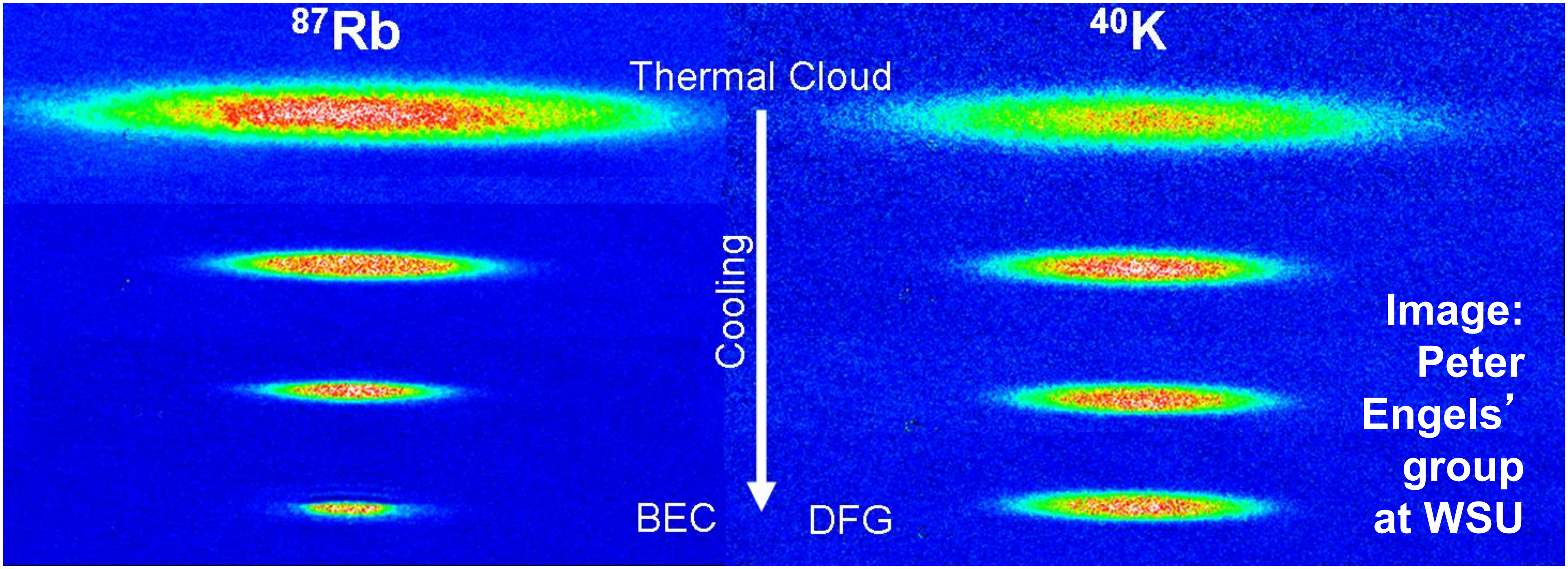

Static and Dynamic Properties of One-Dimensional Few-Atom Systems

Doerte Blume

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Supported by NSF.

Few-Body Physics in Cold Gases

- "Traditionally": Loss measurements of large cold samples provide insights into two-, three- and higher-body processes. Important work on three-body Efimov effect.
- Recent advances: Few-body systems can be prepared in an isolated environment and probed (single atom detection).

Cold molecular beam experiment: Imaging of quantum mechanical density of Efimov helium trimer.

Science 348, 551 (2015)

THREE-BODY PHYSICS

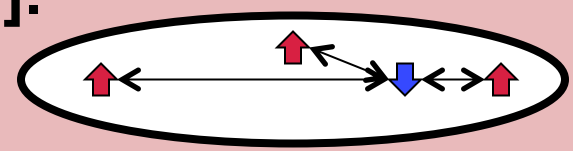
Observation of the Efimov state of the helium trimer

Maksim Kunitski,[1*] Stefan Zeller,[1] Jörg Voigtsberger,[1] Anton Kalinin,[1] Lothar Ph. H. Schmidt,[1] Markus Schöffler,[1] Achim Czasch,[1] Wieland Schöllkopf,[2] Robert E. Grisenti,[1,3] Till Jahnke,[1] Dörte Blume,[4] Reinhard Dörner[1*]

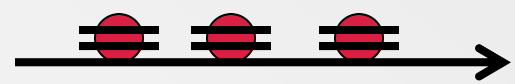
Ultracold fermions in microtrap (Selim Jochim's group): Deterministic state preparation. Radio-frequency spectroscopy. Tunneling spectros-copy with single atom detection.

Outline of This Talk

- **Static properties of one-dimensional few-atom gases:**
  - **Non-interacting Fermi gas with a single impurity [(N,1) system with delta-function interaction].**

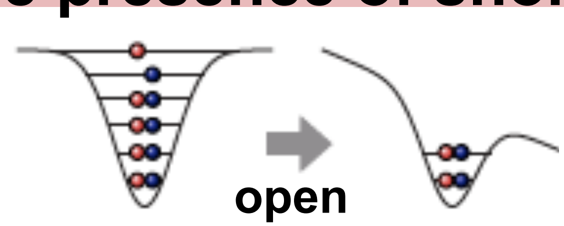


  - **Strongly-interacting gas (identical bosons or identical fermions) with spin-orbit and Raman couplings.**

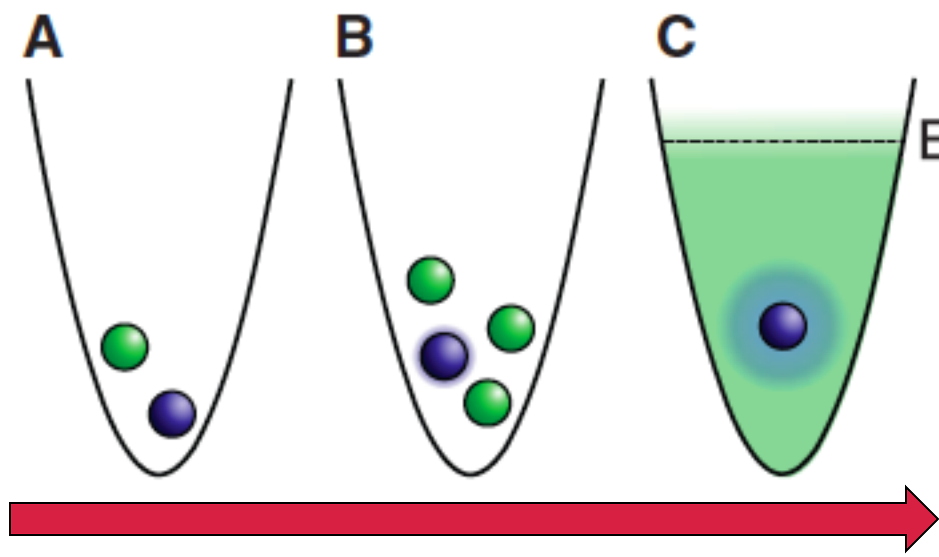


- **Dynamic properties of one-dimensional few-atom gases:**
  - **Tunneling dynamics in the presence of short-range interactions.**

Serwane et al., Science 332, 6027 (2011)

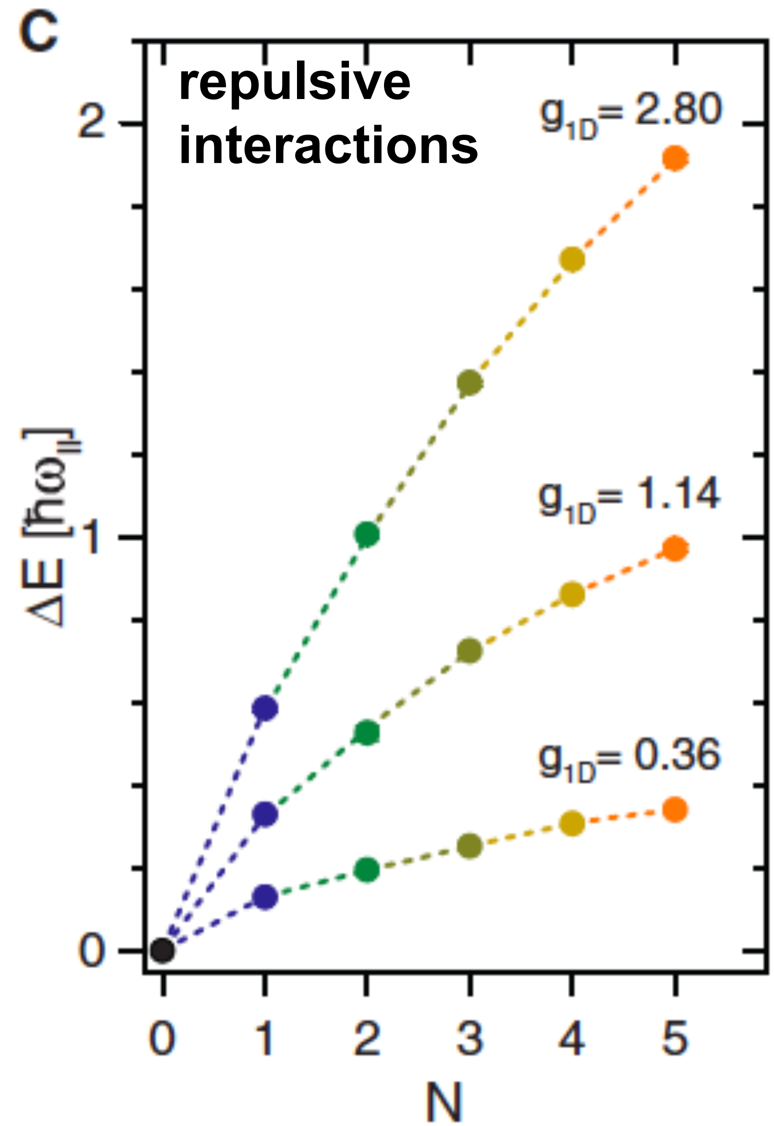


Motivation: Transition to Fermi Sea of Spin-Up Fermions with Single Impurity



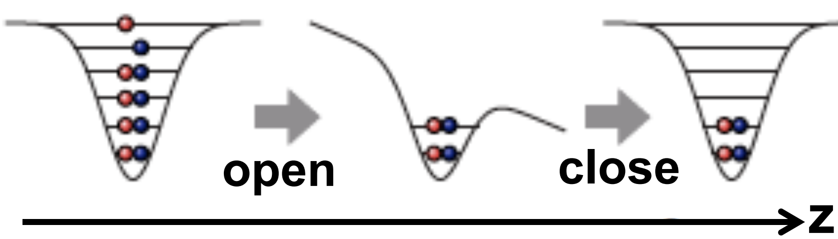
few-body to many-body
(effectively 1D geometry)

Radio-frequency spectroscopy yields interaction energy ΔE (i.e., energy relative to NI system): ΔE goes up with increasing N and g_{1D}.
Wenz et al., Science 342, 457 (2013).



