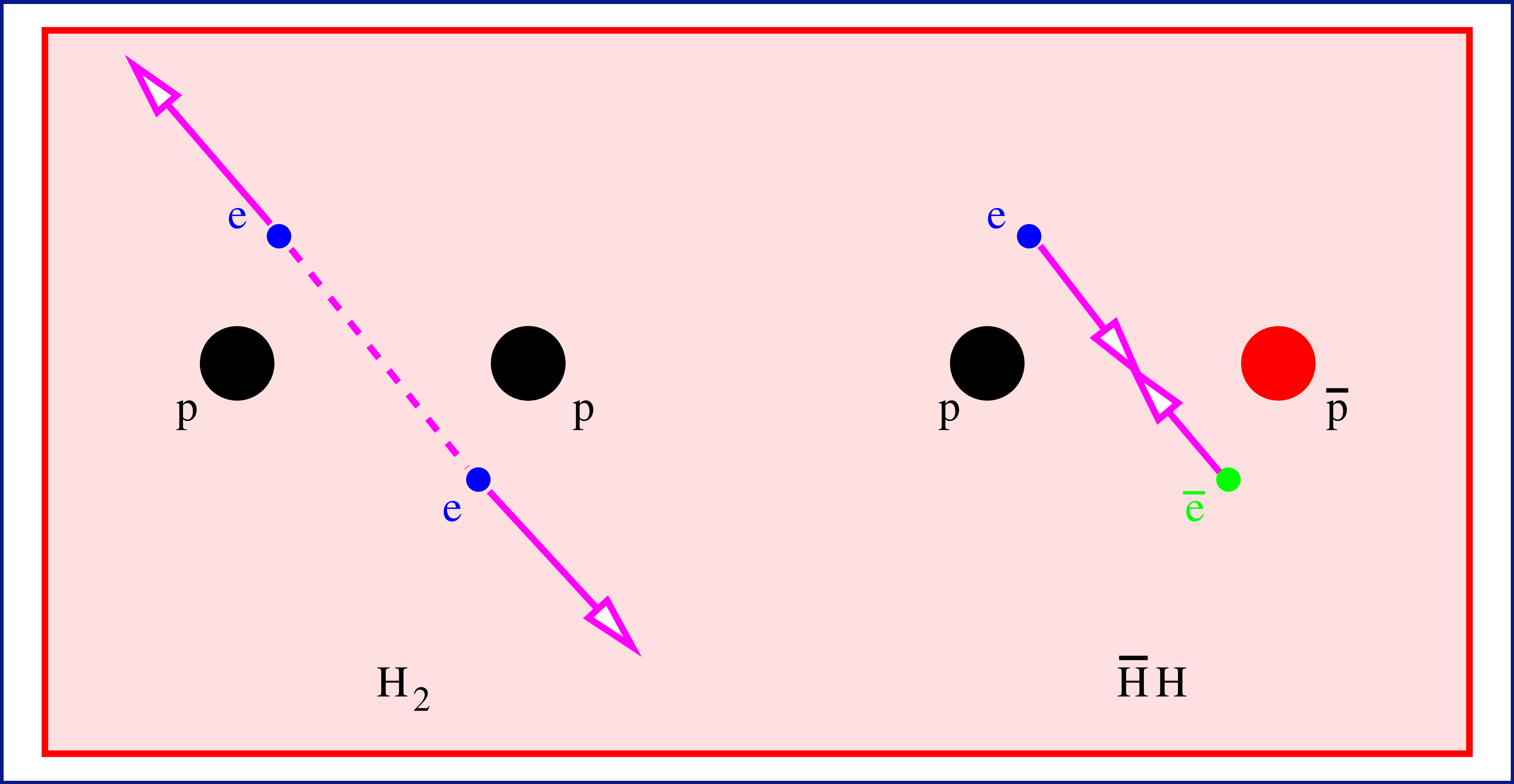
Comparison of $H\bar{H}$ and H_2



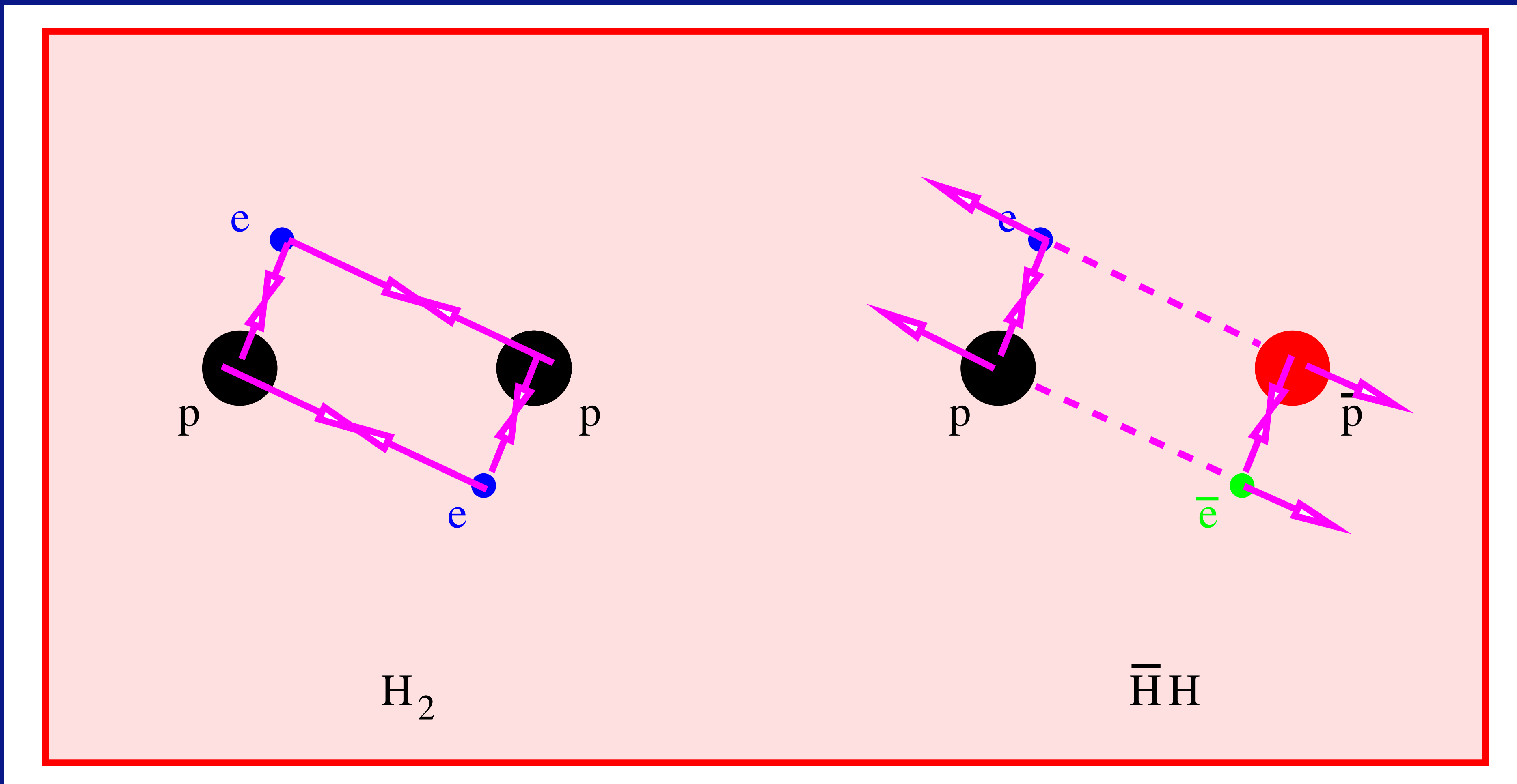
Comparison of $H\bar{H}$ and H_2



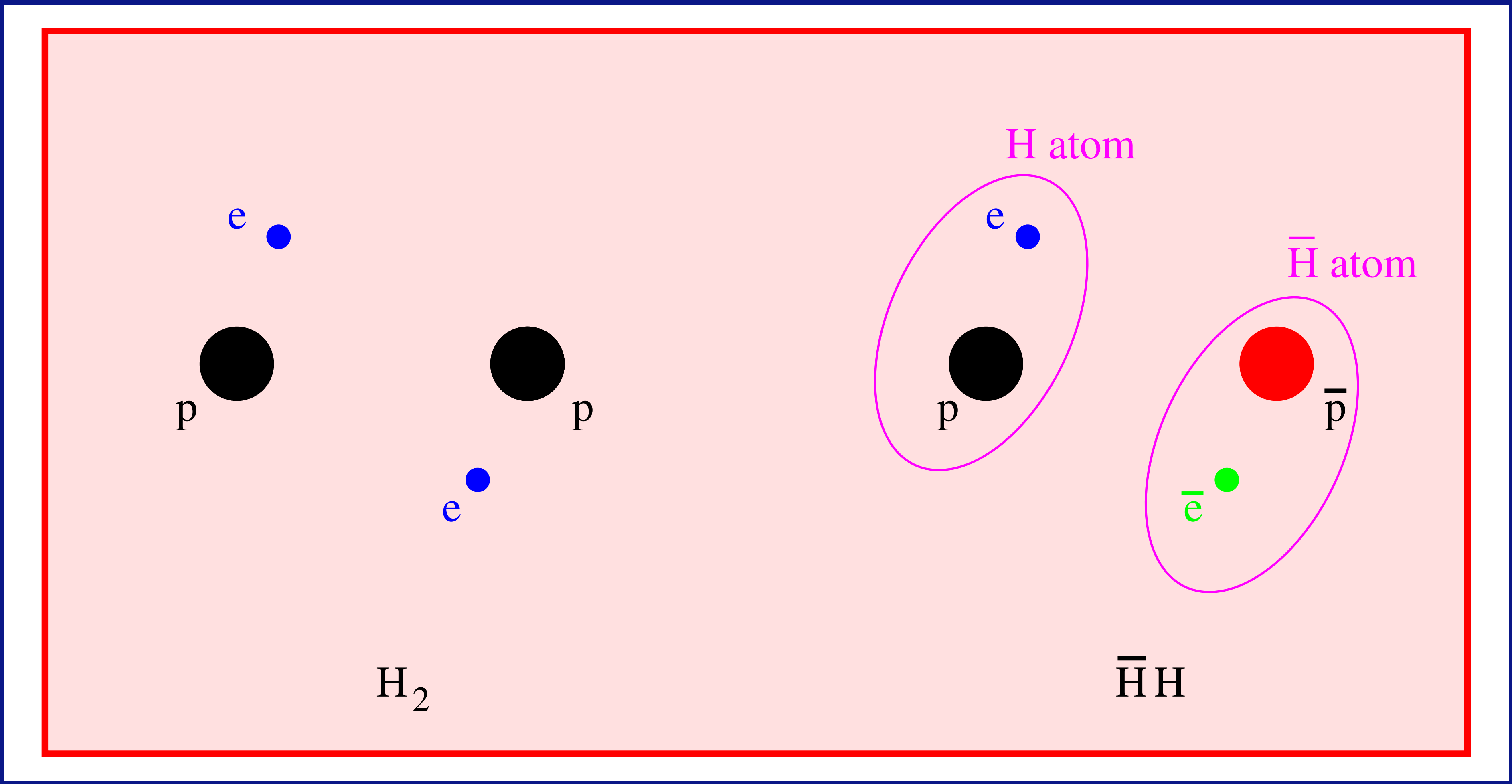
Comparison of $H\bar{H}$ and H_2



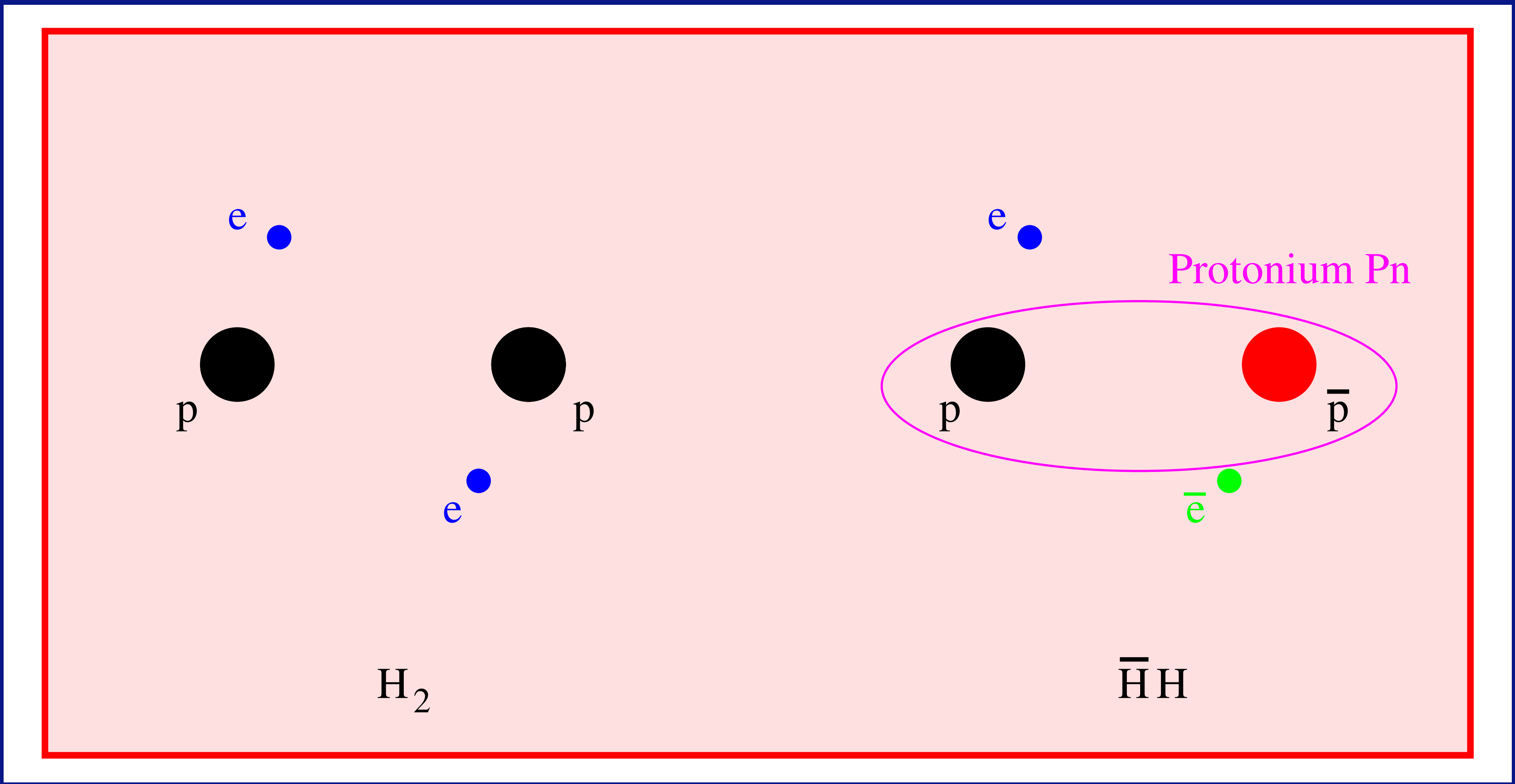
Comparison of $H\bar{H}$ and H_2



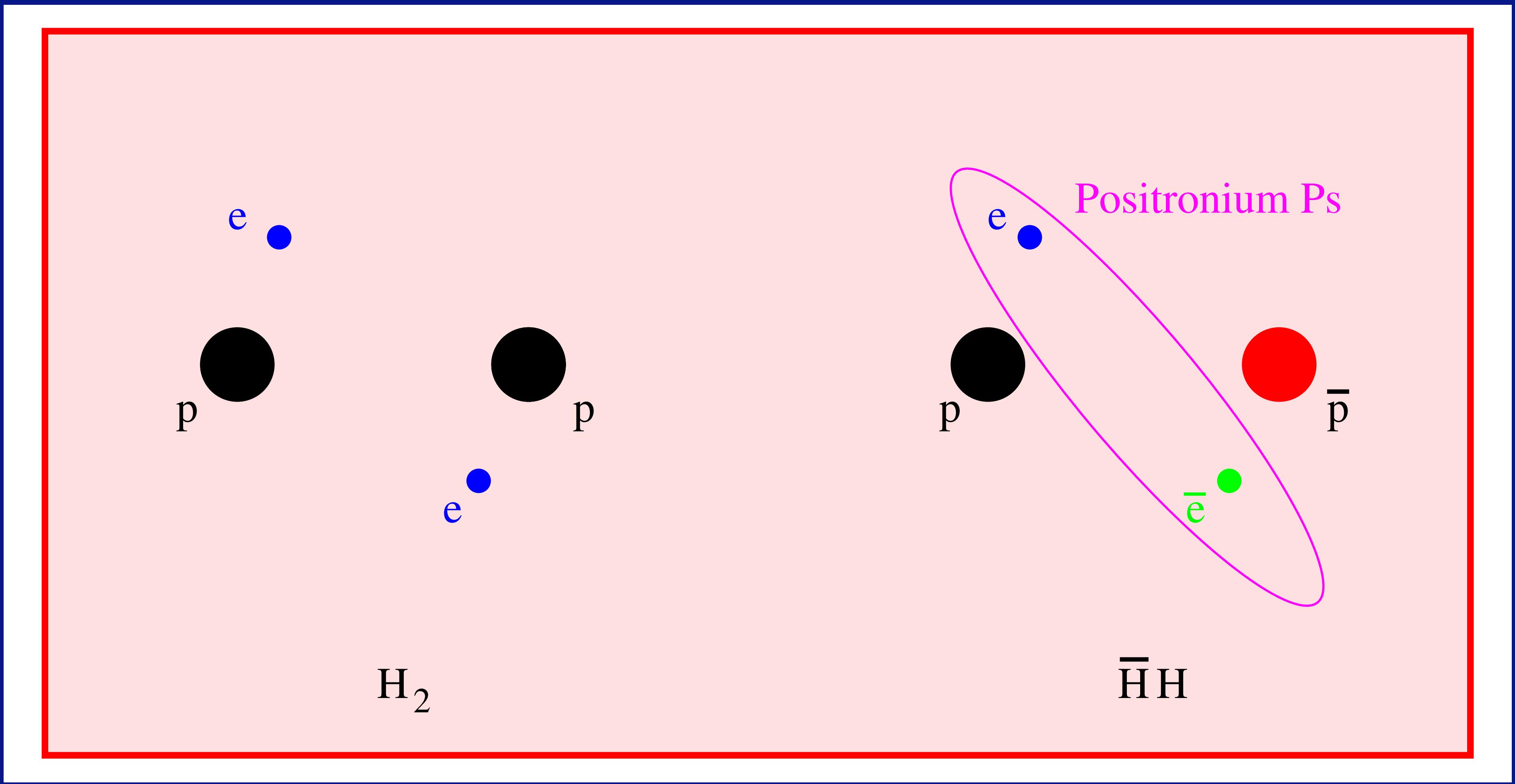
Comparison of $H\bar{H}$ and H_2



Comparison of $H\bar{H}$ and H_2



Comparison of $H\bar{H}$ and H_2



Symmetries of H$\bar{\text{H}}$ (I)

Leptonic non-relativistic Born-Oppenheimer Hamiltonian of H$\bar{\text{H}}$
(in atomic units):

$$\hat{\mathrm{H}}_{\mathrm{lep}} = -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{pe}} - \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

Symmetries of $\mathrm{H\bar{H}}$ (I)

Leptonic non-relativistic Born-Oppenheimer Hamiltonian of $\mathrm{H\bar{H}}$ (in atomic units):

$$\hat{\mathrm{H}}_{\mathrm{lep}} = -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{pe}} - \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

Leptonic permutation $\hat{\mathrm{O}}_l\,\vec{r}_e = \vec{r}_{\bar{e}}, \quad \hat{\mathrm{O}}_l\,\vec{r}_{\bar{e}} = \vec{r}_e$:

$$\hat{\mathrm{O}}_l\,\hat{\mathrm{H}}_{\mathrm{lep}} = -\frac{\nabla_{\bar{e}}^2}{2} - \frac{\nabla_e^2}{2} - \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{pe}} - \frac{1}{r_{\bar{e}e}}$$

$$= -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} + \frac{1}{r_{pe}} + \frac{1}{r_{\bar{p}\bar{e}}} - \frac{1}{r_{\bar{p}e}} - \frac{1}{r_{\bar{p}e}} - \frac{1}{r_{e\bar{e}}}$$

$\longrightarrow$ **no symmetry of** $\hat{\mathrm{H}}_{\mathrm{lep}}$

Symmetries of $\mathrm{H}\bar{\mathrm{H}}$ (I)

