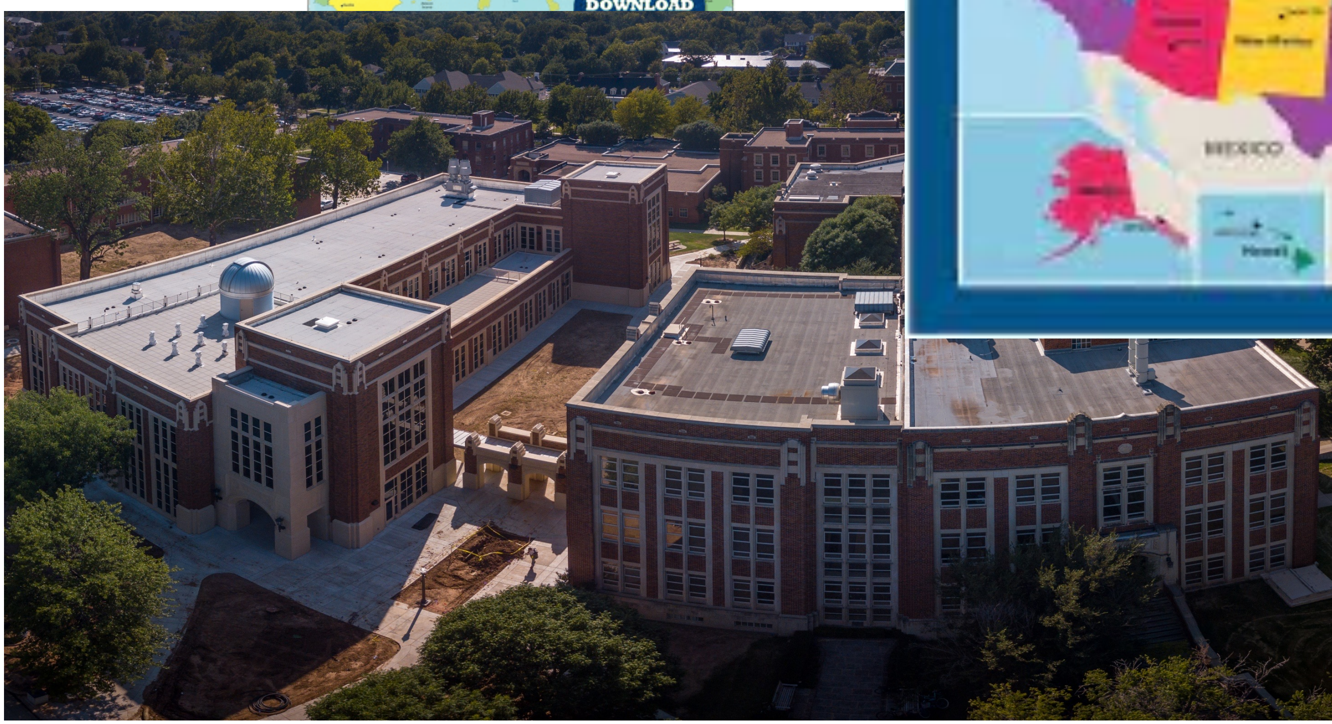
One-Dimensional Fermions: Statics and Dynamics

Doerte Blume

Homer L. Dodge Department of Physics and Astronomy
Center for Quantum Research and Technology
University of Oklahoma, Norman

Supported by the NSF.

Where Have I Been and Where Am I Now?



What You Might Not Know About Oklahoma

Eastern collared lizard (Oklahoma's state lizard).

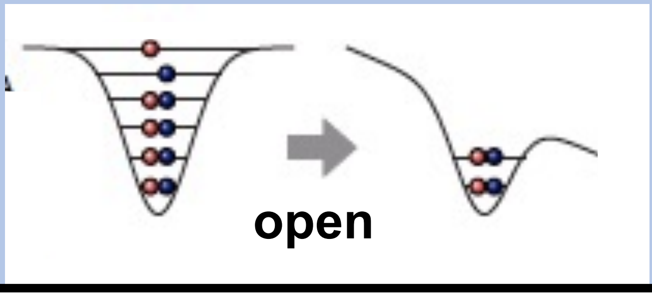
Wichita Mountains Wildlife Refuge is the largest bison refuge managed by the U.S. Fish and Wildlife Service.

This Lecture:
One-Dimensional Fermions

Dynamic properties of one-dimensional few-atom gases:

Tunneling dynamics in the presence of short-range interactions.

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



To understand dynamics, it is helpful to look at static properties.

Throughout today's lecture, the presentation is strongly influenced by ultracold atom experiments: To obtain quantitative agreement between theory and experiment, theorists and experimentalists have to work quite hard…

Why Do We Care About Dynamics?

Most processes that occur in nature are not in equilibrium.

(Ultra-) cold atoms provide test bed: Clean, good preparation fidelity,…

Probing and imaging are continually improving:

Single-particle resolution.

Interferometric probes.