Energy Spectra: Rf Spectroscopy Data versus 3D and 1D Calculations

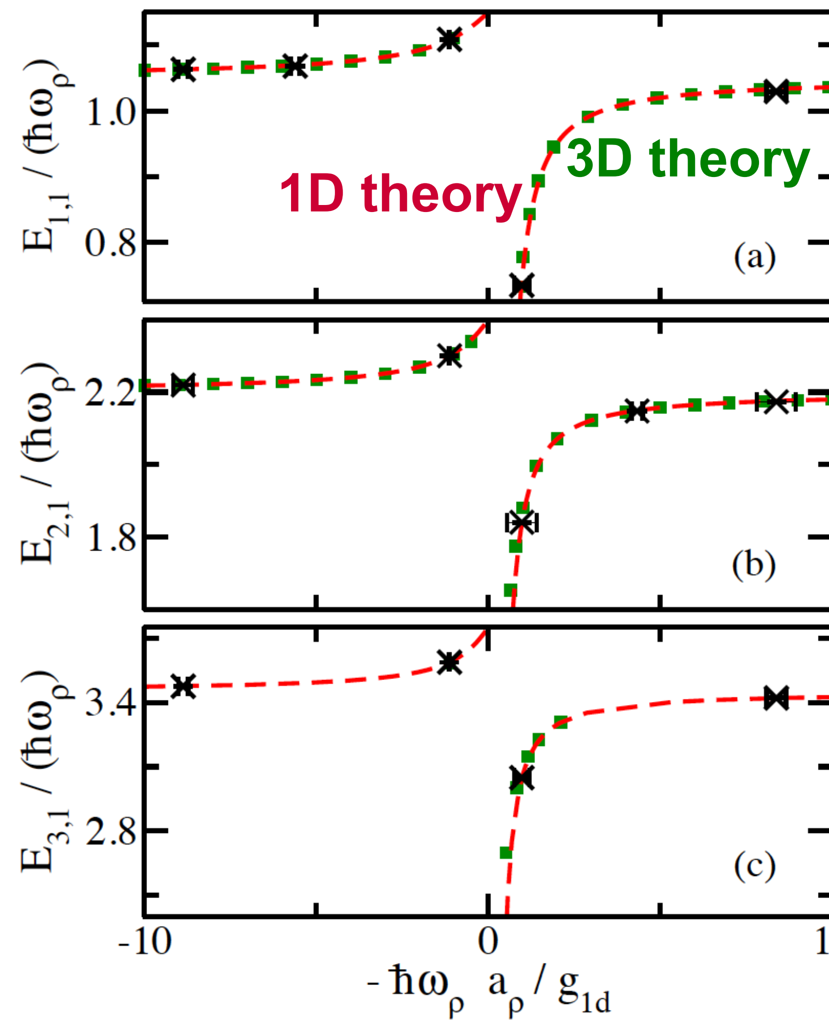
In the tight xy-directions, the confinement is approximately harmonic. Tunneling in z allows for preparation of (1,1), (2,1), (3,1), (2,2),… systems:



Serwane et al., Science 332, 6027 (2011)

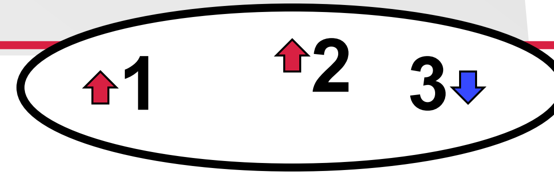
Experimental data: G. Zuern, Ph.D. thesis, Heidelberg (2012).
Theory: Gharashi, Yin, Blume, PRA 89, 023603 (2014).

Experiment: rf spectroscopy



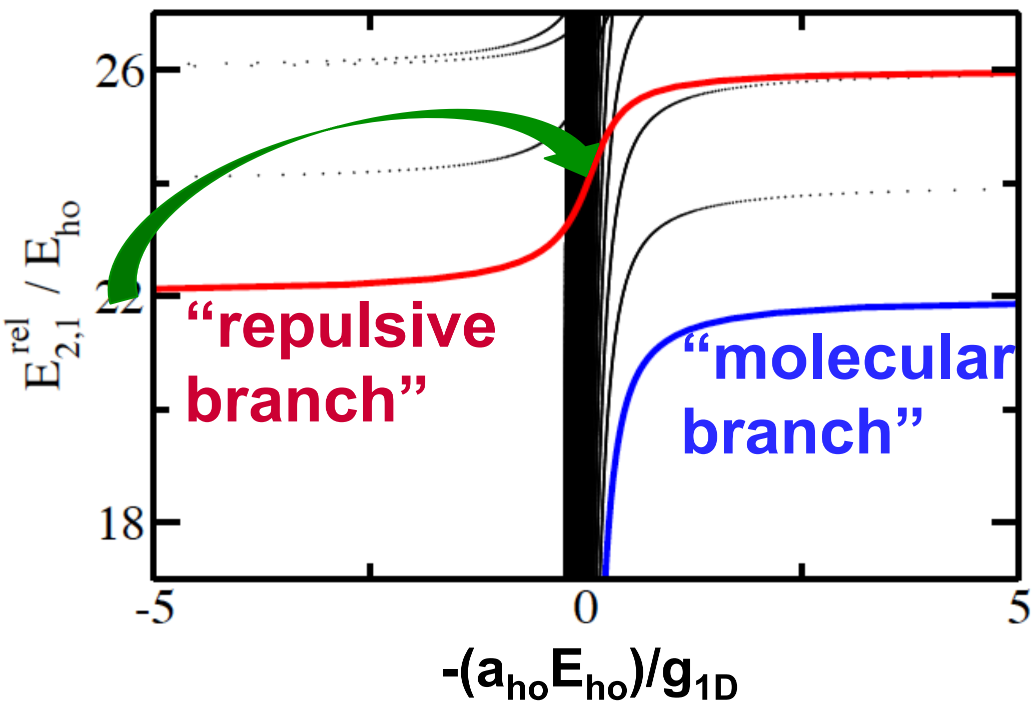
1 / (two-body interaction strength)

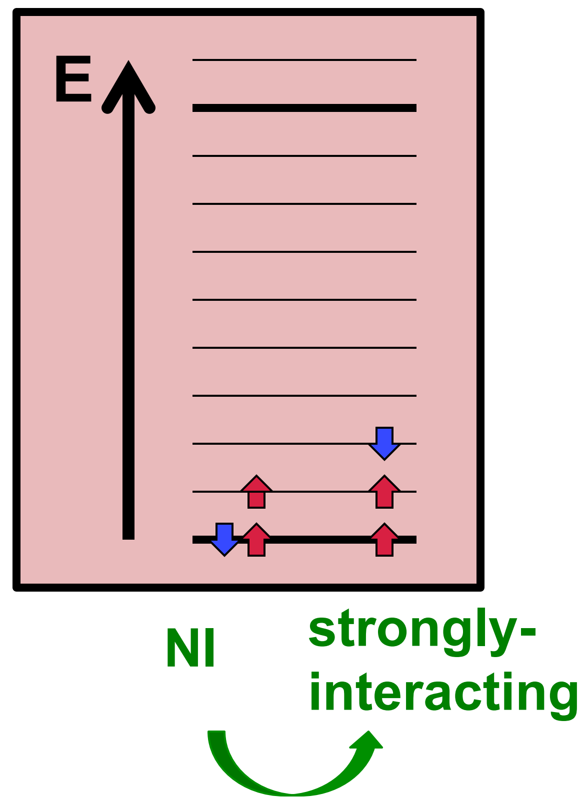
Detailed Spectrum: (2,1) Fermi System in Highly-Elongated Trap



1 and 3 interact.
2 and 3 interact.

3D energy spectrum for elongated trap with aspect ratio 10 (but shown as a function of $-1/g_{1D}$):





Gharashi, Daily and Blume, PRA 86, 042702 (2012) (calculations based on Lippmann-Schwinger equation).

Building a Fermi Sea with a Single Impurity One Atom at a Time

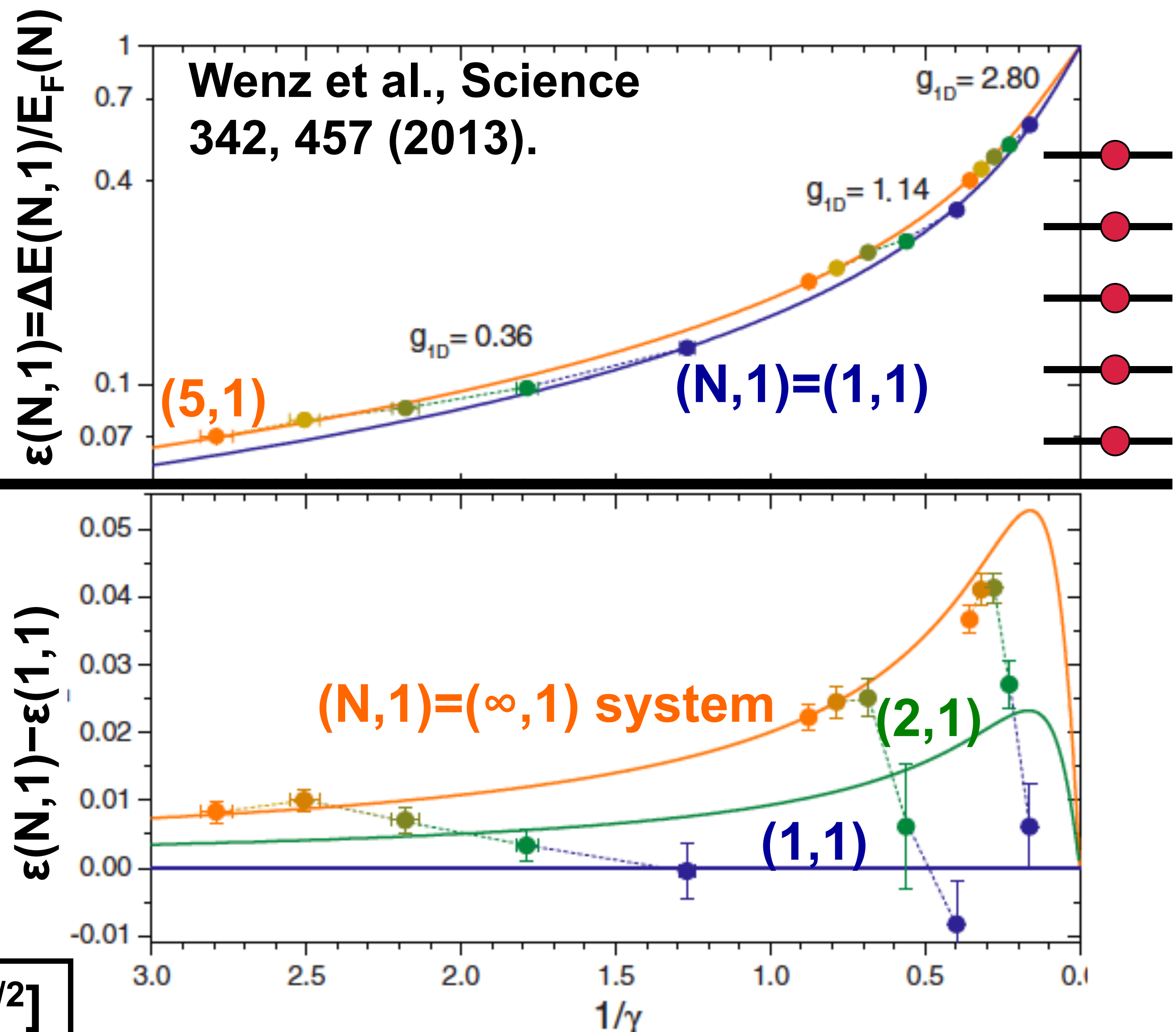
Scale interaction energy ΔE(N,1) by Fermi energy $E_F(N)$.

$E_F(N) = N E_{ho}$

N: # of majority atoms.

Subtract scaled two-body energy ε(1,1) ("residue" beyond one interacting pair at a time).

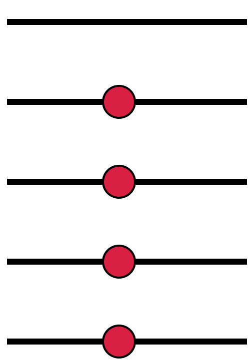
$\gamma = \pi g_{1D}/[E_{ho}a_{ho}(2N)^{1/2}]$



Semi-Analytical Expression for Interaction Energy of True 1D System?