Leptonic non-relativistic Born-Oppenheimer Hamiltonian of $\mathrm{H}\bar{\mathrm{H}}$ (in atomic units):

$$\hat{\mathrm{H}}_{\mathrm{lep}} = -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{pe}} - \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

Leptonic inversion $\hat{\mathrm{i}}_l\,\vec{r}_{pe} = -\vec{r}_{\bar{p}e}, \quad \hat{\mathrm{i}}_l\,\vec{r}_{p\bar{e}} = -\vec{r}_{\bar{p}\bar{e}}$:

$$\hat{\mathrm{i}}_l\,\hat{\mathrm{H}}_{\mathrm{lep}} = -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{\bar{p}e}} - \frac{1}{r_{p\bar{e}}} + \frac{1}{r_{pe}} + \frac{1}{r_{\bar{p}\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

$$= -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} + \frac{1}{r_{pe}} + \frac{1}{r_{\bar{p}\bar{e}}} - \frac{1}{r_{\bar{p}e}} - \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

$\longrightarrow$ **no symmetry of** $\hat{\mathrm{H}}_{\mathrm{lep}}$

Symmetries of H$\bar{\text{H}}$ (I)

Leptonic non-relativistic Born-Oppenheimer Hamiltonian of H$\bar{\text{H}}$ (in atomic units):

$$\hat{\mathrm{H}}_{\mathrm{lep}} \quad = \quad -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{pe}} - \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}}$$

Q symmetry (leptonic permutation and inversion)

$\hat{\mathrm{Q}}_l\, \vec{r}_{pe} = \hat{\mathrm{i}}_l\, \hat{\mathrm{O}}_l\, \vec{r}_{pe} = -\vec{r}_{\bar{p}\bar{e}}, \quad \hat{\mathrm{Q}}_l\, \vec{r}_{p\bar{e}} = \hat{\mathrm{i}}_l\, \hat{\mathrm{O}}_l\, \vec{r}_{p\bar{e}} = -\vec{r}_{\bar{p}e}$:

$$\begin{aligned} \hat{\mathrm{Q}}_l\, \hat{\mathrm{H}}_{\mathrm{lep}} \quad &= \quad -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{\bar{p}\bar{e}}} - \frac{1}{r_{pe}} + \frac{1}{r_{p\bar{e}}} + \frac{1}{r_{\bar{p}e}} - \frac{1}{r_{e\bar{e}}} \\ &= \quad -\frac{\nabla_e^2}{2} - \frac{\nabla_{\bar{e}}^2}{2} - \frac{1}{r_{pe}} - \frac{1}{r_{\bar{p}\bar{e}}} + \frac{1}{r_{\bar{p}e}} + \frac{1}{r_{p\bar{e}}} - \frac{1}{r_{e\bar{e}}} \end{aligned}$$

$\longrightarrow$ **symmetry of** $\hat{\mathrm{H}}_{\mathrm{lep}}$

Symmetries of H$\bar{\text{H}}$ (II)

- The Q symmetry ($\hat{\mathrm{Q}}_l = \hat{\mathrm{i}}_l\,\hat{\mathrm{O}}_l$) acts exclusively on the spatial coordinates of the leptons.

- The leptonic inversion ($\hat{\mathrm{i}}_l$) is closely related to the leptonic parity $\hat{\mathrm{P}}_l$, but the latter includes the internal parities (the ones of a fermion and an antifermion being opposite).

- It is possible to show that the combined Q and leptonic spin-exchange $\hat{\mathrm{S}}_l$ operations correspond to the leptonic charge-conjugation $\hat{\mathrm{C}}_l$ and parity $\hat{\mathrm{P}}_l$ operations:

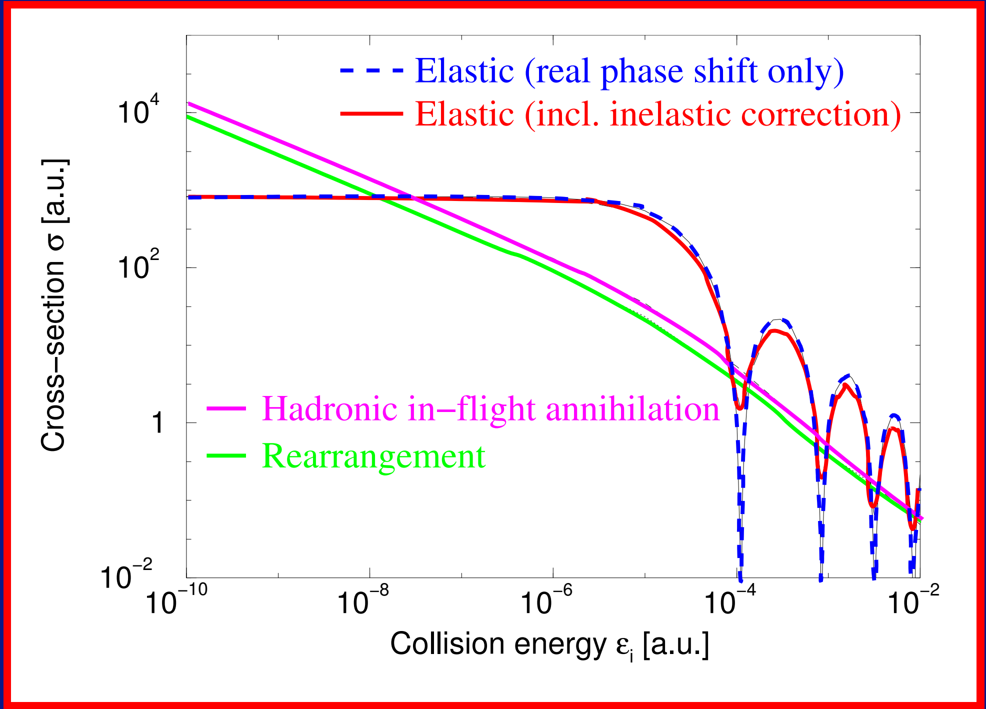
$$\hat{\mathrm{C}}_l\,\hat{\mathrm{P}}_l\,|\Psi_{\mathrm{lep}}\rangle \;=\; \hat{\mathrm{Q}}_l\,\hat{\mathrm{S}}_l\,|\Psi_{\mathrm{lep}}\rangle$$

- The $\hat{\mathrm{Q}}_l$ operator is only a coordinate transformation, this is useful for coding (generation of symmetry-adapted basis functions).

Processes in $H\bar{H}$ collisions

Possible low-energy scattering events:

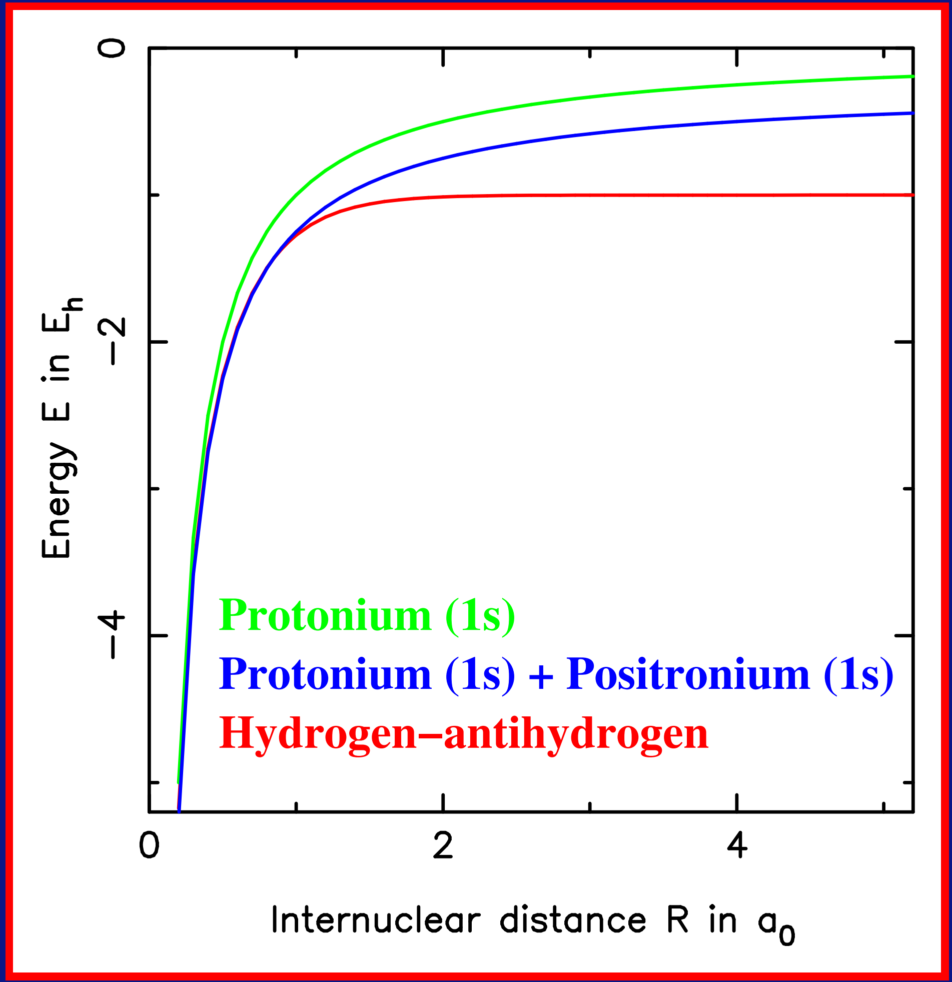
- $\oplus$ **elastic scattering** (responsible for cooling)
- $\ominus$ e^+/e^- **annihilation in flight**
- $\ominus$ $p/\bar{p}$ **annihilation in flight**
- $\ominus$ **rearrangement reactions**, especially $H + \bar{H} \rightarrow p\bar{p} + e^+e^-$, and
- $\ominus$ **radiative association**, $H + \bar{H} \rightarrow H\bar{H} + h\nu$.