Non-destructive imaging.

Want to identify general, underlying/governing principles.

Correlations in universal regime.

Role of interactions.

Things To Keep In Mind

<u>Time-independent Hamiltonian:</u>

Eigen states evolve with time (trivial space-independent phase):
$\exp\left(-\frac{\iota E_j t}{\hbar}\right)\psi_j.$

Energy is conserved (even for superposition state; assuming unitary time evolution).

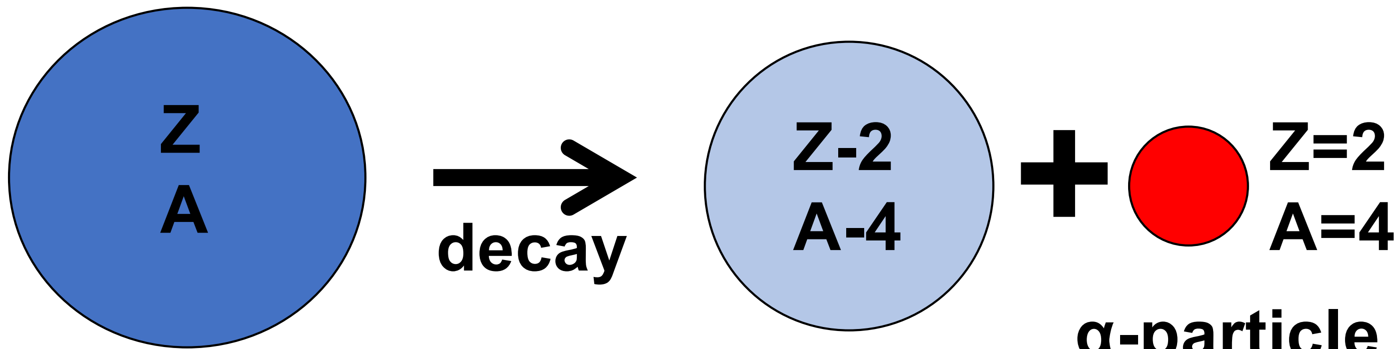
Wave packet dynamics can be thought of as evolution of superposition state.

<u>Time-dependent Hamiltonian:</u>

Energy is not, in general, conserved.

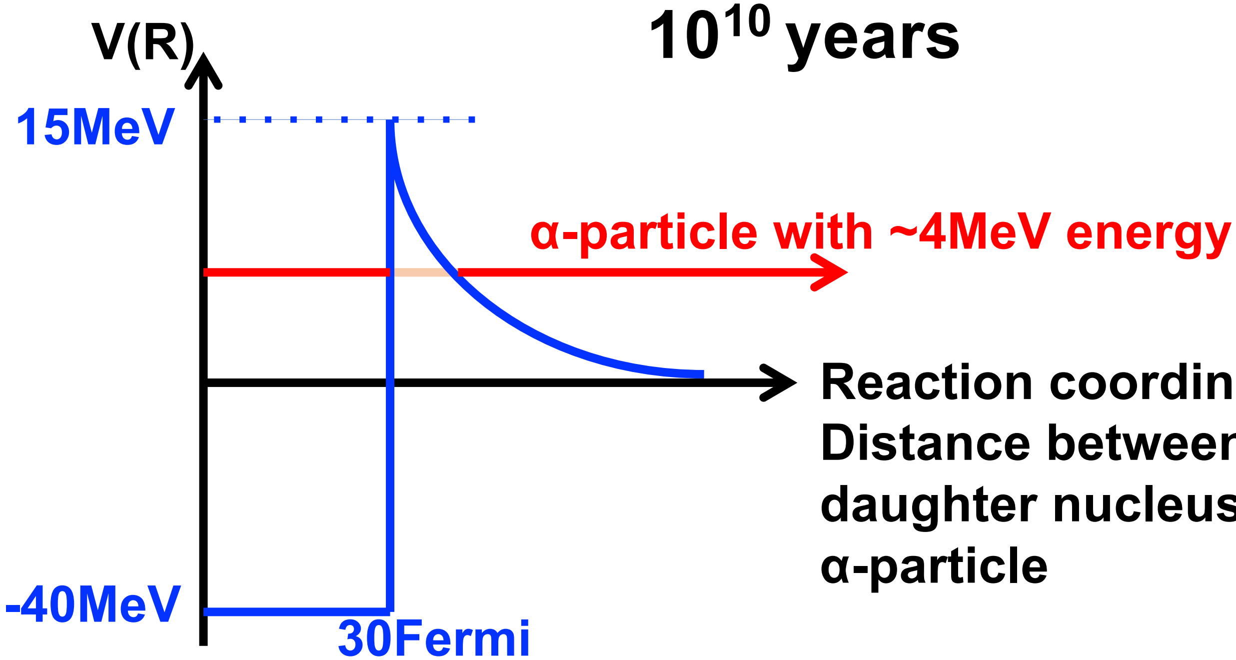
α-Decay (Textbook Example).
E.g.: $^{232}Th \rightarrow {}^{228}U + {}^{4}He$

Parent nucleus with Z protons and A nucleons: Emission of ^{4}He nucleus.