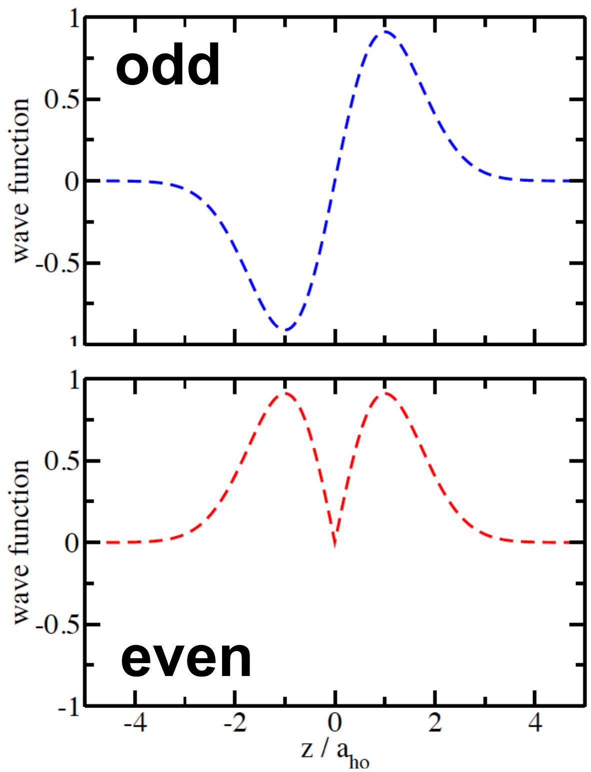
- For systems with periodic boundary conditions, Bethe ansatz. See McGuire (1965).

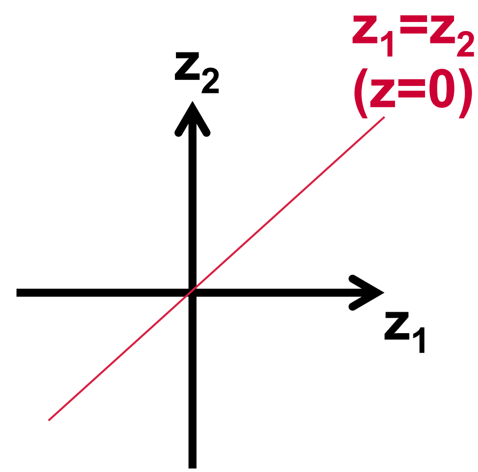
- For harmonically trapped Fermi gas with impurity, $g_{1D}=0$ and $g_{1D}=\infty$ are analytically tractable (Girardeau).



$g_{1D}=\infty$ (wave fct.= Slater determinant)

E.g., (1,1) and $g_{1D}=\infty$:





Node at $z_1=z_2$: Particles cannot penetrate.

Non-symmetrized states:

For $z_1<z_2$: $\mathrm{Det}(\varphi_0(z_1),\varphi_1(z_2))\Theta_{z1<z2}$

For $z_1>z_2$: $\mathrm{Det}(\varphi_0(z_1),\varphi_1(z_2))\Theta_{z2<z1}$

Strategy: Treat Interactions as Perturbation around g_{1D}=0 and $g_{1D}=\infty$

Gharashi, Yin, Yan, Blume, PRA 91, 013620 (2015).

- $g_{1D}=0$ (standard perturbation theory):
  - Interaction $\Sigma_j\, g_{1D}\delta(z_j - z_0)$.
  - Boundary condition: $\Psi'(z_{j0}=0^+)-\Psi'(z_{j0}=0^-)=(g_{1D}m/\hbar^2)\Psi(z_{j0}=0)$.
  - All infinite sums converge.
  - Up up to 3rd order PT: $\varepsilon(N,1) = B^{(1)}(N)\gamma + B^{(2)}(N)\gamma^2 + B^{(3)}(N)\gamma^3$

- $g_{1D}=\infty$ ("non-standard" perturbation theory):
  - Rewrite interaction matrix element $V_{\alpha\beta}$ as $1/g_{1D}$ x integral:
    $V_{\alpha\beta} = \Sigma_j -\hbar^4/(m^2 g_{1D})$ x I_j, where
    $I_j = < \Psi_\alpha'(z_{j0}=0^+)-\Psi_\alpha'(z_{j0}=0^-) \mid \delta(z_{j0}) \mid \Psi_\beta'(z_{j0}=0^+)-\Psi_\beta'(z_{j0}=0^-) >$.

Volosniev et al., Nat. Comm. 5, 5300 (2014).

  - Starting at 2nd order, we see divergencies (need to introduce counterterms).
  - Up to 3rd order PT: $\varepsilon(N,1) = 1 + C^{(1)}(N)\gamma^{-1} + C^{(2)}(N)\gamma^{-2} + C^{(3)}(N)\gamma^{-3}$

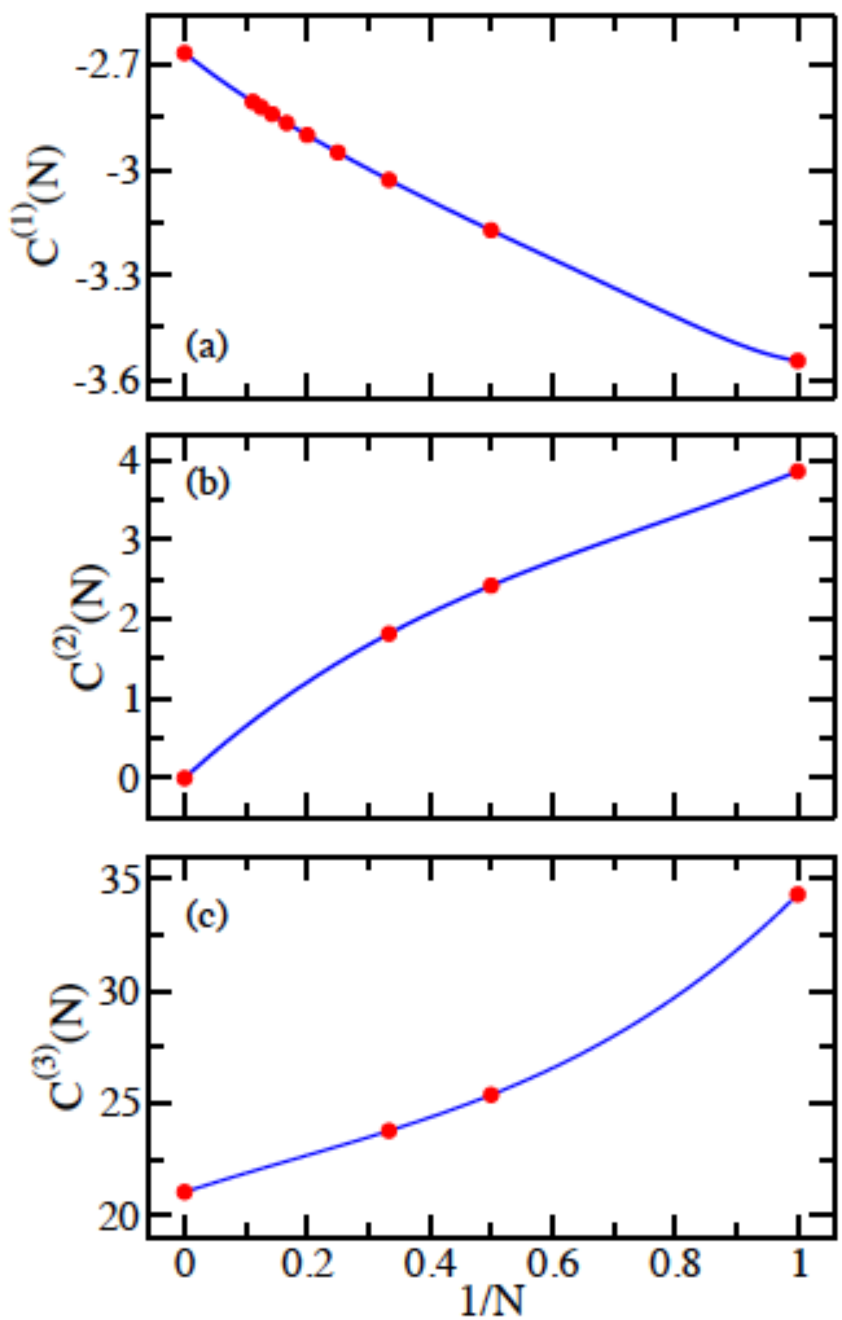
$1/g_{1D}$ Expansion Coefficients

For (N,1)=(1,1), expand transcendental equation by Busch et al. (1998) around γ=0 and 1/γ=0.

For (N,1)=(∞,1), apply local density approximation to McGuire result (1965) and expand around γ and 1/γ.

(N,1)=(1,1) and (N,1)=(∞,1) results connect smoothly.

How well do the expansions work?

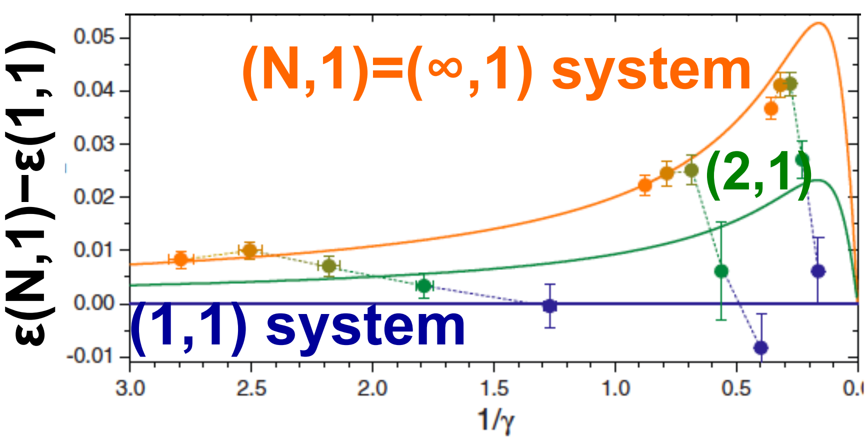


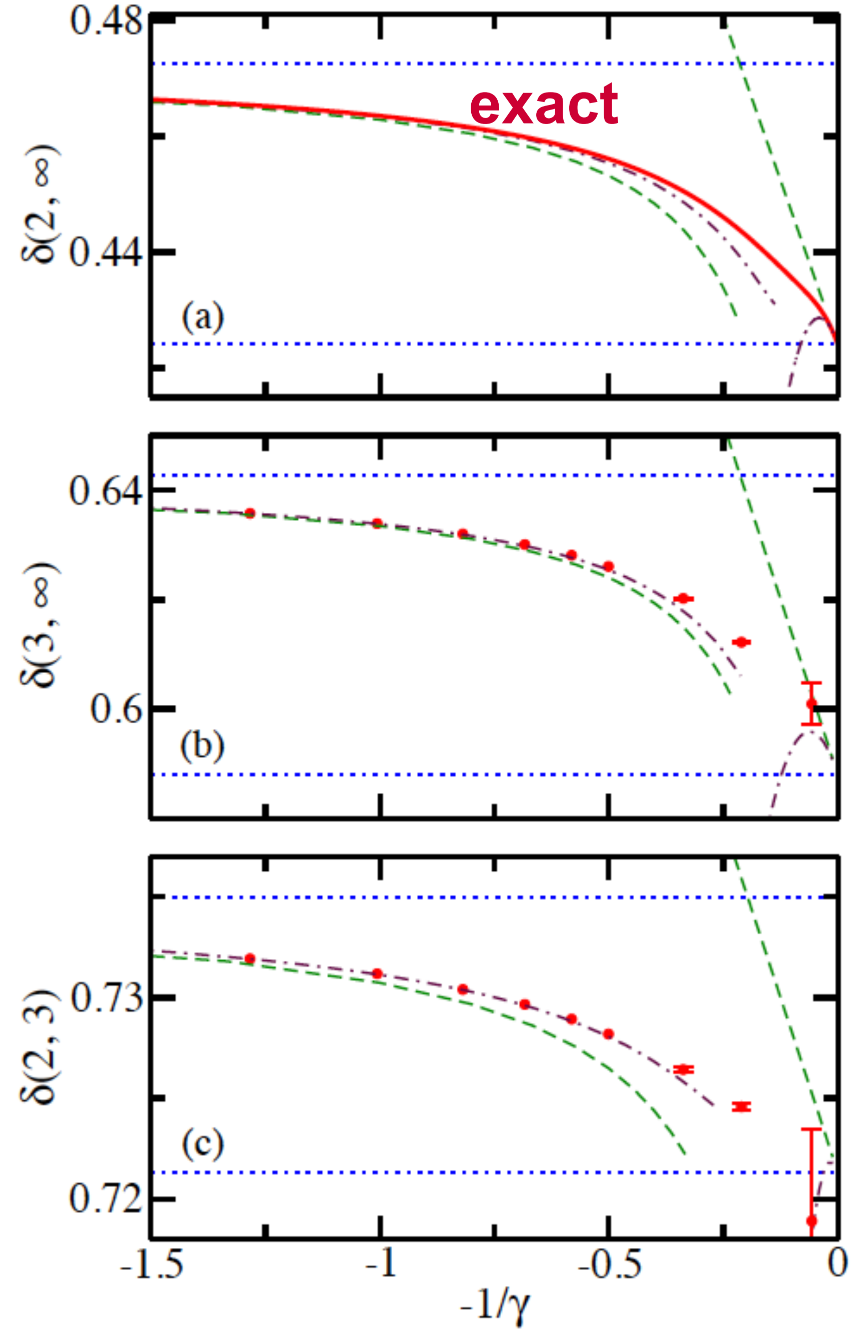
Scaled Interaction Energy

δ(N,N') =
[ε(N,1)−ε(1,1)] / [ε(N',1)−ε(1,1)]