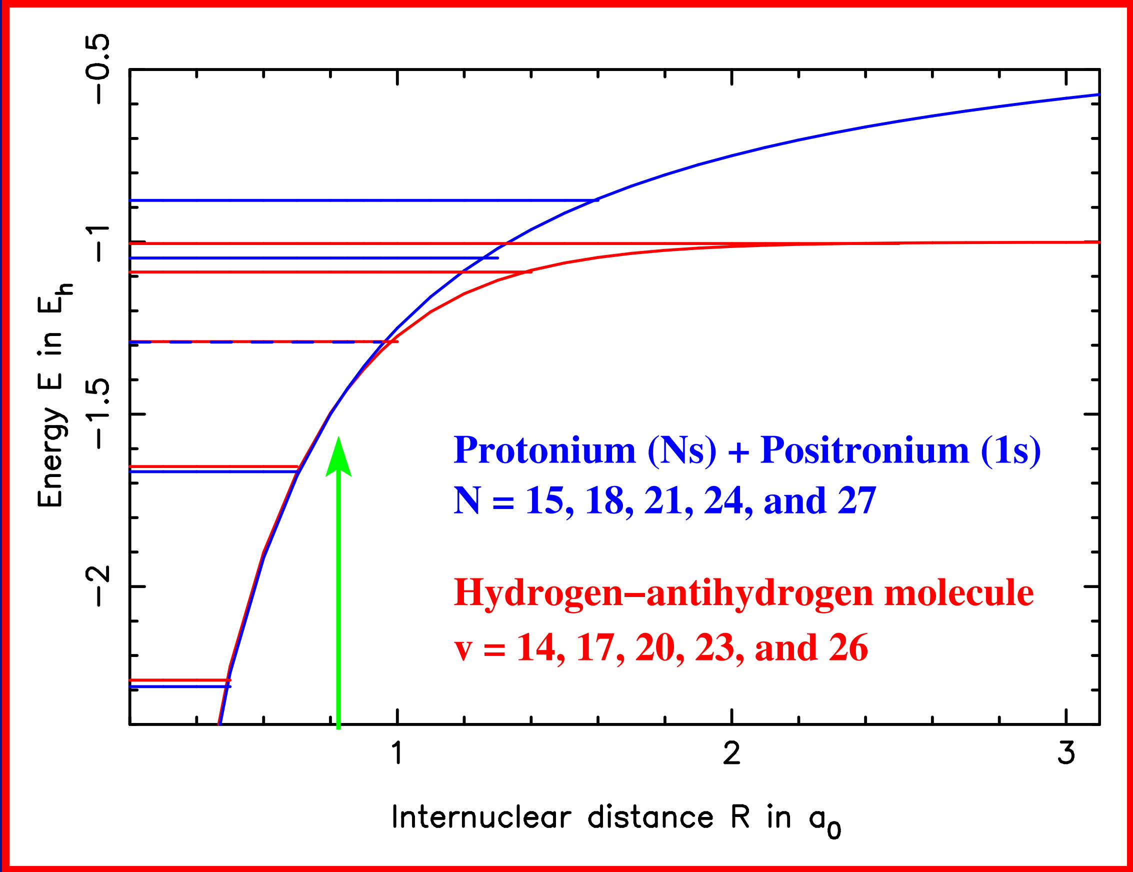
The $H\bar{H}$ "molecule" (I)

$H\bar{H}$:

- "Chemically" bound molecule.
- Potential curve corresponds to slightly distorted protonium potential ($p\bar{p}$).
- The distortion transforms an **infinite** $p\bar{p}$ level series into a **finite number of rovibrational states**.
- However, **$H\bar{H}$ is metastable:**
  - ⋆ **Annihilation** and
  - ⋆ **decay** in protonium and positronium.

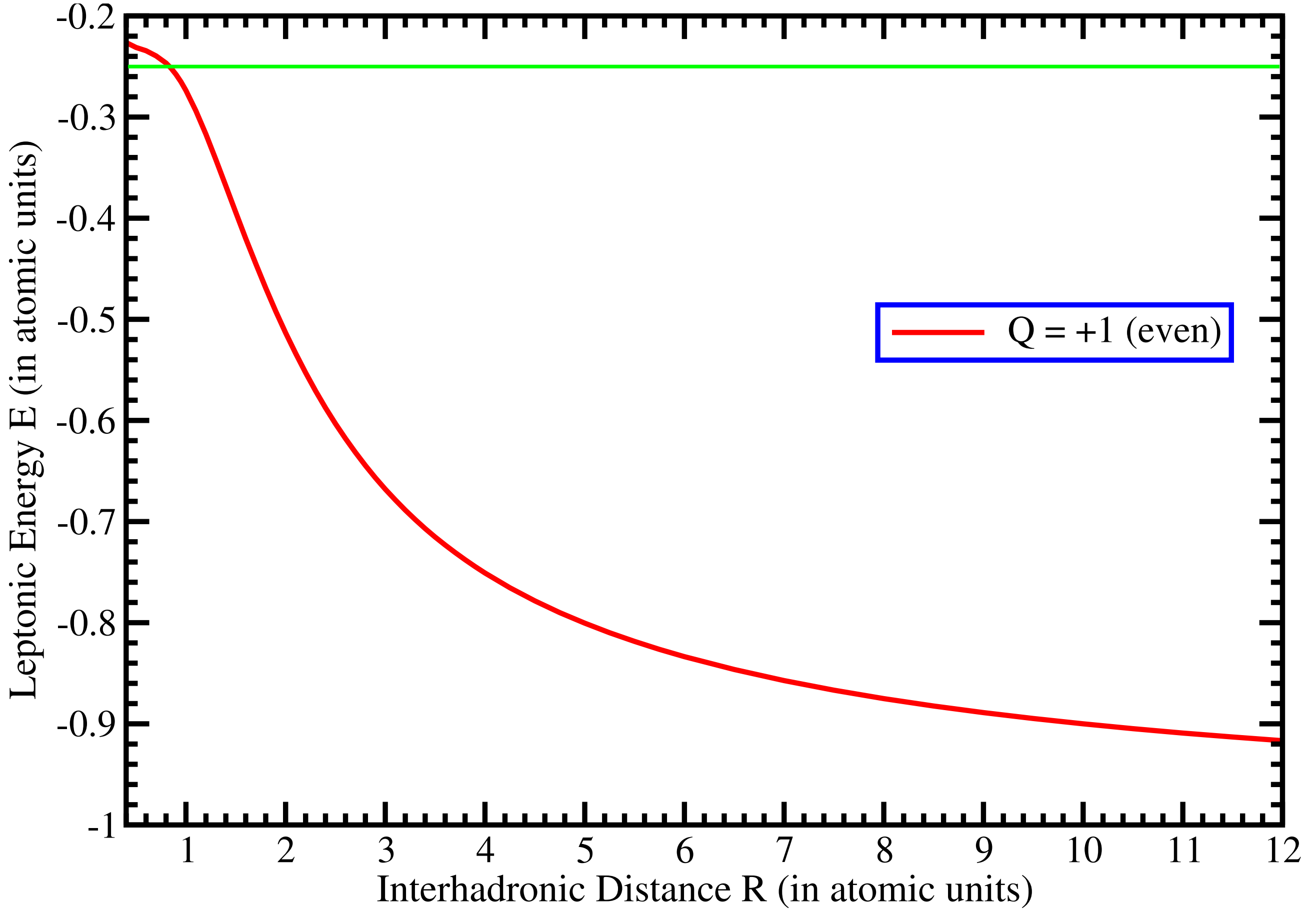


$H\bar{H}$ "molecule" (II)



At the critical distance $R_{\rm cr}$ ↑ opens the decay channel $\rm H\bar{H} \rightarrow p\bar{p} + e\bar{e}$.

Leptonic energy



At the critical distance $R_{\rm cr}$ the leptonic ground-state energy of H$\bar{\rm H}$ equals the one of a freely moving Ps ($E_{\rm Ps(1s)} = -0.25\,{\rm a.\,u.}$).

The critical distance

Basis functions of the used type,

$$\phi_i(\vec{r}_e, \vec{r}_{\bar{e}}) \;=\; \left(\frac{2r_{e,\bar{e}}}{R}\right)^{\mu_i} \xi_e^{u_i} \eta_e^{v_i} \xi_{\bar{e}}^{\bar{u}_i} \eta_{\bar{e}}^{\bar{v}_i} e^{-\alpha\xi_e - \bar{\alpha}\xi_{\bar{e}} + \beta\eta_e + \bar{\beta}\eta_{\bar{e}}} \quad ,$$

allow a very efficient and accurate inclusion of electron-electron correlation for H_2,

The critical distance

Basis functions of the used type,

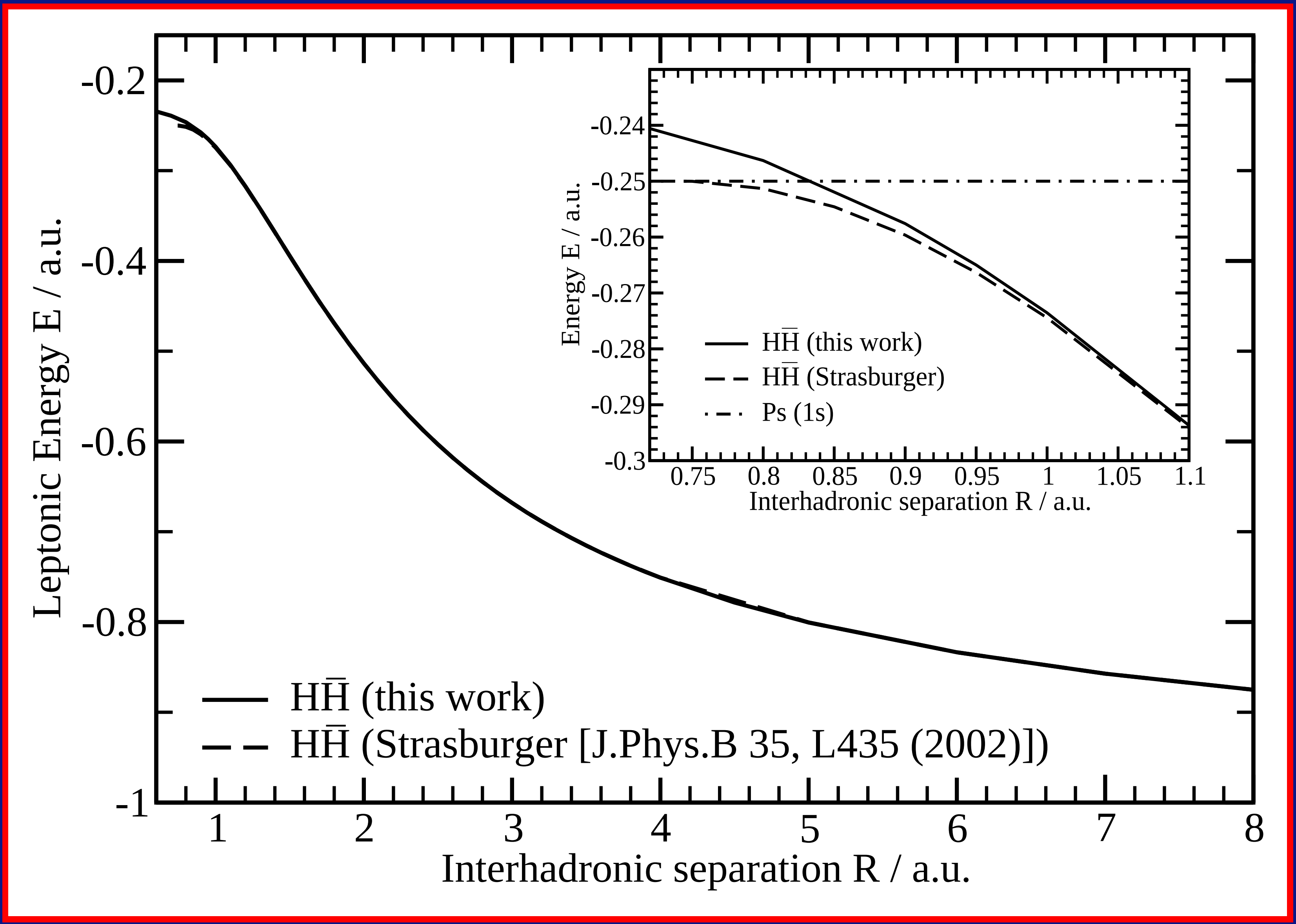
$$\phi_i(\vec{r}_e, \vec{r}_{\bar{e}}) \;=\; \left(\frac{2r_{e,\bar{e}}}{R}\right)^{\mu_i} \xi_e^{u_i} \eta_e^{v_i} \xi_{\bar{e}}^{\bar{u}_i} \eta_{\bar{e}}^{\bar{v}_i} e^{-\alpha\xi_e - \bar{\alpha}\xi_{\bar{e}} + \beta\eta_e + \bar{\beta}\eta_{\bar{e}}} \quad ,$$