Lifetime of 10^{10} years

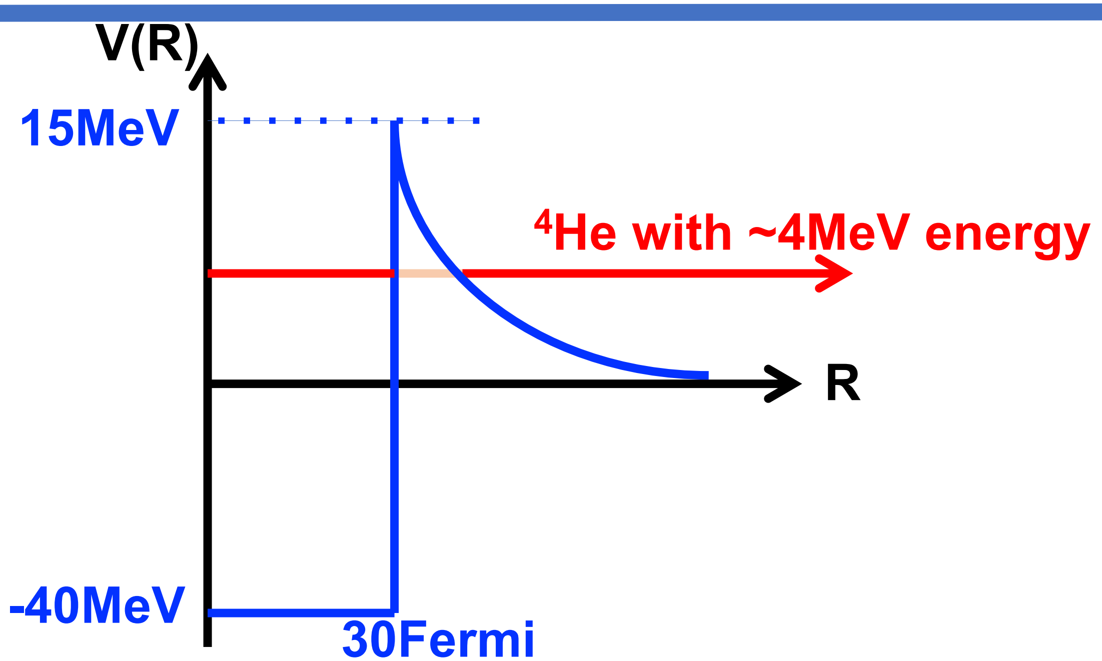
α-particle has ~4MeV energy



Reaction coordinate R: Distance between daughter nucleus and α-particle

Classically: α-particle is stuck inside.
Quantum mechanically: Tunneling.

Alpha Decay Through Tunneling



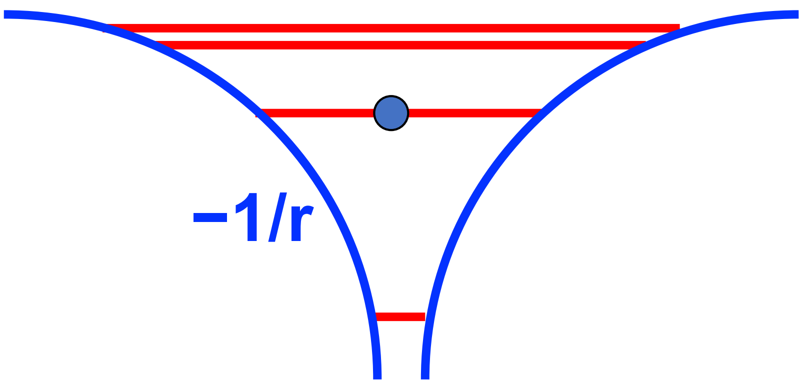
Explanation:
α-particle repeatedly hits the barrier and each time there is a probability to get out.

Short-comings: ^{4}He is not just repeatedly hitting the barrier (^{4}He does not even exist before it has been separated from the daughter nucleus).