Small γ:
$\delta(N,N') = \xi^{(0)} + \xi^{(1)}\gamma + \xi^{(2)}\gamma^2$

Large γ:
$\delta(N,N') = \zeta^{(0)} + \zeta^{(1)}\gamma^{-1} + \zeta^{(2)}\gamma^{-2}$





Scaled Interaction Energy

δ(N,N') =
[ε(N,1)−ε(1,1)] / [ε(N',1)−ε(1,1)]

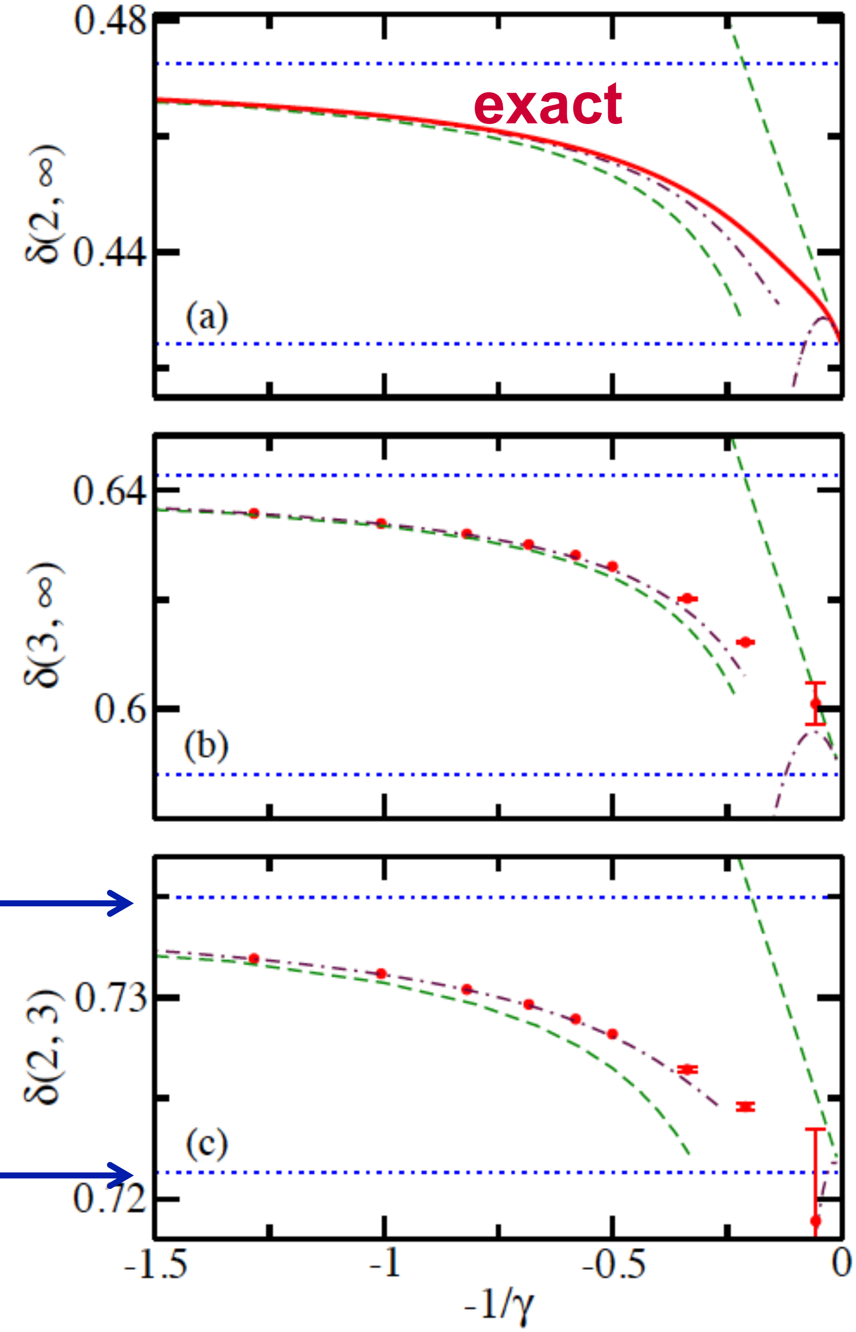
Small γ:
$\delta(N,N') = \xi^{(0)} + \xi^{(1)}\gamma + \xi^{(2)}\gamma^2$

Large γ:
$\delta(N,N') = \zeta^{(0)} + \zeta^{(1)}\gamma^{-1} + \zeta^{(2)}\gamma^{-2}$

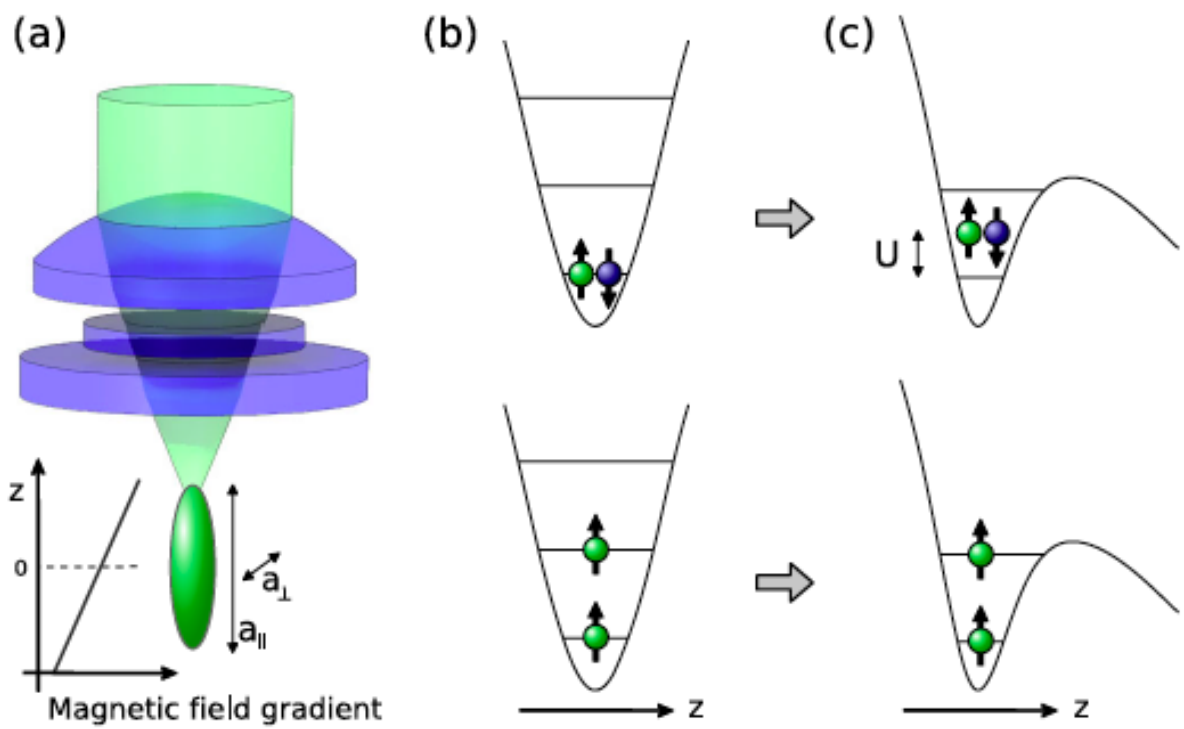
Radius of convergence:
N=2: $1/\gamma=(1.0745\ 2\pi)^{-1}$ ~0.148.
N=∞: $1/\gamma=(2\pi)^{-1}$

small γ

large γ



Change from Statics to Dynamics: Tunneling for Two Interacting Particles



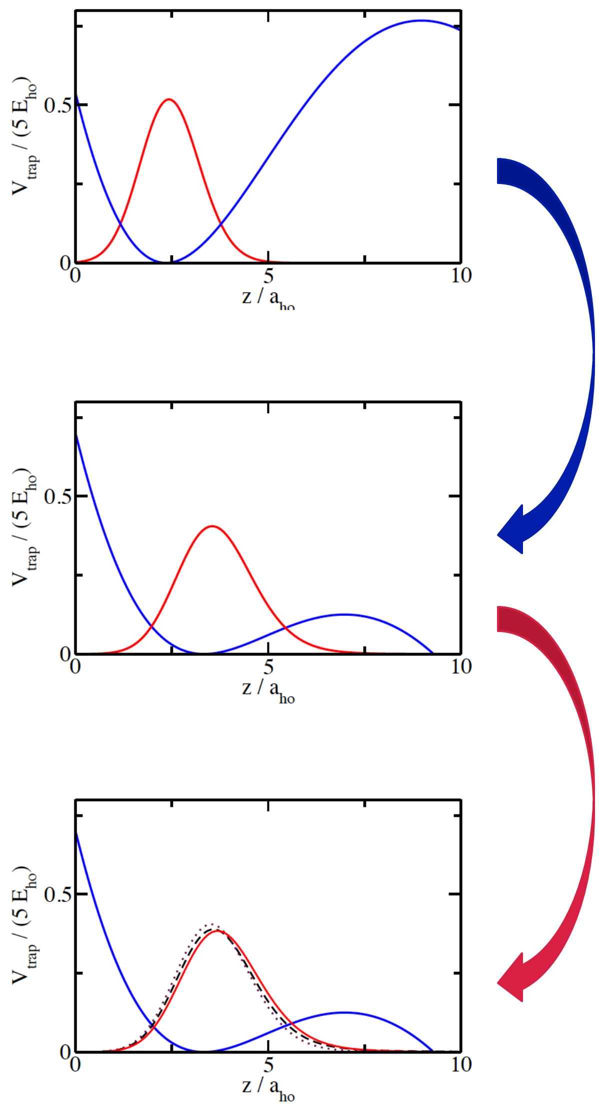
From Zuern et al., PRL 108, 075303 (2012).

Somewhat similar to He atom (two electrons) in external field.

A key difference: The cold-atom experiments are effectively one-dimensional.

Electrons: Atoms in particular hyperfine state.
Electron-electron Coulomb potential: Zero-range contact potential.
Electron-nucleus Coulomb potential: External harmonic trap.

Look at Tunneling in Detail: Start with Single-Particle System



lower the barrier in about 2ms

wavepacket is no longer in "eigenstate": follow time evolution for ~100-1000ms

Functional form of $V_{trap}(z)$:

$V_{trap}(z) =$

$pV_0[1-1/[1+(z/z_r)^2]]-\mu_m c_{|j>} B'z$

First task:

Can we look at outward flux and determine p and $c_{|j>}B'$ through comparison with experimental data?

Second task:

What happens if we prepare two-atom state?

Look at upper branch.

Look at molecular branch.

How to Calculate the Flux out of the Trap (Tunneling Rate)?