allow a very efficient and accurate inclusion of electron-electron correlation for H_2,

but the highest power of $r_{1,2}$ ($\mu_{\rm max}$) still limits the Taylor expansion describing free positronium:

$\mu_{\rm max}$	0	1	2	3
$\mathcal{E}_{1s}^{Ps}$	-0.1376	-0.1913	-0.2193	-0.2348
rel. error [%]	45.0	23.5	12.3	6.1

Improved calculation



Excited states

- Reminder: all 4 leptonic spin states are degenerate in the non-relativistic limit.
- There are 2 Σ states converging asymptotically to the H(n=2)+$\bar{\text{H}}$(1s), and 2 Σ states converging asymptotically to the H(1s)+$\bar{\text{H}}$(n=2) limit:

$$\text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(2\text{p}_\text{z})$$
$$\text{H}(2\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(2\text{p}_\text{z}) + \bar{\text{H}}(1\text{s})$$

- 2 of the states have Q *even* symmetry, 2 have Q *odd* symmetry.

Excited states

- Reminder: all 4 leptonic spin states are degenerate in the non-relativistic limit.

- There are 2 Σ states converging asymptotically to the H(n=2)+$\bar{\text{H}}$(1s), and 2 Σ states converging asymptotically to the H(1s)+$\bar{\text{H}}$(n=2) limit:

$$\text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(2\text{p}_\text{z})$$
$$\text{H}(2\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(2\text{p}_\text{z}) + \bar{\text{H}}(1\text{s})$$

- 2 of the states have Q *even* symmetry, 2 have Q *odd* symmetry.

- There are 3 Σ states converging asymptotically to the H(n=3)+$\bar{\text{H}}$(1s), and 3 Σ states converging asymptotically to the H(1s)+$\bar{\text{H}}$(n=3) limit:

$$\text{H}(1\text{s}) + \bar{\text{H}}(3\text{s}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(3\text{p}_\text{z}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(3\text{d}_{\text{z}^2})$$
$$\text{H}(3\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(3\text{p}_\text{z}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(3\text{d}_{\text{z}^2}) + \bar{\text{H}}(1\text{s})$$

Excited states

- Reminder: all 4 leptonic spin states are degenerate in the non-relativistic limit.

- There are 2 Σ states converging asymptotically to the H(n=2)+$\bar{\text{H}}$(1s), and 2 Σ states converging asymptotically to the H(1s)+$\bar{\text{H}}$(n=2) limit:

$$\text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(2\text{p}_\text{z})$$
$$\text{H}(2\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(2\text{p}_\text{z}) + \bar{\text{H}}(1\text{s})$$

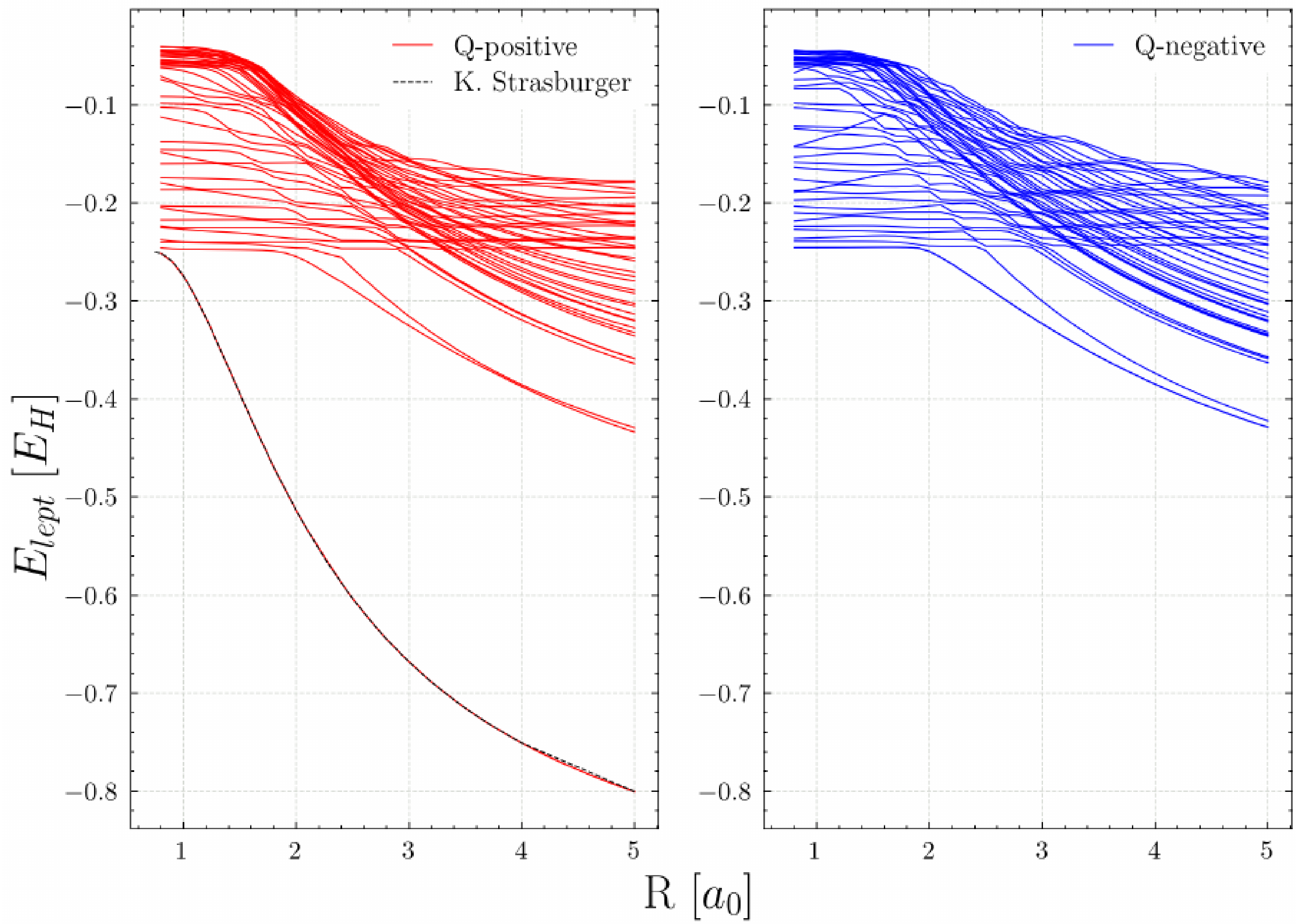
- 2 of the states have Q *even* symmetry, 2 have Q *odd* symmetry.

- There are 3 Σ states converging asymptotically to the H(n=3)+$\bar{\text{H}}$(1s), and 3 Σ states converging asymptotically to the H(1s)+$\bar{\text{H}}$(n=3) limit:

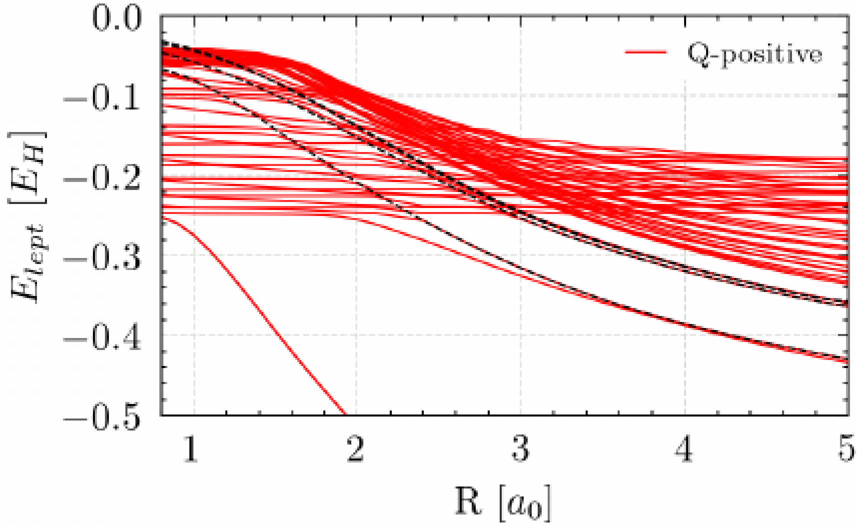
$$\text{H}(1\text{s}) + \bar{\text{H}}(3\text{s}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(3\text{p}_\text{z}) \qquad \text{H}(1\text{s}) + \bar{\text{H}}(3\text{d}_{\text{z}^2})$$
$$\text{H}(3\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(3\text{p}_\text{z}) + \bar{\text{H}}(1\text{s}) \qquad \text{H}(3\text{d}_{\text{z}^2}) + \bar{\text{H}}(1\text{s})$$