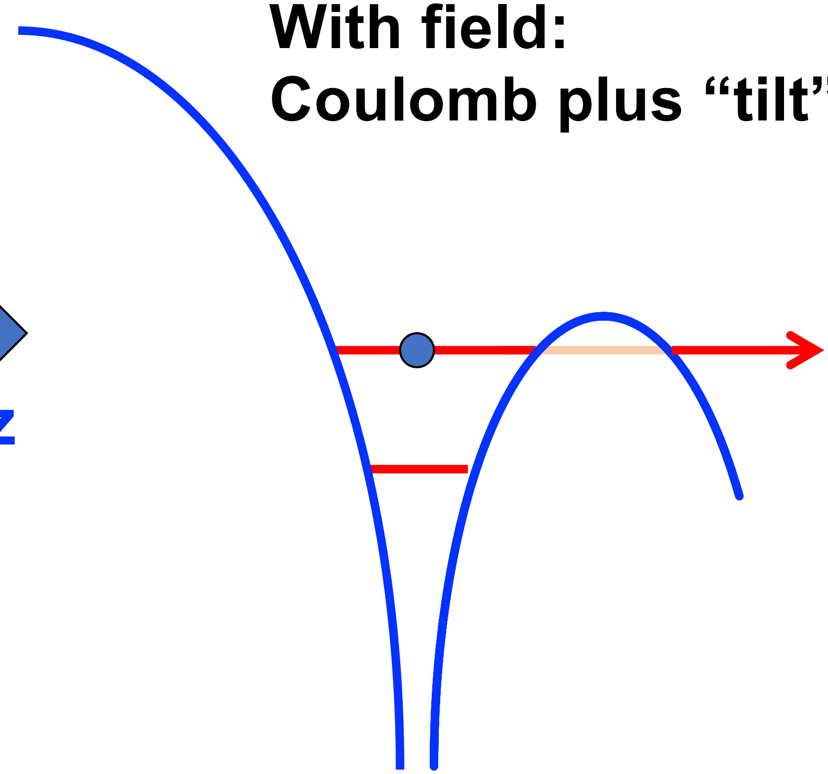
In reality: We have a complicated (open) A-body quantum system with certain final state distribution.

Different Example: H-Atom In External Field

No field: just Coulomb



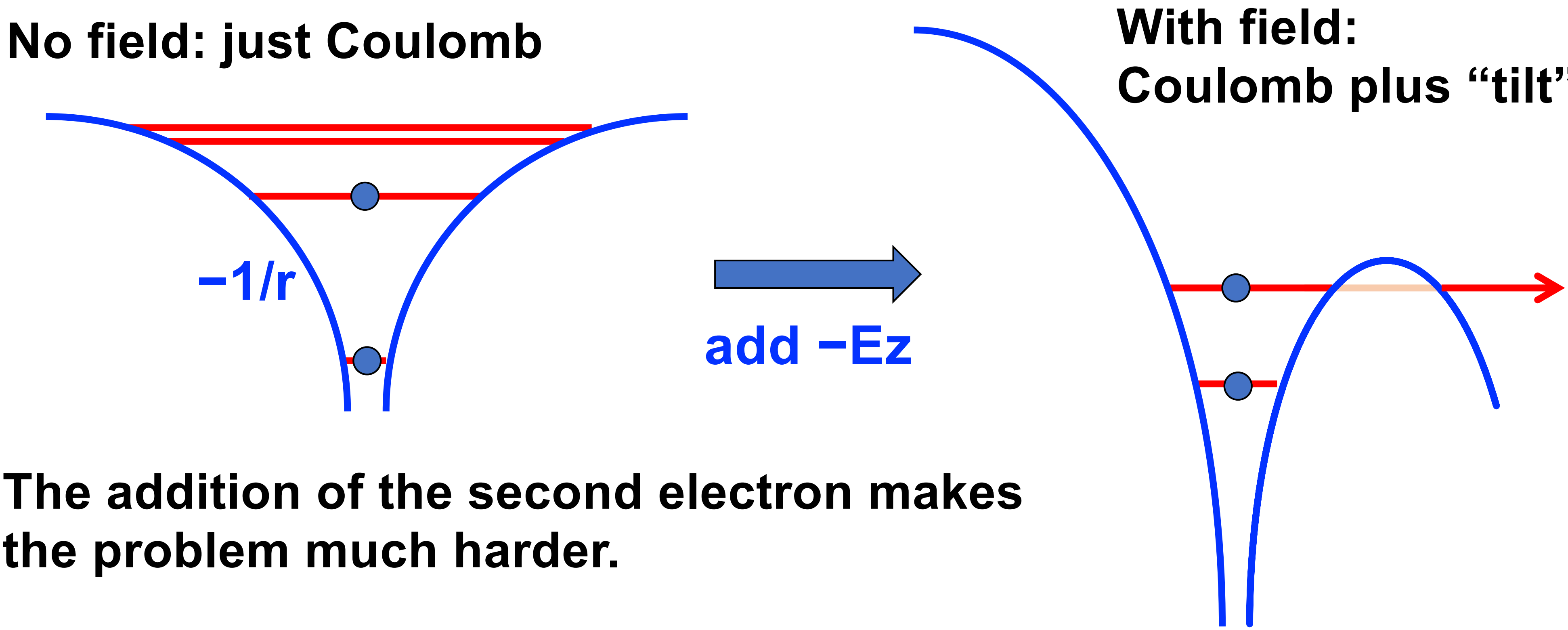
With field:
Coulomb plus "tilt"



Without relativistic effects ($2n^2$ degeneracy): $n=1,2,\ldots$ and $E_n = -13.6\,\text{eV} / n^2$

Relatively simple single-electron problem.
What happens when we go to He-atom? Two electrons…