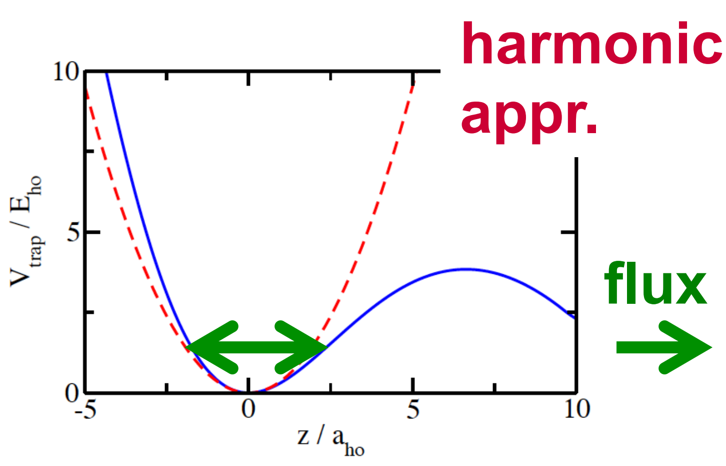
Solve time-dependent Schroedinger equation

$i\hbar\, \delta\Psi(x,t)/\delta t = H\, \Psi(x,t)$ for initial state $\Psi(x,0)$.

Hamiltonian H = (kinetic energy operator) + (potential energy).

For single particle: potential energy = trapping potential $V_{trap}(z)$.

For two particles: $V_{trap,1}(z_1) + V_{trap,2}(z_2)$ + (interaction potential).

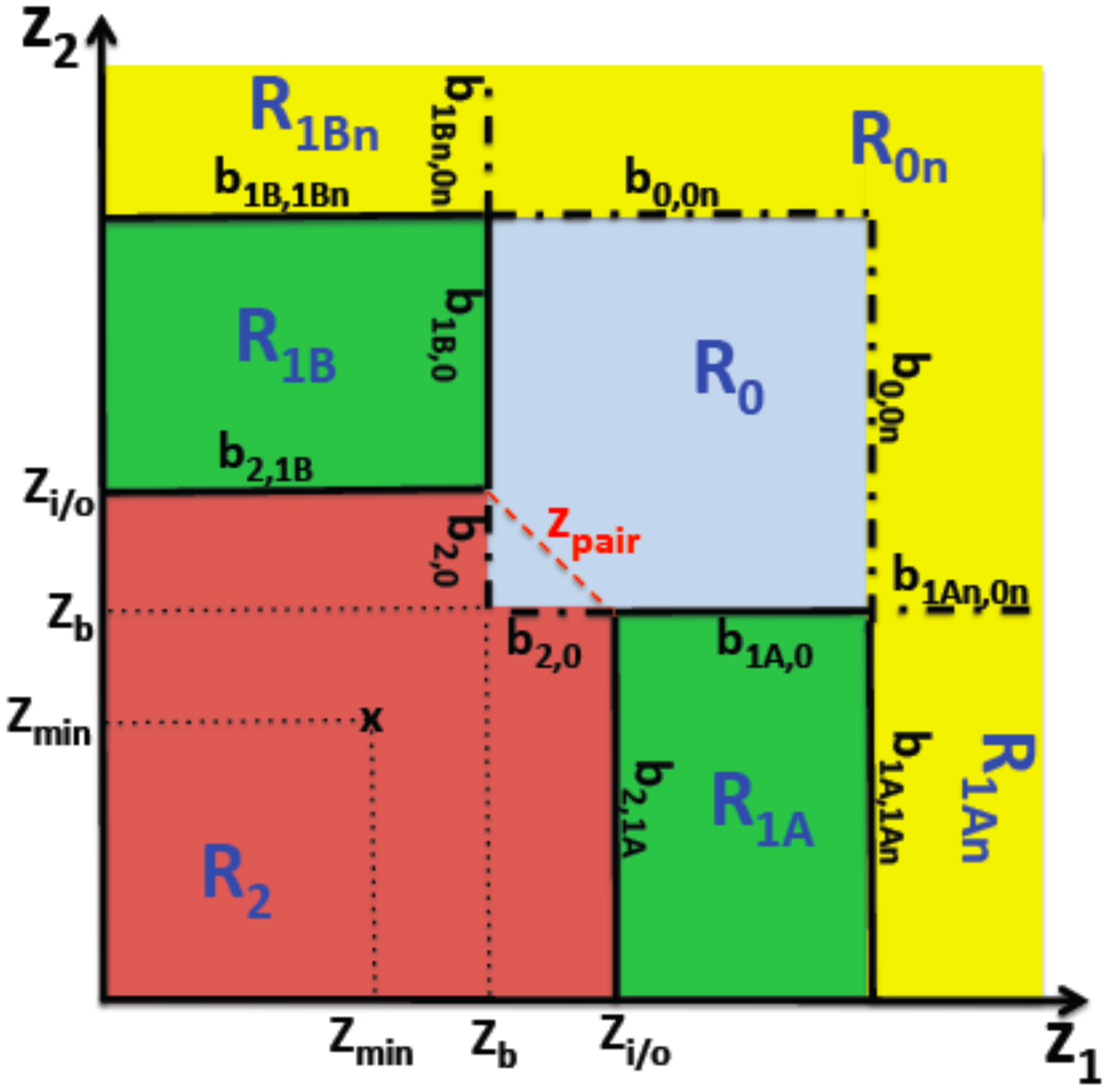


Trap time scale: $T_{ho}=\omega^{-1}$.

"Many runs against the barrier": Need to go to $t \gg T_{ho}$.

Use absorbing boundary conditions or damping so that wave packet will not get reflected by the box.

Our 2D Numerics: Three Different Length Scales ($z_0 << a_{ho} <<$ Num. Box L)

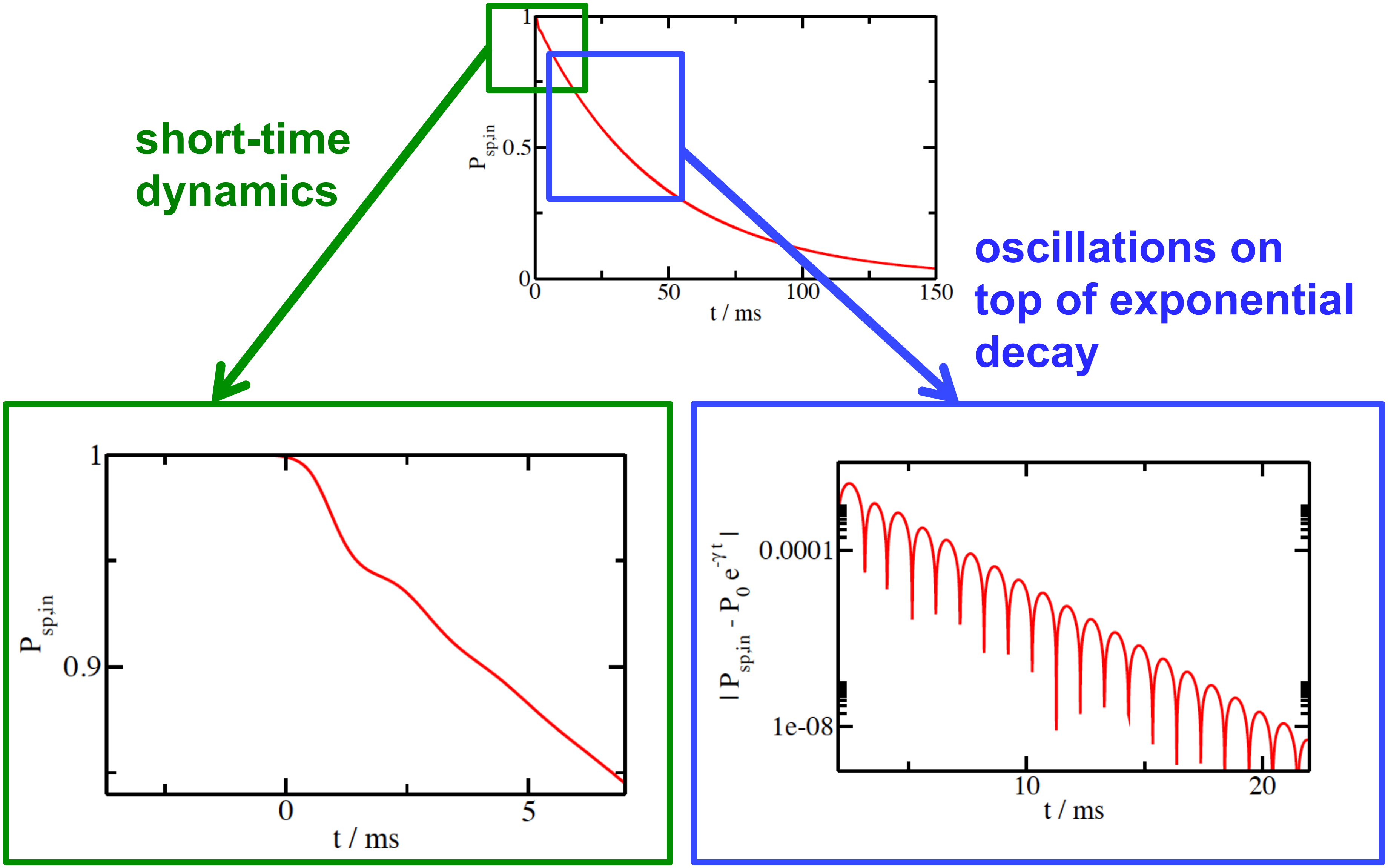


Two different time propagation schemes:
1) Expand propagator in Chebychev polynomials (only for finite-range two-body potentials; "fast").
2) Use exact zero-range propagator ("slow").

Region with two trapped particles (R_2), regions with one trapped particle (R_{1A} and R_{1B}) and region with zero trapped particles (R_0).

To get average number of particles in trap, we monitor flux through $b_{2,1A}$, $b_{2,1B}$, $b_{2,0}$.

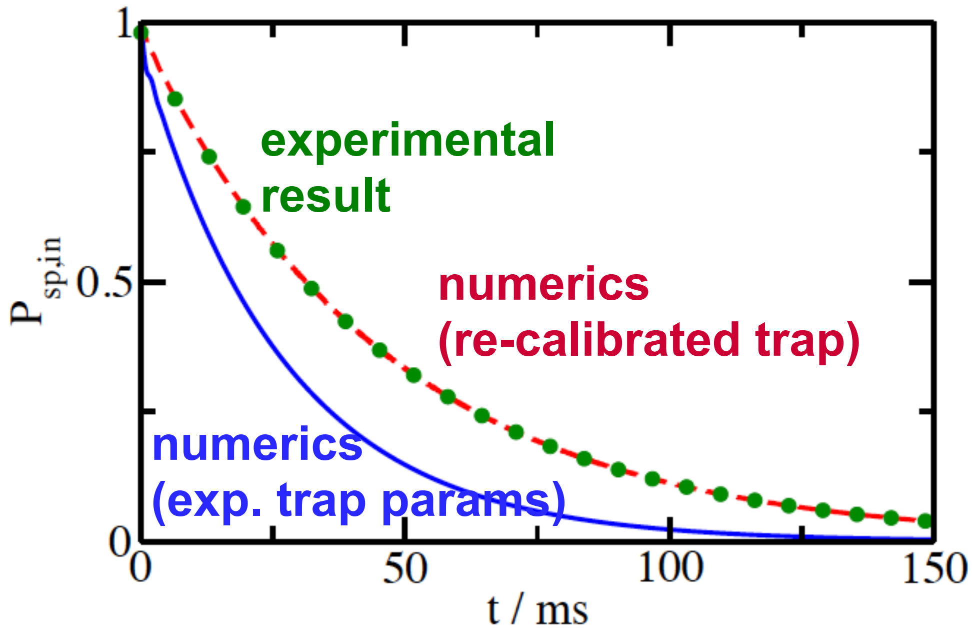
Fraction $P_{sp,in}$ Inside the Trap: Exponential Decay with Extra Features



Compare Single-Particle Dynamics with Experimental Results

Experimental paper contains trap parameters p and $c_{|j>}B'$ [Zuern et al., PRL 108, 075303 (2012)].
When we use these parameters, our tunneling rate γ differs by up to a factor of two from experimentally measured tunneling rate.

$P_{sp,in}(t) = P_{sp,in}(0) \exp(-\gamma t)$.