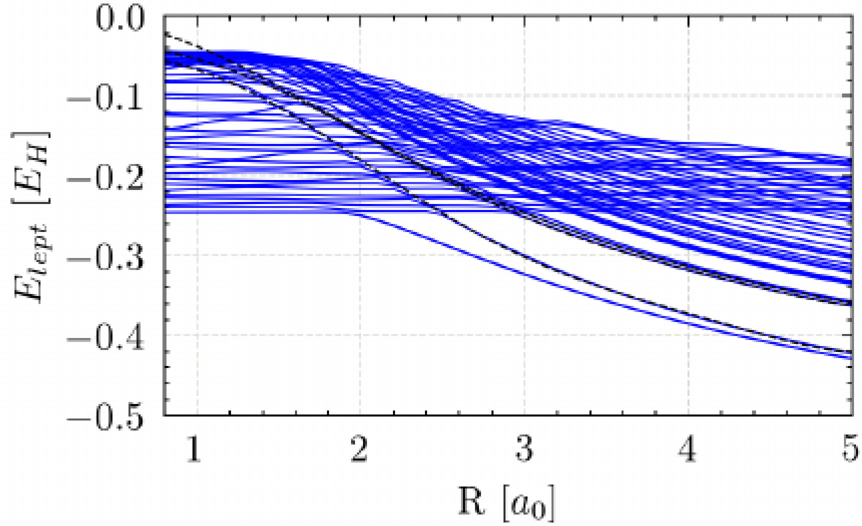
- In the non-relativistic limit there are $2n$ Σ states for every main quantum number n (n states are Q *even* and n are *odd*).

Excited states (new results)



Excited states (zoom)



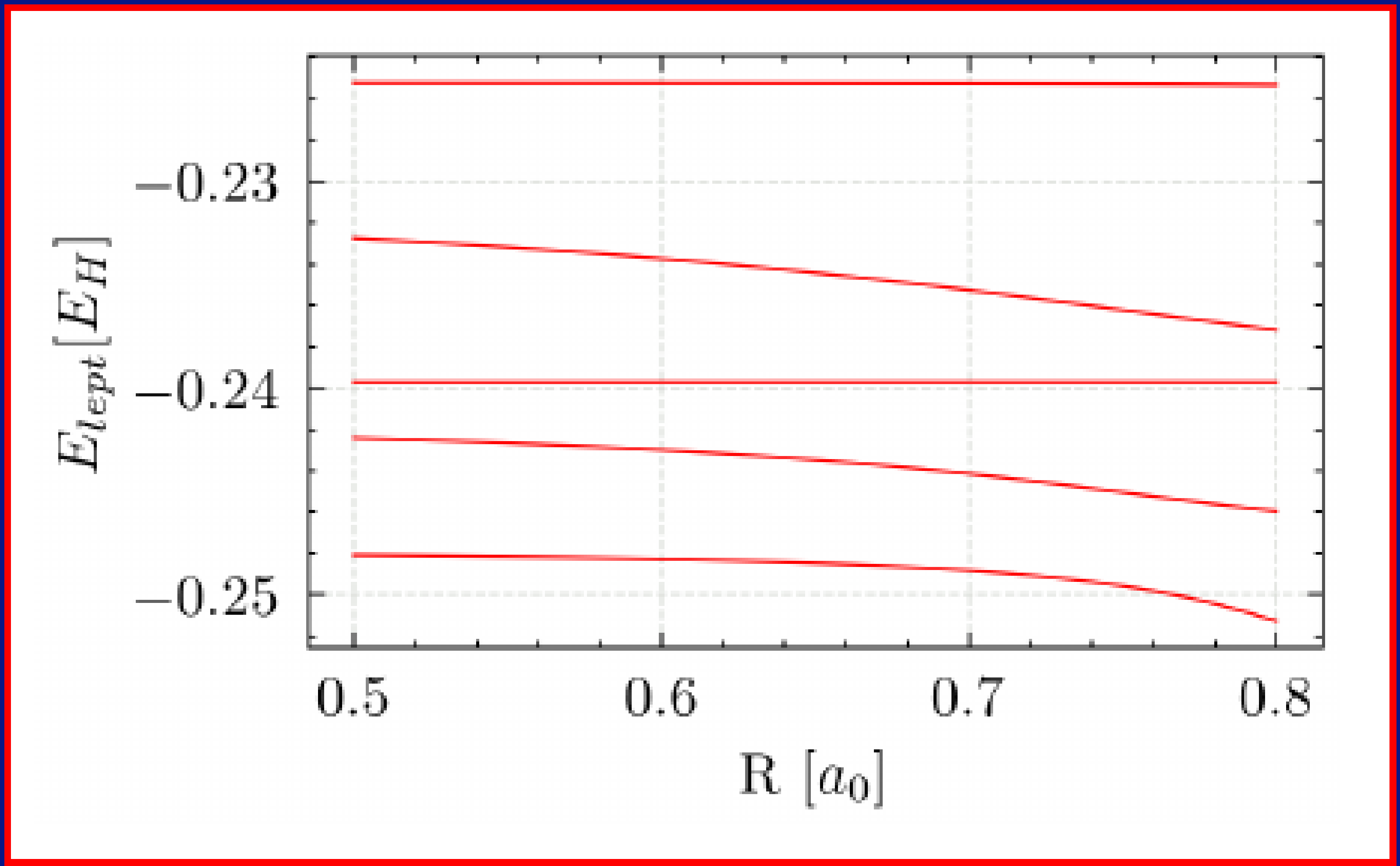


New code allows for more systematic basis-set enlargement.

In contrast to previous calculations with this basis-set type, now the (free) positronium states appear in the spectrum.

$\longrightarrow$ **Avoided crossings (resonances) between molecular and positronium states.**

Ground state (zoom)



Critical distance: avoided crossing???

Deexcitation of excited $\bar{\mathrm{H}}$

Resonant deexcitation transfer: $\mathrm{H}(1s) + \bar{\mathrm{H}}(nl) = \mathrm{H}(nl) + \bar{\mathrm{H}}(1s)$

- Using calculated excited-state potential curves, elastic and excitation transfer cross-sections were obtained.
- For example, the following scattering cross-sections are obtained:

$$\mathrm{H}(1s) + \bar{\mathrm{H}}(2s) \longrightarrow \mathrm{H}(1s) + \bar{\mathrm{H}}(2s) \qquad \sigma_{\mathrm{el}} = 706\,\mathrm{a.u.}$$
$$\mathrm{H}(1s) + \bar{\mathrm{H}}(2s) \longrightarrow \mathrm{H}(2s) + \bar{\mathrm{H}}(1s) \qquad \sigma_{\mathrm{et}} = 8468\,\mathrm{a.u.}$$

- The excitation-transfer cross-section is quite large, thus it may be a way for deexcitation of $\bar{\mathrm{H}}$.

Deexcitation of excited $\bar{\text{H}}$

Resonant deexcitation transfer: $\text{H}(1\text{s}) + \bar{\text{H}}(\text{nl}) = \text{H}(\text{nl}) + \bar{\text{H}}(1\text{s})$

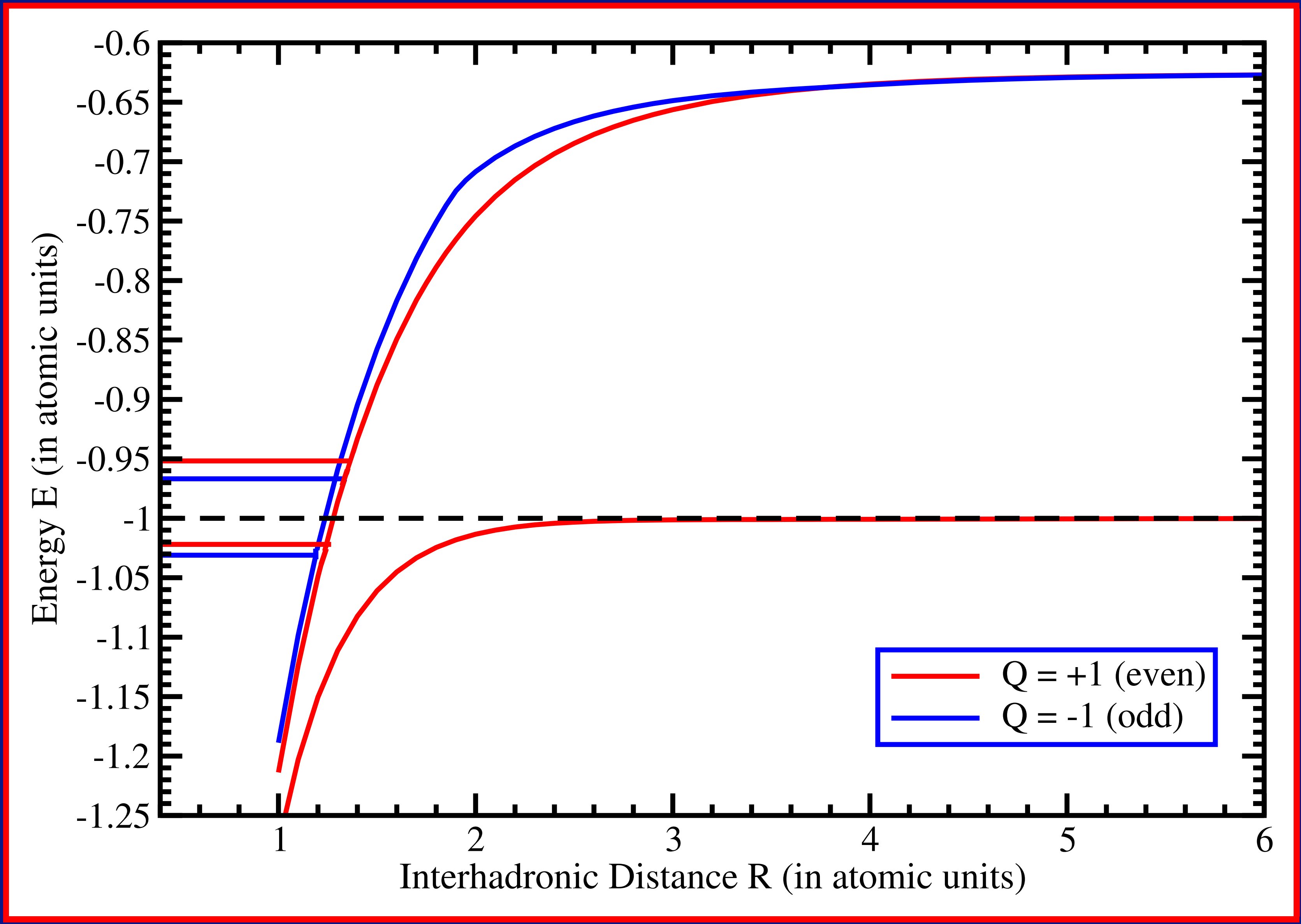
- Using calculated excited-state potential curves, elastic and excitation transfer cross-sections were obtained.
- For example, the following scattering cross-sections are obtained:

$$\text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \longrightarrow \text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \qquad \sigma_{\text{el}} = 706\,\text{a. u.}$$
$$\text{H}(1\text{s}) + \bar{\text{H}}(2\text{s}) \longrightarrow \text{H}(2\text{s}) + \bar{\text{H}}(1\text{s}) \qquad \sigma_{\text{et}} = 8468\,\text{a. u.}$$