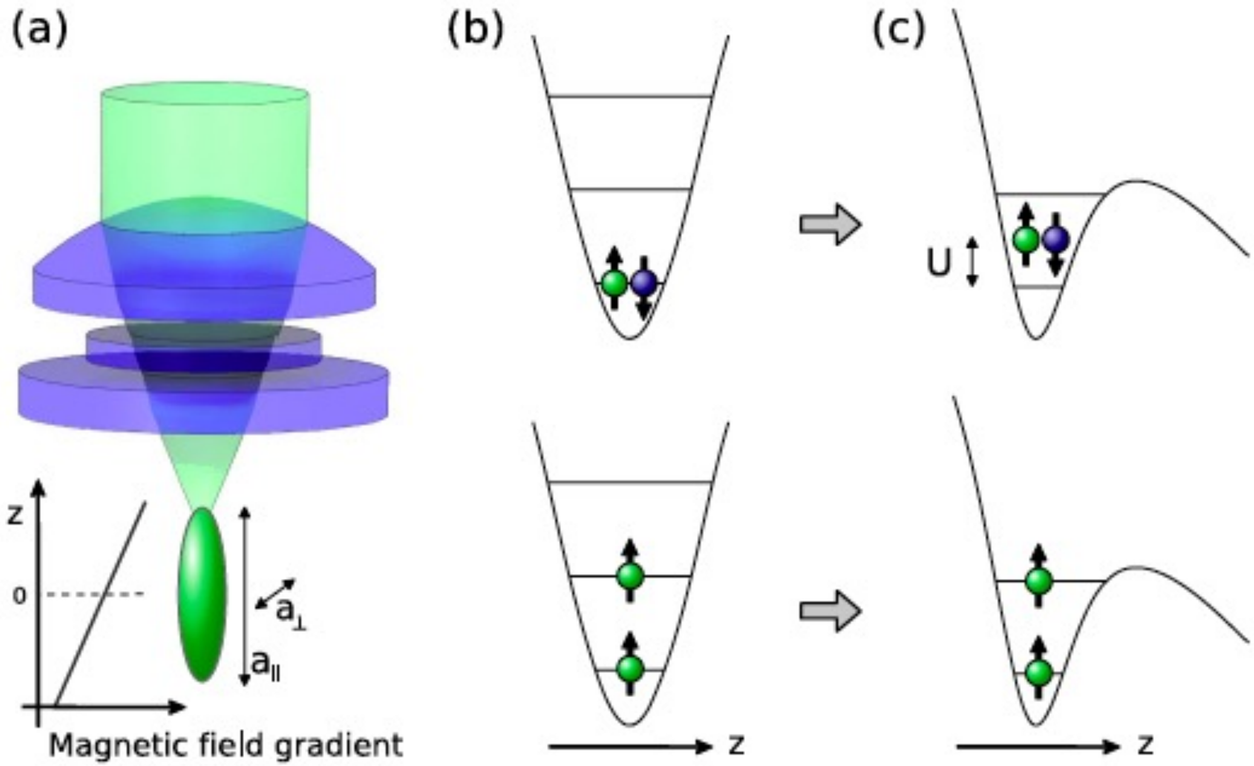
He-Atom In External Field: Single-Particle Vs. Pair Tunneling



The addition of the second electron makes the problem much harder.

Why do we care? Highly non-trivial particle-particle correlations are of fundamental interest.
Emitted electrons serve as a probe: The system is its own probe (we don’t have any other microscopes available…).

Tunneling Dynamics Of 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.

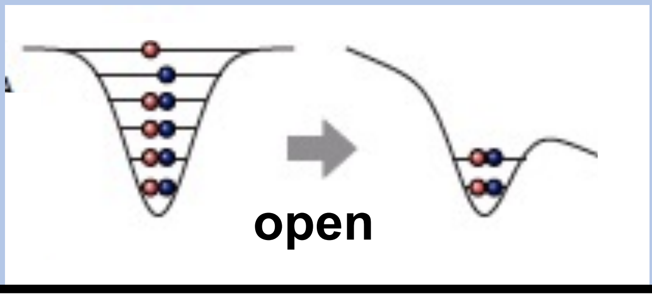
Electrons: Atoms in particular hyperfine state.
Electron-electron Coulomb potential: Zero-range contact potential.
Electron-nucleus Coulomb potential: External harmonic trap.

“Simple” Non-Trivial Open Quantum System

Dynamic properties of one-dimensional few-atom gases:

Tunneling dynamics in the presence of short-range interactions.

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



In cold atom context:
Tunneling as spectroscopy.

More generally:
Weird quantum mechanical phenomenon.

Details:
Gharashi, Blume, PRA 92, 033629 (2015).