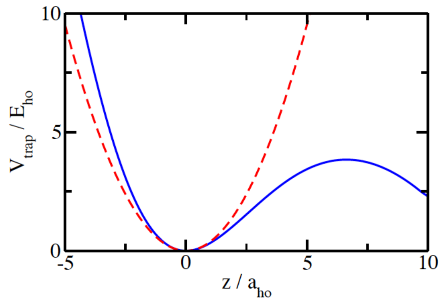
Why? Trap parameters p and $c_{|j>}B'$ are calibrated using semi-classical WKB approximation. WKB tunneling rate is inaccurate.

See also Lundmark et al., PRA 91, 041601(R) (2015).

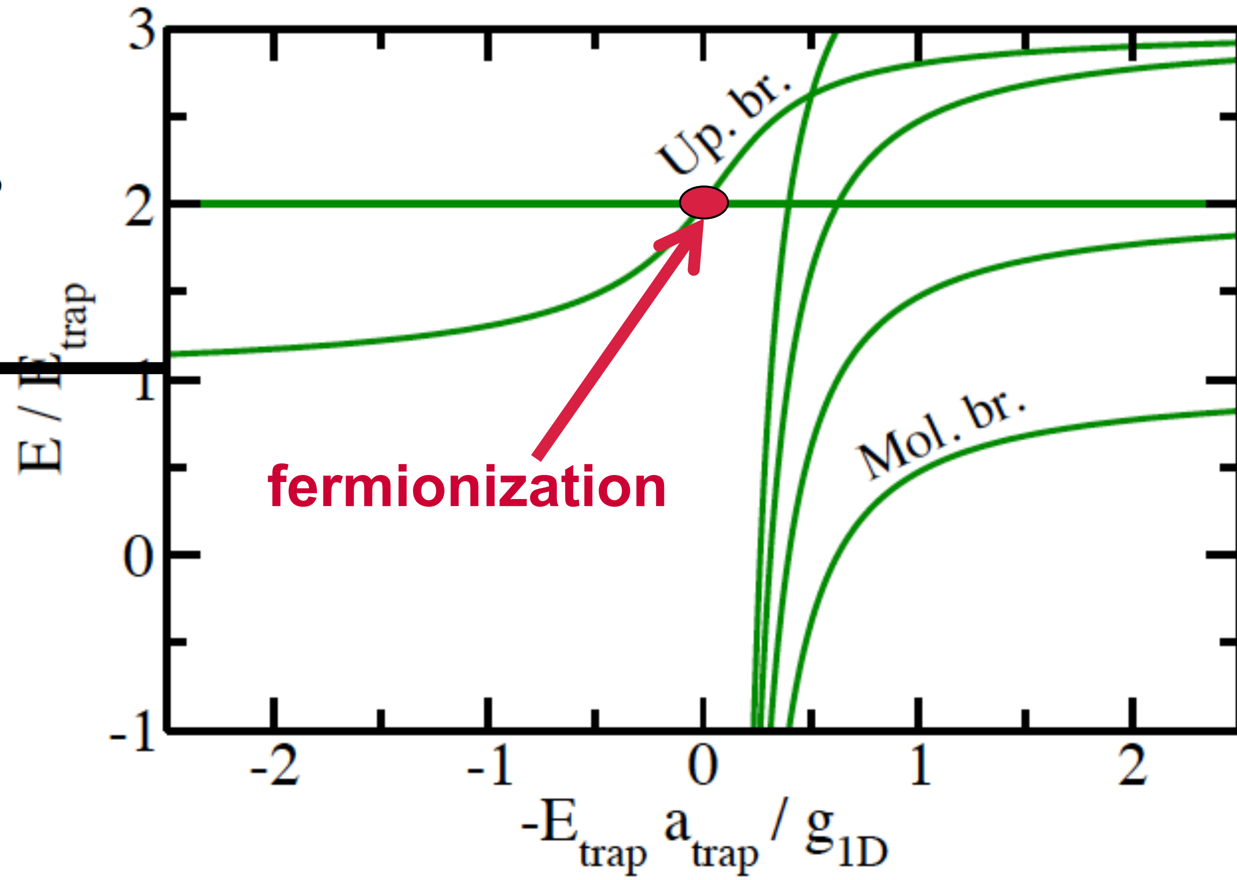
Re-parameterize trap: Find parameters such that our γ agrees with experimental γ.

Overview: Upper Branch and Molecular Branch for Deep Trap (Quasi-Eigenstates)

Harmonic approximation



Two-body energy spectrum:



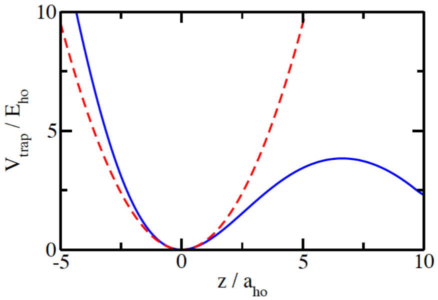
non-interacting (NI)

NI

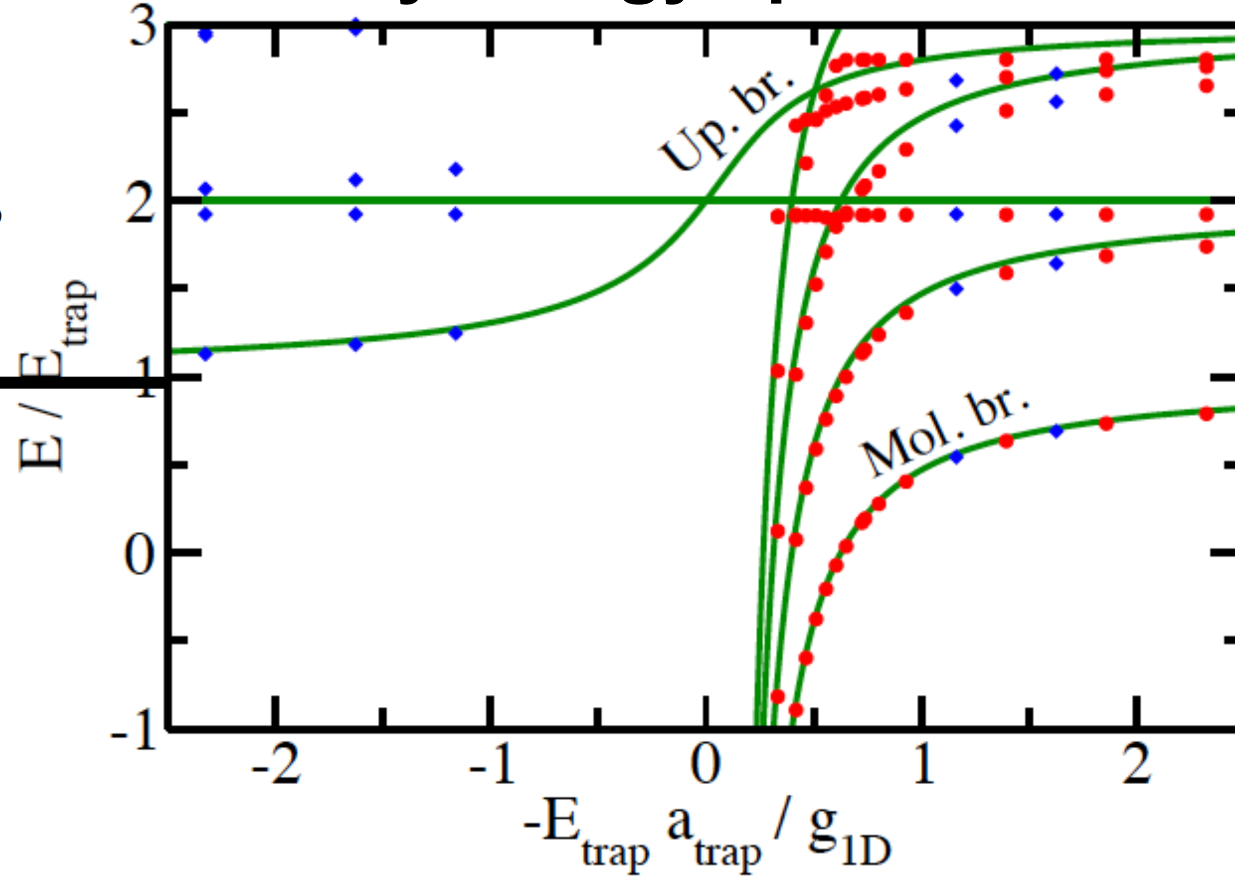
1 / (two-body interaction strength)

Overview: Upper Branch and Molecular Branch for Deep Trap (Quasi-Eigenstates)

Anharmonic confinement



Two-body energy spectrum:



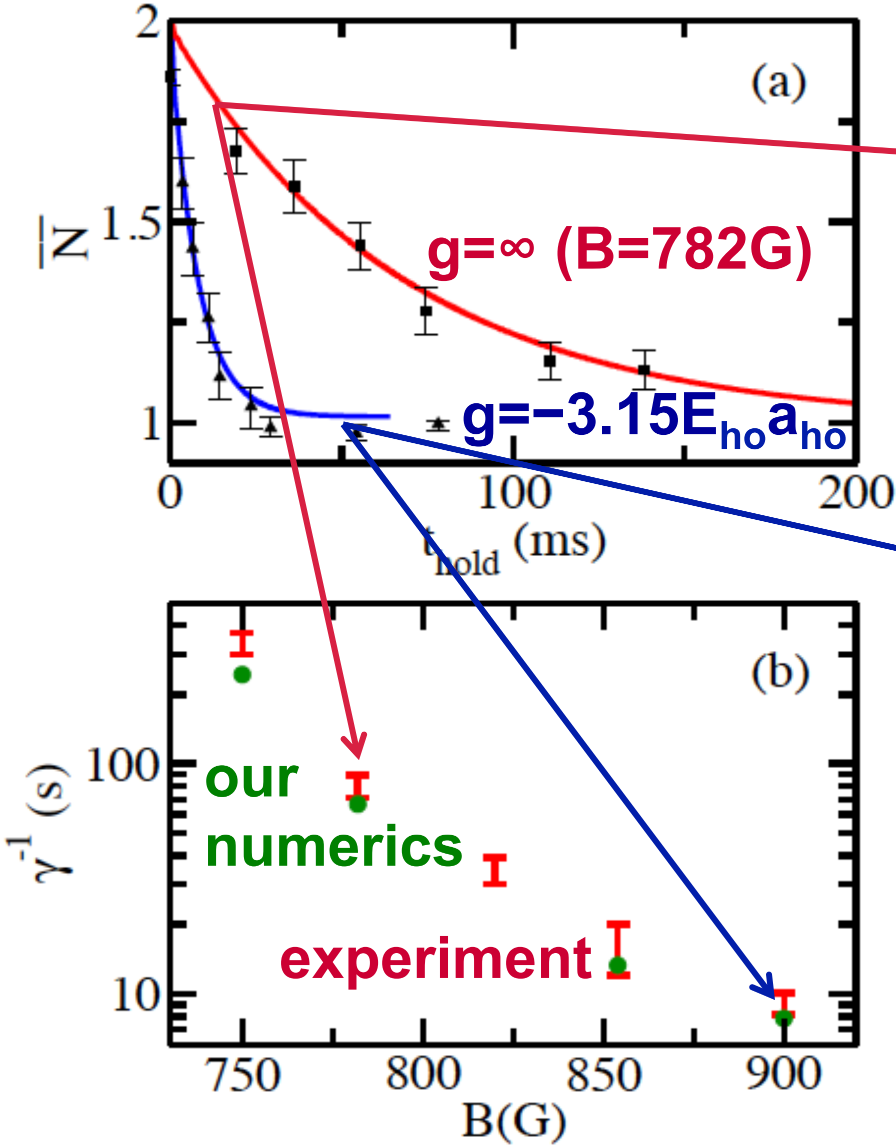
non-interacting (NI)

NI

1 / (two-body interaction strength)

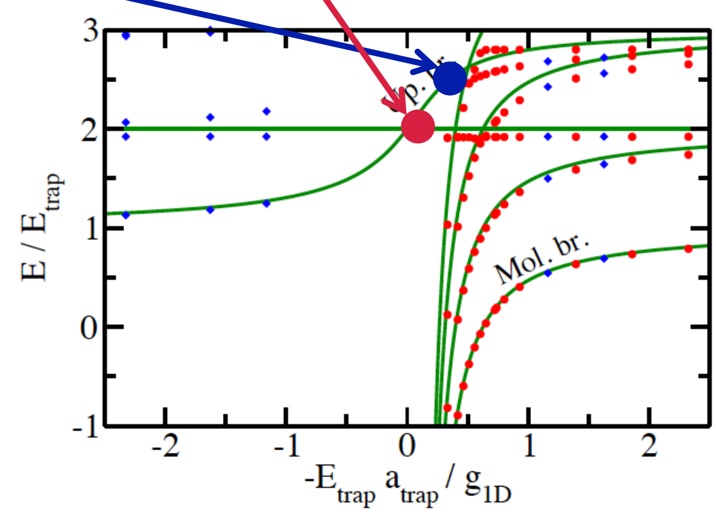
We consider zero-range and finite-range interactions (tiny range dependence).