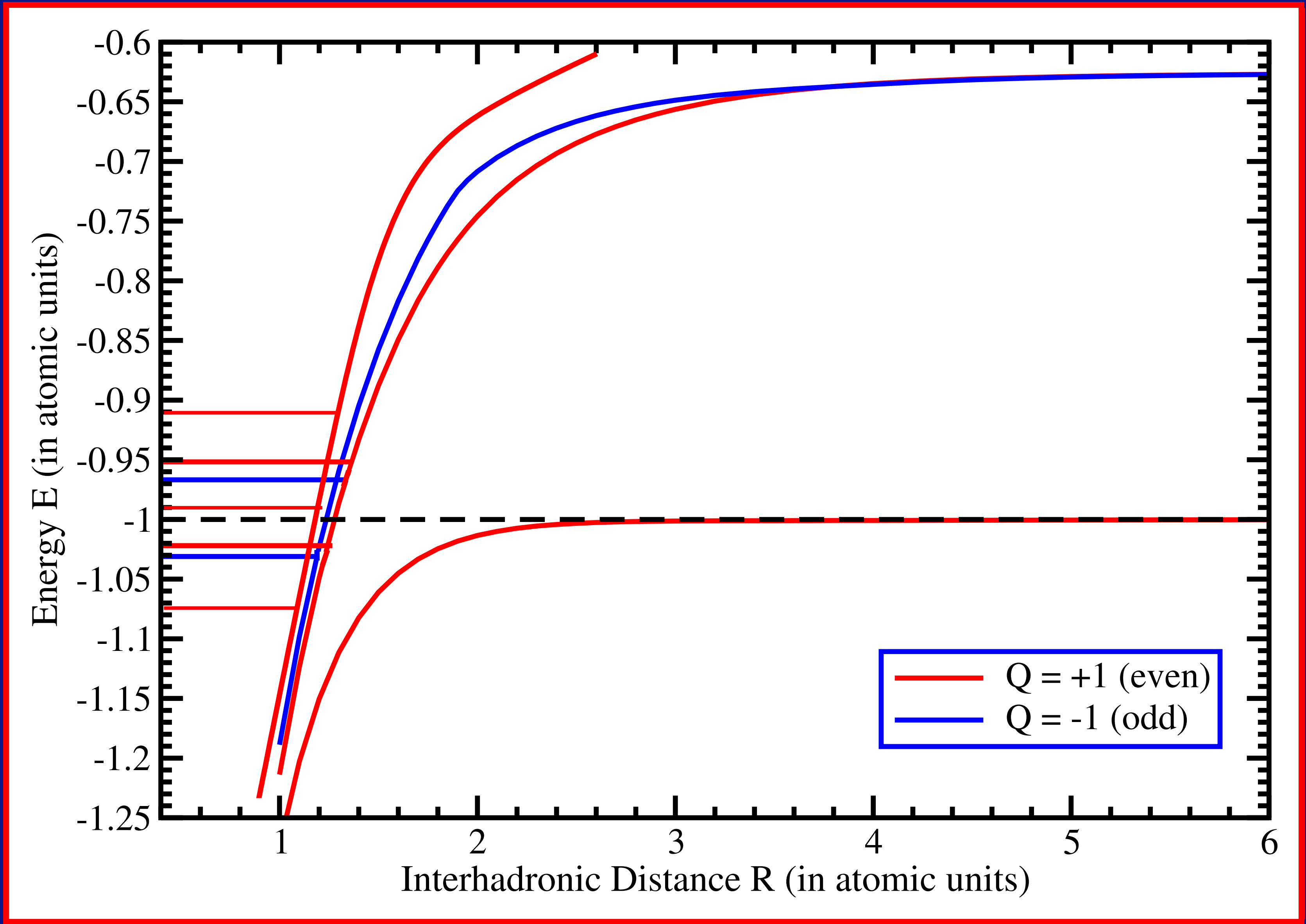
- The excitation-transfer cross-section is quite large, thus it may be a way for deexcitation of $\bar{\text{H}}$.

However, the excited states indicate new complications!

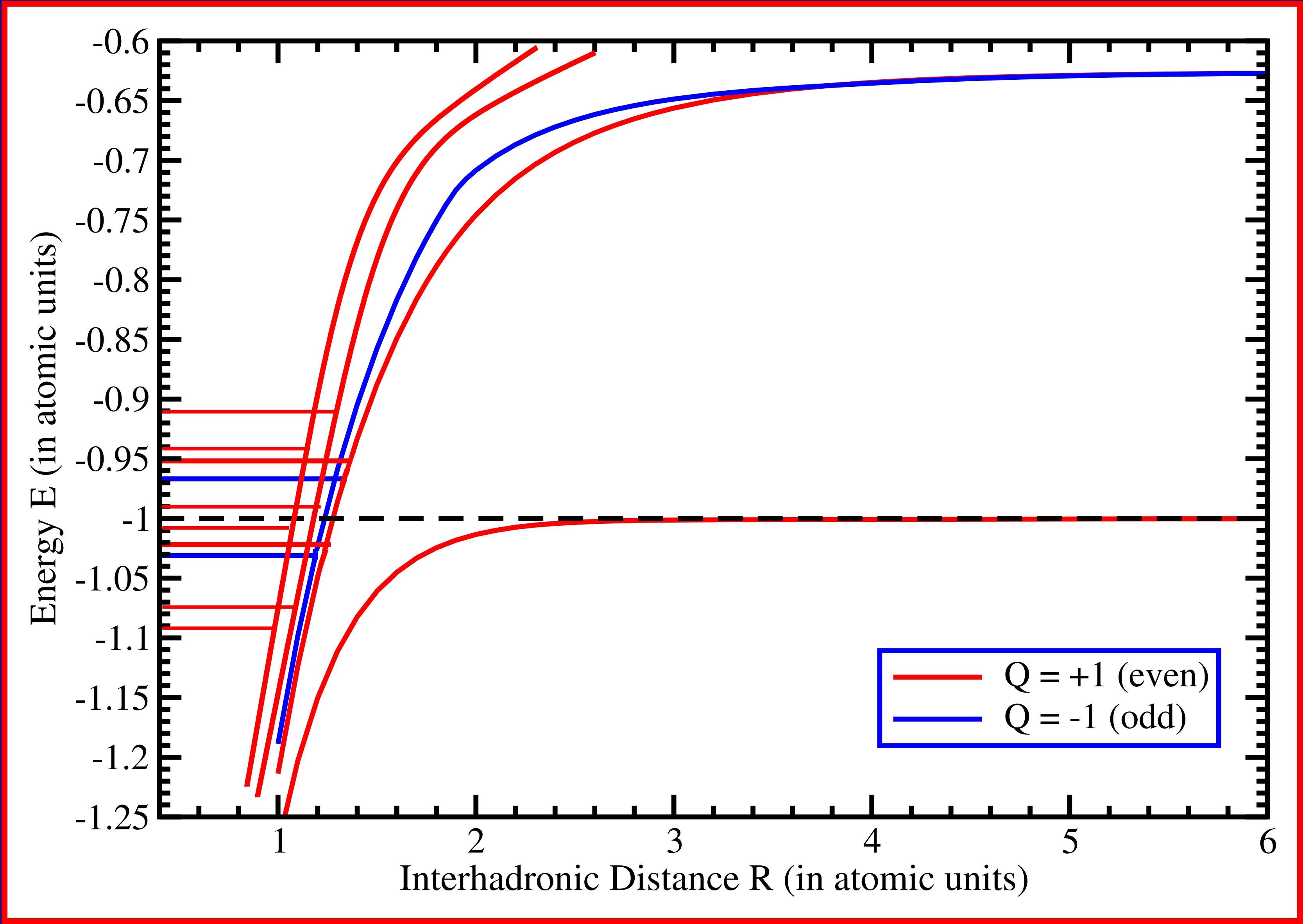
Vibrational states / Feshbach resonances