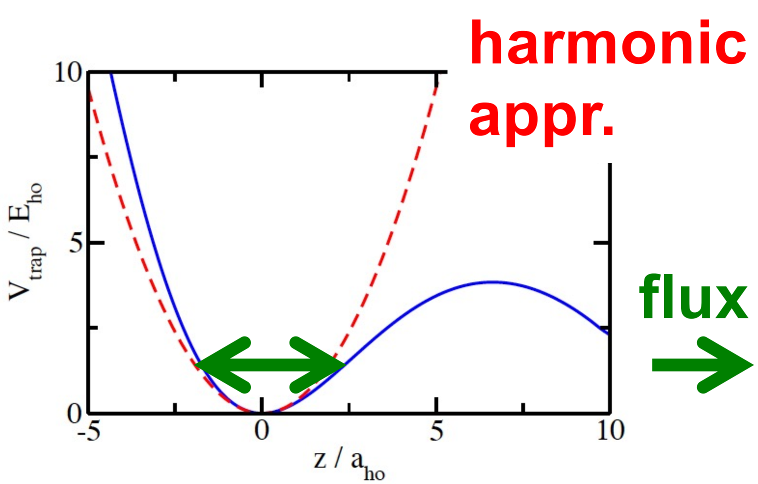
Other works:
Rontani, PRL 108, 115302 (2012); PRA 88, 043633 (2013).
Lundmark et al., PRA 91, 041601(R) (2015).

General Considerations

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).

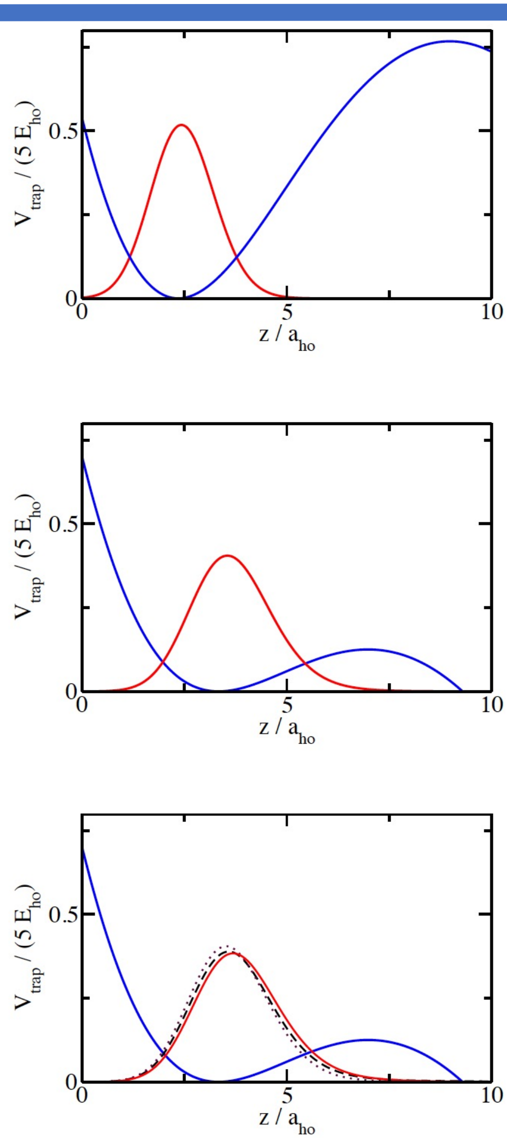


Trap time scale: $T_{ho}=\omega^{-1}$.

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

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

Start With Single-Particle System



lower the barrier in about 2ms (adiabatic)

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?

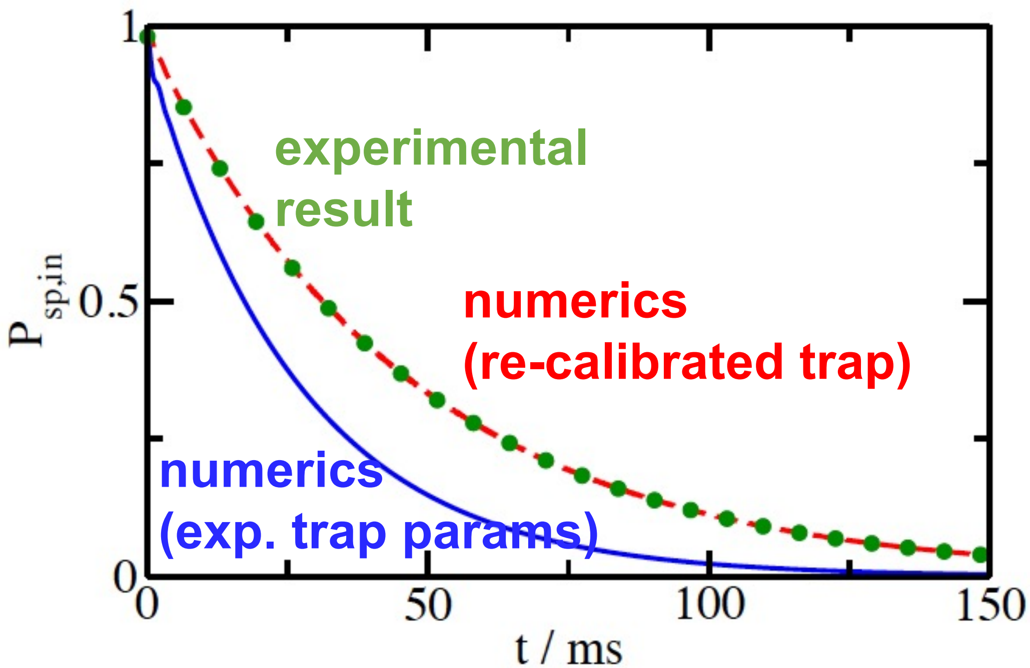
Second task:
What happens if we prepare two-atom state?
Look at "upper and molecular" branches.