Upper Branch: Comparison with Experimental Data



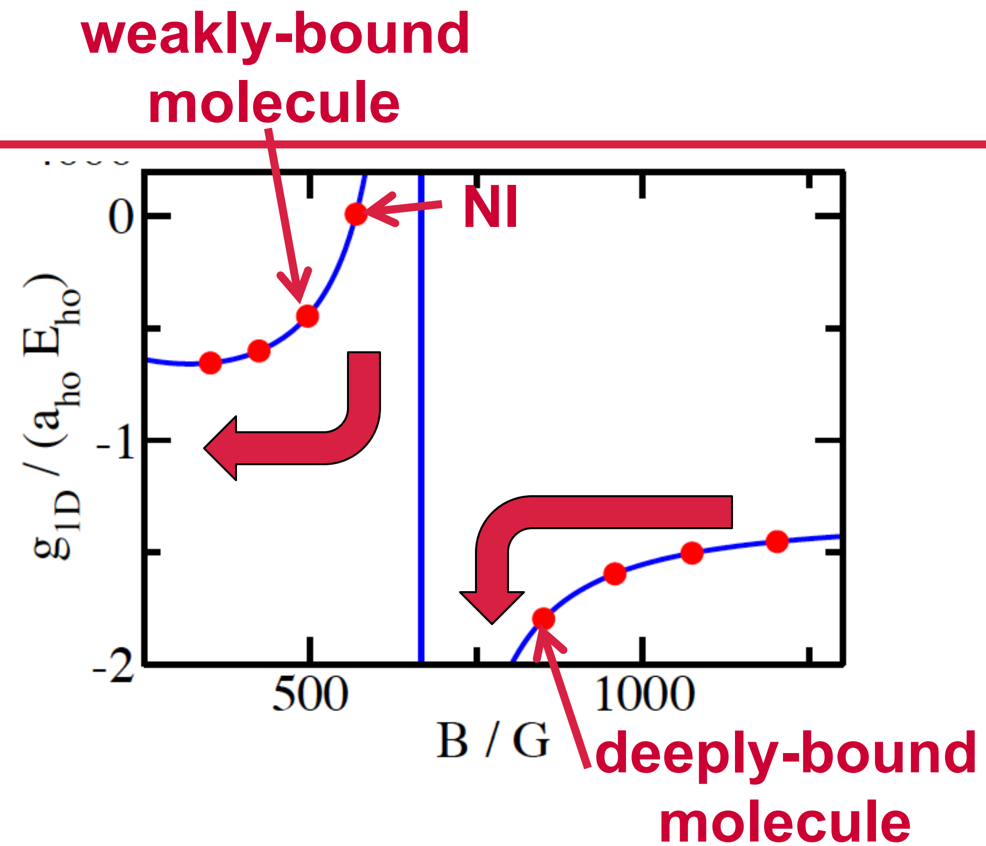
Very good agreement with experimental results.

The “further up” the upper branch the system is, the faster the decay.



Molecular Branch

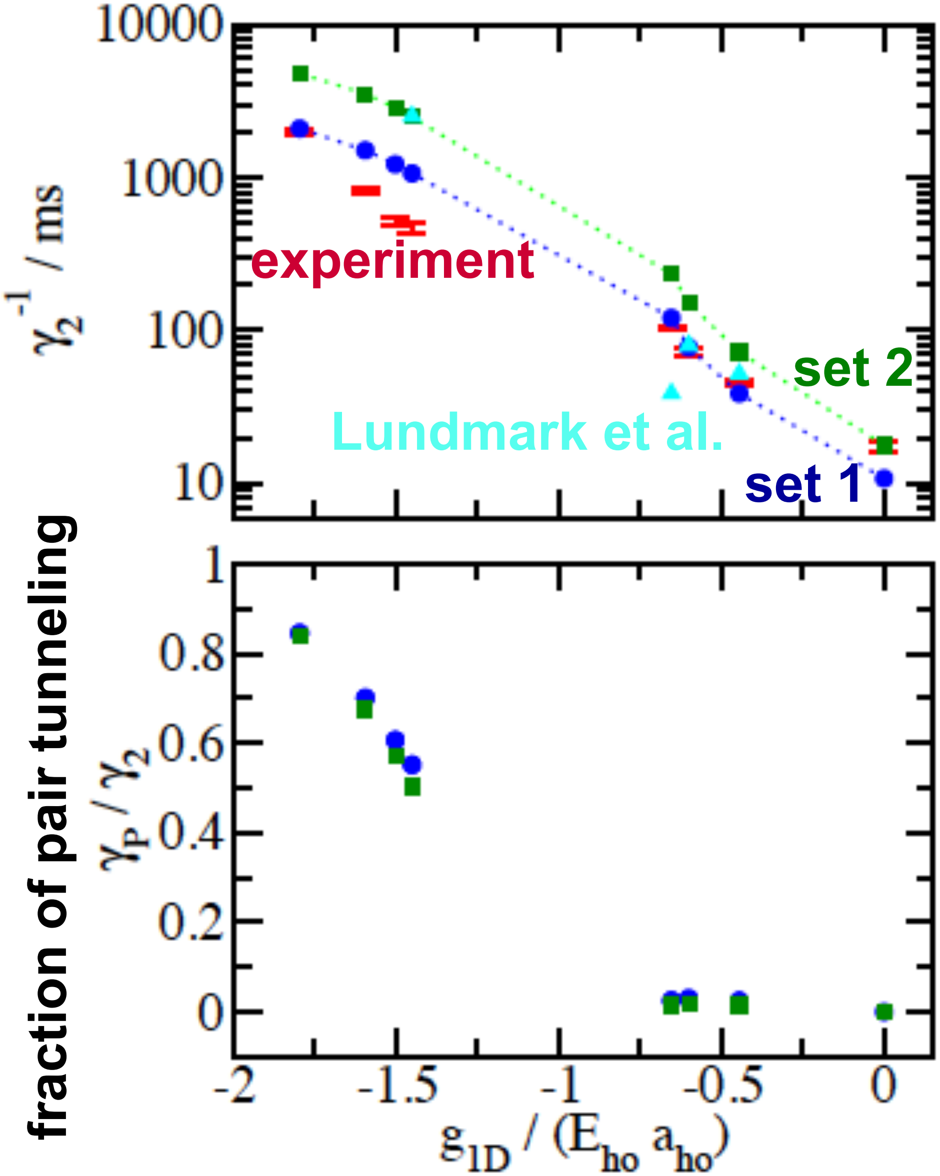
"Molecular branch" means that the interaction energy is negative (|F=1/2,M_F=1/2> and |F=3/2,M_F=−3/2> states). In free space, the two-body system would form a molecule of size ~ $-2/g_{1D}$.



Getting the single-particle tunneling rates to agree with experiment (=our re-calibration approach), does not guarantee agreement of two-body tunneling dynamics.

We unsuccessfully tried to "tweak" trap parameters such that we agree at one- and two-body level (non-unique inversion problem at single-particle level). May not be possible…

Results for Tunneling Dynamics of Molecular Branch



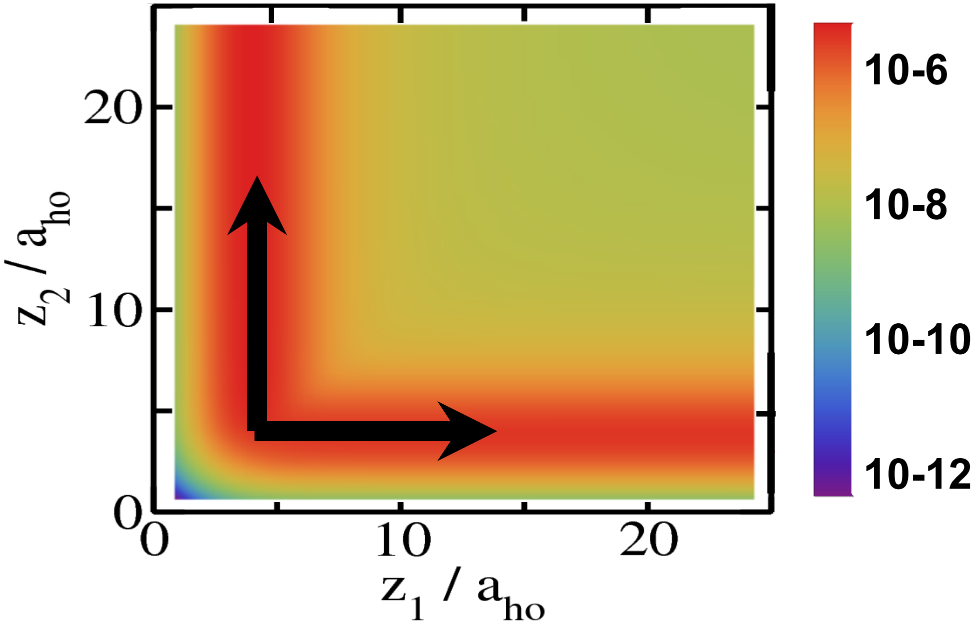
Set 1: We use the trap parameters determined by Heidelberg WKB analysis. Problem: Single particle tunneling rate is off by factor of 2.

Set 2: We use parameters that reproduce single-particle tunneling rate. Problem: Tunneling rates for interacting systems are off.

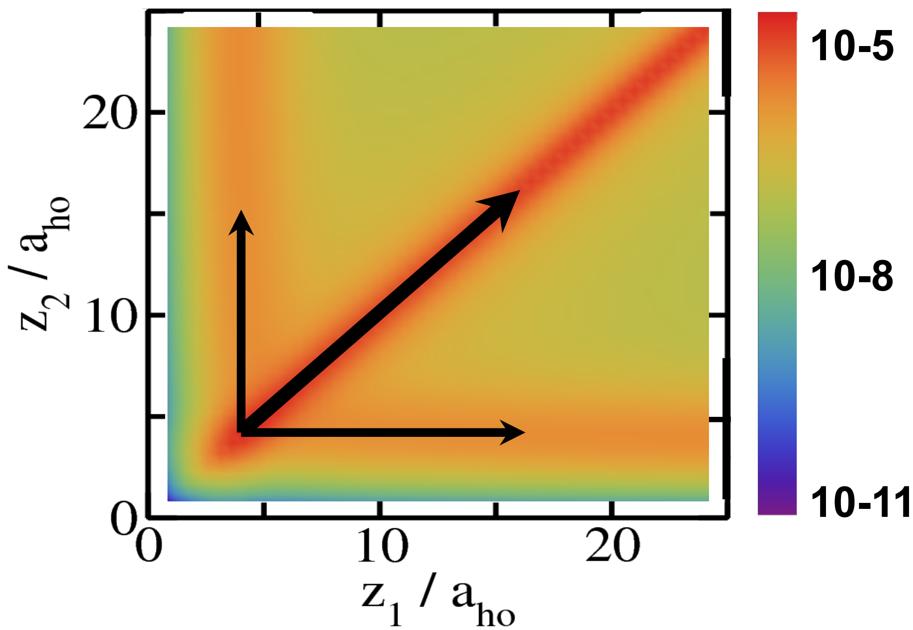
We disagree with results by Lundmark et al., PRA 91, 041601(R) (2015).

Magnitude of the Flux

Non-interacting system (g=0): Particles tunnel independently.