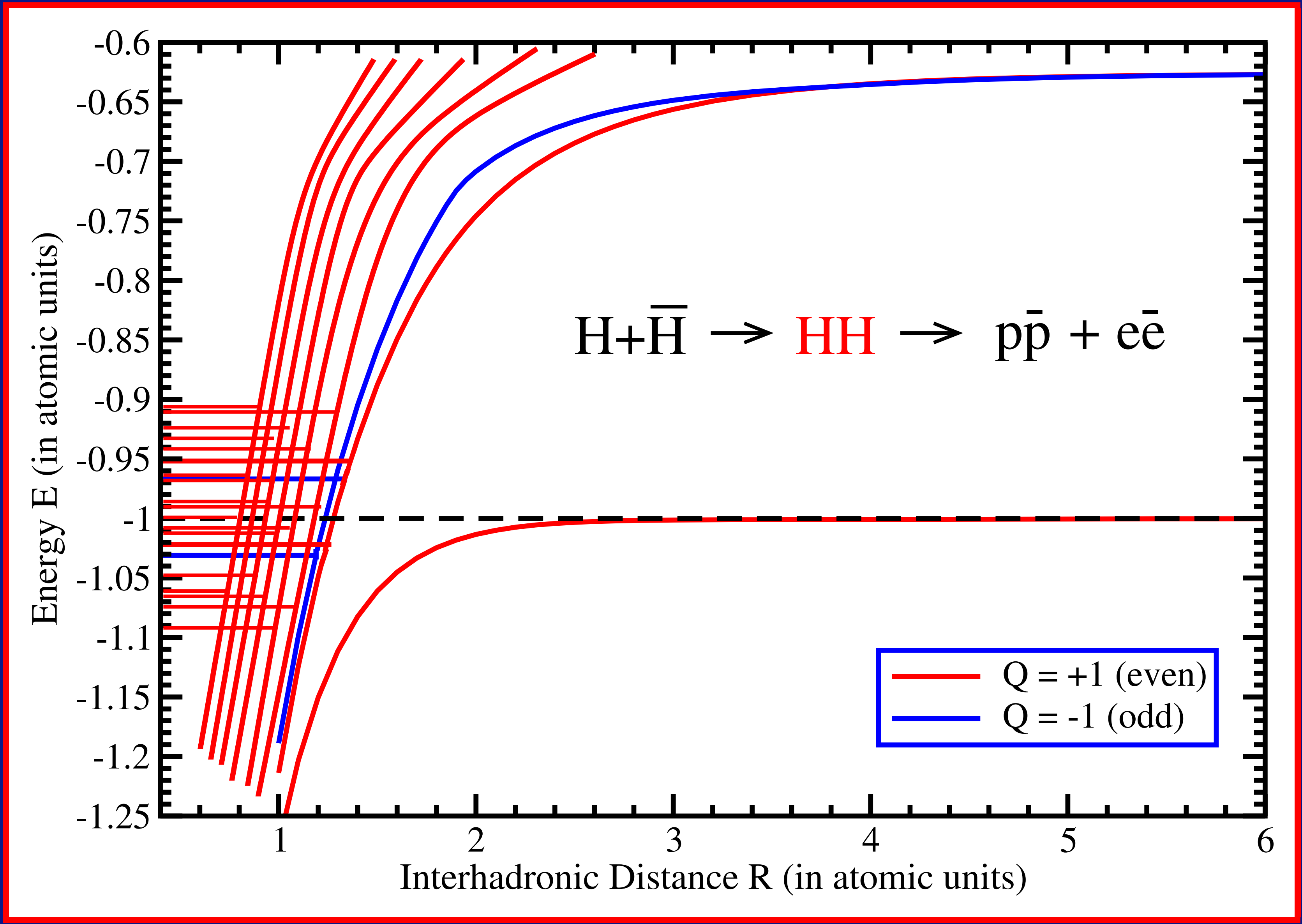
Vibrational states / Feshbach resonances



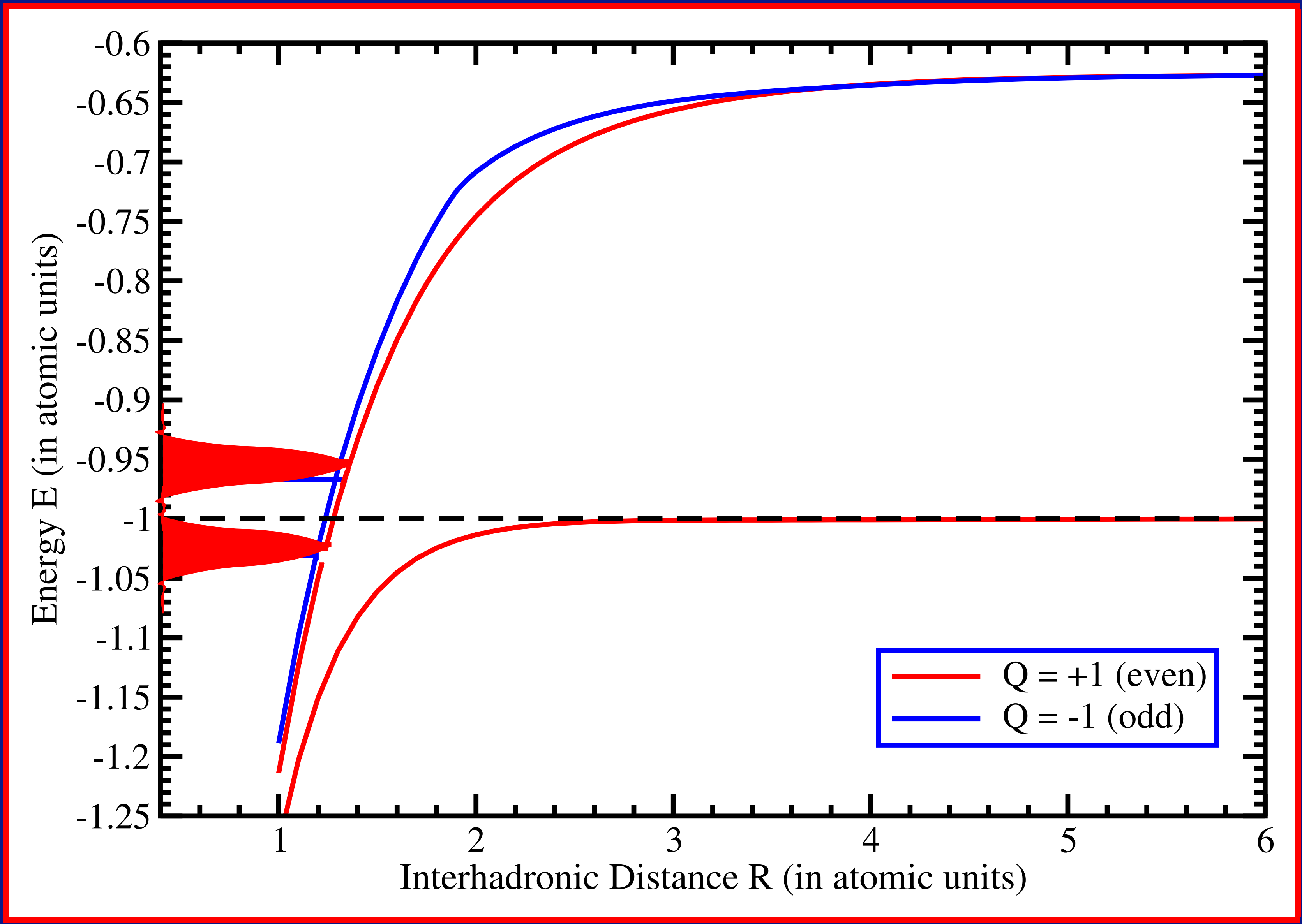
Vibrational states / Feshbach resonances



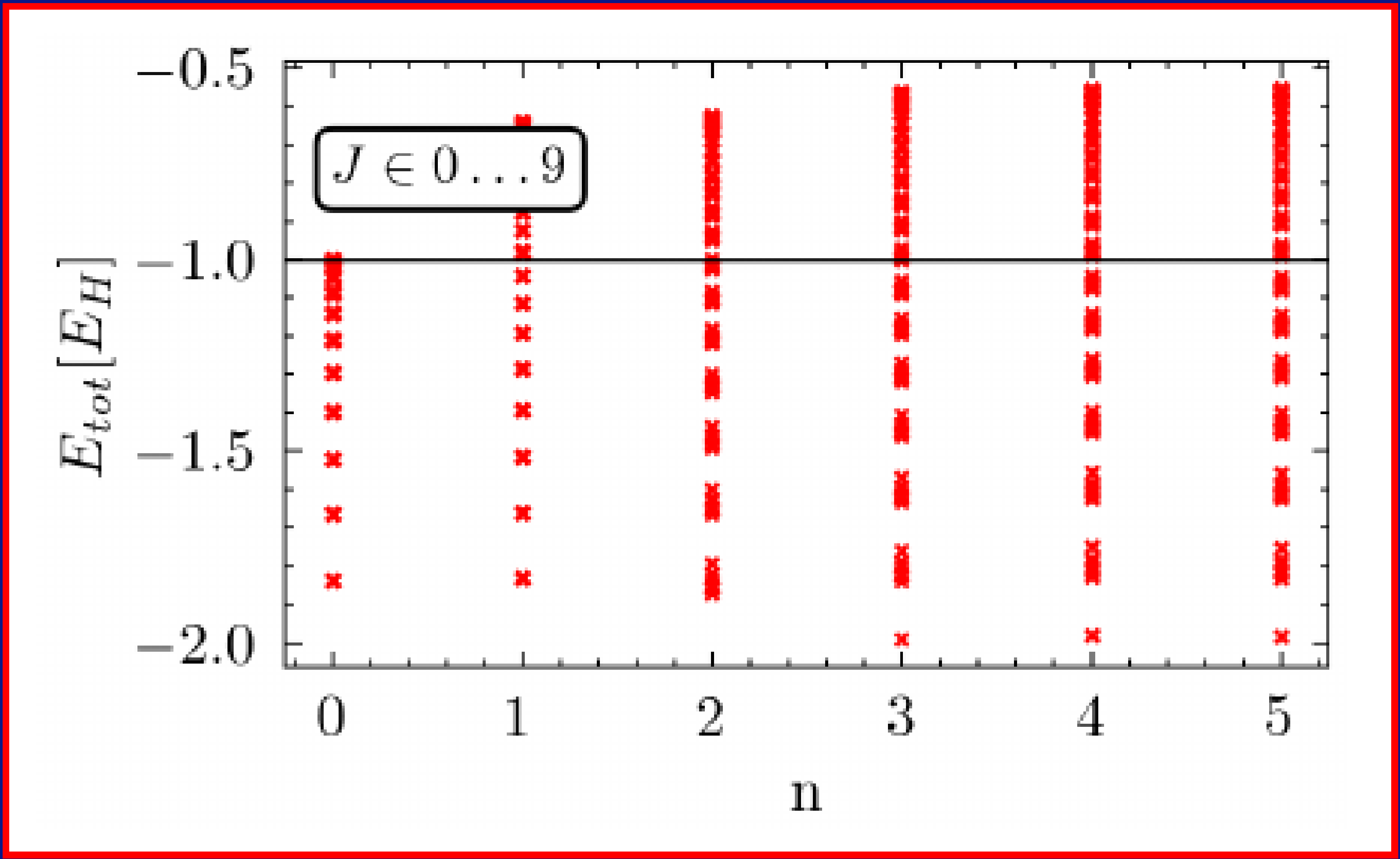
Vibrational states / Feshbach resonances



Vibrational states / Feshbach resonances



Density of states at threshold



Many states at threshold (only Q positive ones are shown).

Summary

1. Confined particles (ultracold atoms in optical lattices or tweezers)
   - Influence of the confining potential.
   - Confinement-induced resonances (CIR).
2. Hydrogen-antihydrogen interaction.

Resonances in few-body systems are ubiquitous.

The influence of confining potentials can usually not be ignored.