Single-Particle Dynamics: Experiment Versus Theory

Experimental paper contains trap parameters p and $c_{|j>}B'$ [Zuern et al., PRL 108, 075303 (2012)].

When we use those 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.

Semi-Classical WKB Approximation

Energy quantization condition determines energy ε:

$$\int_{z_{\epsilon,1}}^{z_{\epsilon,2}} \sqrt{2m[\epsilon - V_{\text{trap}}(z)]}dz = \left(n + \frac{1}{2}\right)\pi\hbar.$$

Tunneling rate:

$$\gamma_{\text{sp}}^{\text{WKB}} = f^{\text{WKB}}\mathcal{T}$$

$$\mathcal{T} = \exp\left[-2\int_{z_{\epsilon,2}}^{z_{\epsilon,3}} \sqrt{\frac{2m}{\hbar^2}|\epsilon - V_{\text{trap}}(z)|}dz\right]$$

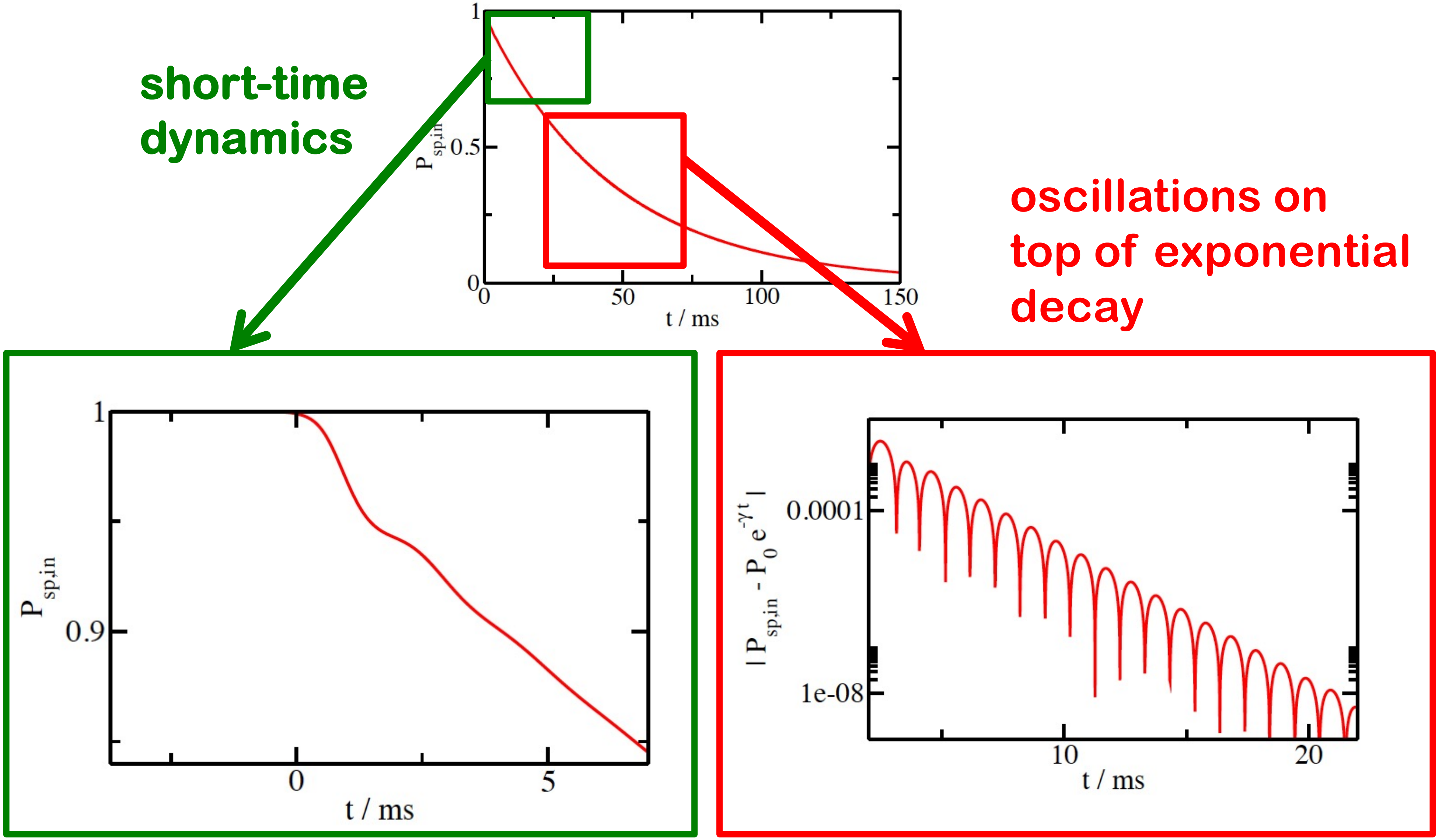
tunneling coefficient

$$f^{\text{WKB}} = \frac{\epsilon - V_{\text{trap}}(z_{\min,t=0})}{2\pi\hbar}$$

frequency

Tunneling is an exponential process and very sensitive to small variations. WKB approximation is qualitative but not quantitative (tunneling rates can be too large or too small).

Fraction $P_{sp,in}$ Inside The Trap: Exponential Decay + Extras



How Do We Perform Time-Dynamics?

Given: $\Psi(\vec{r}, t_0)$. Wanted: $\Psi(\vec{r}, t)$.

Act with time evolution operator: $\Psi(\vec{r}, t) = U(t - t_0)\Psi(\vec{r}, t_0)$.

$$U(t - t_0) = \exp\left(-\frac{\imath}{\hbar}\int_{t_0}^{t} H(t')dt'\right) \xrightarrow[H \text{ time-indep.}]{\quad\quad} \exp\left(-\frac{\imath H(t-t_0)}{\hbar}\right).$$

Assume that H is independent of time for each $t - t_0$ interval.

How to implement $U(t - t_0)\Psi(\vec{r}, t_0)$ operation?

1) Expand U in terms of Chebychev polynomials (requires smooth potential).

2) Split-operator approach + zero-range interactions.

Expansion In Terms Of Chebychev Polynomials

Expand $U(t - t_0) = \sum_{k=0}^{N} a_k \phi_k \left(\frac{-\iota H(t-t_0)}{\hbar R}\right)$.

Tal-Elzer et al., JCP 81, 3967 (1984). Leforestier et al., J. Comp. Phys. 94, 59 (1991).