Attractive interaction (a_{1D}=1.38a_{ho}, g <0): Pair tunneling.



Summary of Time-Dependent Studies

- **Single-particle dynamics: WKB analysis should not be used to calibrate trapping potential.**

- **Two-particle tunneling dynamics in the presence of short-range interactions:**

  - **Upper branch tunneling dynamics (initial state is an excited state…) observed in Heidelberg experiment is reproduced nicely by our numerics.**

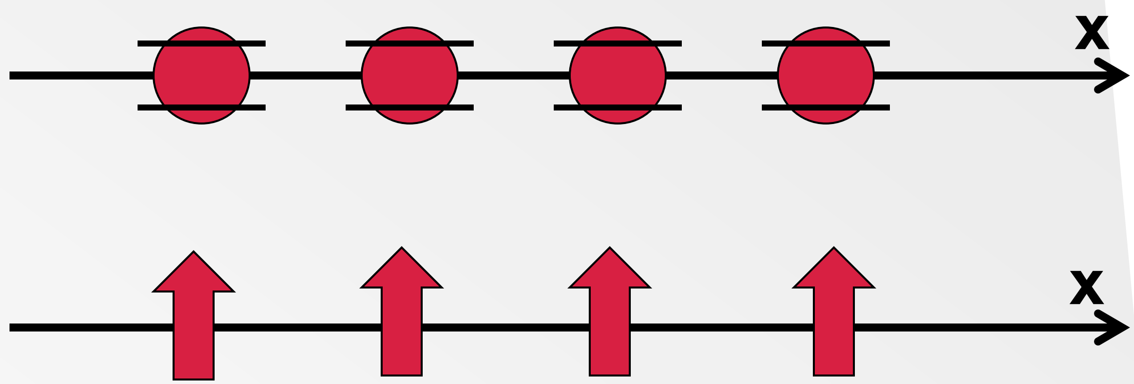
  - **Molecular branch tunneling dynamics observed in Heidelberg experiment turns out to be more challenging to reproduce: We find qualitative but not quantitative agreement.**
  - **Functional form of trap? Other molecular levels?**

N Trapped 1D Particles with $g_{1D}=\infty$: Spin-Orbit and Raman Coupling

Single particle terms (equal mixture of Rashba and Dresselhaus): Raman coupling $(\Omega/2)\sigma_{x,j}$ and spin-orbit coupling $(\hbar k_{so}/m)p_{x,j}\sigma_{y,j}$.

Unitary transformation $U_j=\exp(-ik_{so}x_j\sigma_{y,j})$: $-(\hbar k_{so})^2/(2m) + V_{R,j}$, where $V_{R,j} = (\Omega/2)\,(U_j)^+\,\sigma_{x,j}\,U_j$.

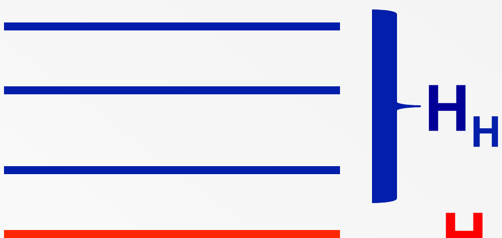
Weak couplings: Effective spin Hamiltonian of the form $(\Omega/2)\,\Sigma_j\,\underline{B}_j\,\underline{\sigma}_j$. Spin spiral due to “spiraling” of effective B-field at slot j [Cui and Ho, PRA 89, 013629 (2014)].



First-order degenerate perturbation theory yields $\Sigma_j\,\underline{B}_j\,\underline{\sigma}_j$ term (“matrix elements factorize”). Beyond 1st order?

How To Go Beyond First Order?

- Construct and diagonalize Hamiltonian matrix using “rotated” $g=\infty$ states as basis.
- Using 2nd order degenerate PT, construct effective low-energy Hamiltonian H_{eff} that is accurate to order Ω^2:
  $H_{eff} = \Sigma_{l,l' \text{ in } HL} |\psi_l\rangle\langle\psi_l| (\Omega^2/8)\, \Sigma_{k \text{ in } HH} ((A_{ll'})_k)\, |\psi_{l'}\rangle\langle\psi_{l'}|$.



H_L: $(N!) \times 2^N$ states

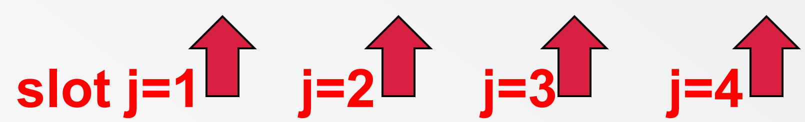
number of distinct particle orderings

two states per spin-1/2 atom

Matrix elements for any N can be rewritten as finite sums (one numerical integration for N>2): This allows for evaluation with arbitrary (controlled) accuracy.

Integrate over the spatial degrees of freedom:

$(\Omega/2)\, \Sigma_j\, \underline{B}_j\, \underline{\sigma}_j + (\Omega^2/8)\, \Sigma_{j,j'}\, \underline{\sigma}_j\, \underline{M}_{jj'}\, \underline{\sigma}_{j'}$.

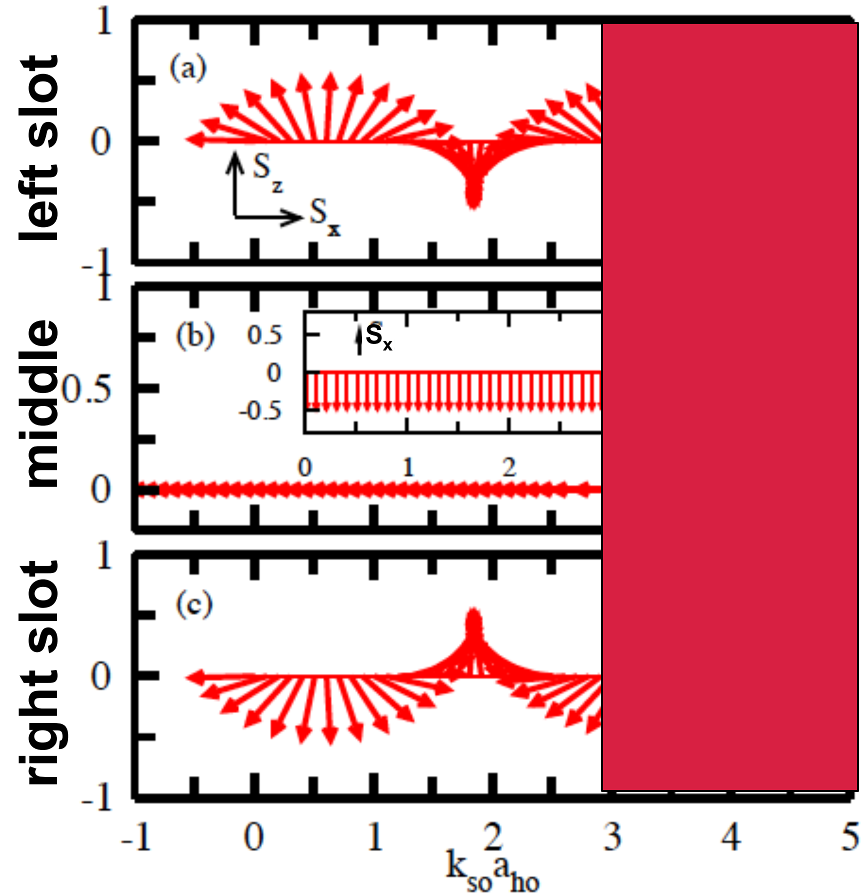


Three-Particle Example: Spin Structure as a Function of k_{so} (Fixed Ω)

Observable:
2D vector ($\langle S_{x,j}\rangle$,$\langle S_{z,j}\rangle$) for each slot j. Note $\langle S_{y,j}\rangle$=0.

Infinitely strongly-interacting 1D gases with spin-orbit and Raman couplings can be described by spin Hamiltonian H_{spin}: spin-spin interactions can be designed (not as much flexibility as for ions…).

H_{spin} offers means to understand the system dynamics.

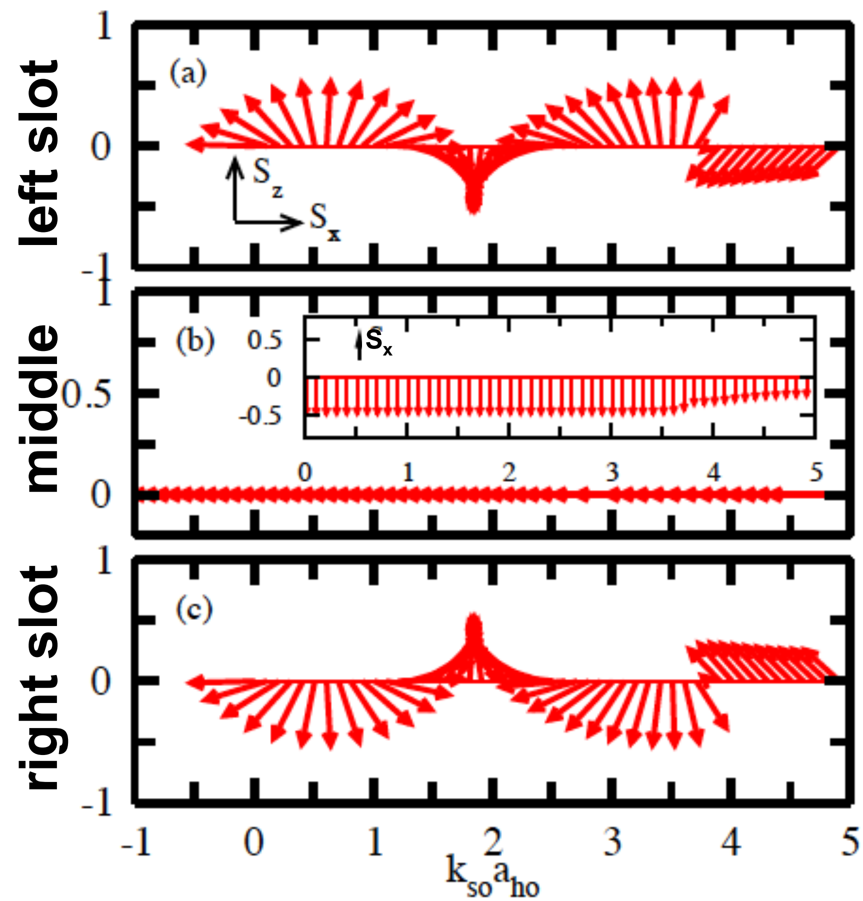


Three-Particle Example: Spin Structure as a Function of k_{so} (Fixed Ω)

Observable:
2D vector ($\langle S_{x,j}\rangle$,$\langle S_{z,j}\rangle$) for each slot j. Note $\langle S_{y,j}\rangle$=0.

Infinitely strongly-interacting 1D gases with spin-orbit and Raman couplings can be described by spin Hamiltonian H_{spin}: spin-spin interactions can be designed (not as much flexibility as for ions…).

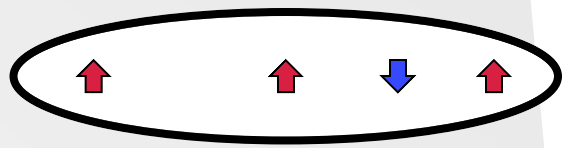
H_{spin} offers means to understand the system dynamics.



Summary: Harmonically Trapped One-Dimensional Atomic Gases

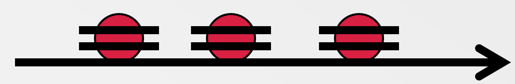
- Static properties of one-dimensional few-atom gases:
  - Non-interacting Fermi gas with a single impurity [(N,1) system with delta-function interaction].

Perturbative expressions for g=0 and 1/g=0.



  - Strongly-interacting gas (identical bosons or identical fermions) with spin-orbit and Raman couplings.

Spin-chain with effective magnetic field and spin-spin interactions.



- Dynamic properties of one-dimensional few-atom gases:
  - Tunneling dynamics in the presence of short-range interactions.

Simulations of two-particle dynamics.

Serwane et al., Science 332, 6027 (2011)