R: real number chosen such that $\frac{-\iota H(t-t_0)}{\hbar R} \in [-\iota, \iota]$.

k-th Chebychev polynomial is obtained recursively:
$\phi_k(X) = 2X\phi_{k-1}(X) + \phi_{k-2}(X)$.

Initialization: $\phi_0(X) = \Psi(\vec{r}, t_0)$ and $\phi_1(X) = X\Psi(\vec{r}, t_0)$.

a_k: expansion coefficients (k-th order Bessel fct. of first kind).

Advantages: Large "time steps" $t - t_0$.
Nice convergence of expansion.

Split-Operator Approach: Zero-Range Interactions

$\boldsymbol{\Psi}(\vec{\boldsymbol{r}}, \boldsymbol{t}+\boldsymbol{\Delta t}) = \int \boldsymbol{\rho}(\vec{\boldsymbol{r}}', \vec{\boldsymbol{r}}; \boldsymbol{\Delta t}) \boldsymbol{\Psi}(\vec{\boldsymbol{r}}', \boldsymbol{t}) \boldsymbol{d}\vec{\boldsymbol{r}}'$.

Blinder, PRA 37, 973 (1988).
Yan, Blume, PRA 91, 043607 (2015).

$$\boldsymbol{\rho}(\vec{\boldsymbol{r}}', \vec{\boldsymbol{r}}; \Delta \boldsymbol{t}) = \left\langle \vec{\boldsymbol{r}}' \middle| \exp\left(\frac{-\imath \boldsymbol{H} \boldsymbol{\Delta t}}{\hbar}\right) \middle| \vec{\boldsymbol{r}} \right\rangle.$$

Let $H = H_{ref} + V$. Let propagator for H_{ref} be $\rho_{ref}(\vec{r}', \vec{r}; \Delta t)$.

Use Trotter formula:

$$\boldsymbol{\rho}(\vec{\boldsymbol{r}}', \vec{\boldsymbol{r}}; \boldsymbol{\Delta t}) \approx \exp\left(\frac{-\imath V \Delta t}{2\hbar}\right) \boldsymbol{\rho}_{ref}(\vec{\boldsymbol{r}}', \vec{\boldsymbol{r}}; \boldsymbol{\Delta t}) \exp\left(\frac{-\imath V \Delta t}{2\hbar}\right).$$

If H_{ref} contains kinetic energy plus two-body zero-range interaction, then $\rho_{ref}(\vec{r}', \vec{r}; \Delta t)$ is known analytically in 1D and 3D.

Requires small Δt. Integrand oscillates with frequency $\propto (\Delta t)^{-1}$.

Two-Particle System: Need Interactions

Question:
If we want to work with fermions, do we use ^{6}Li or ^{7}Li?

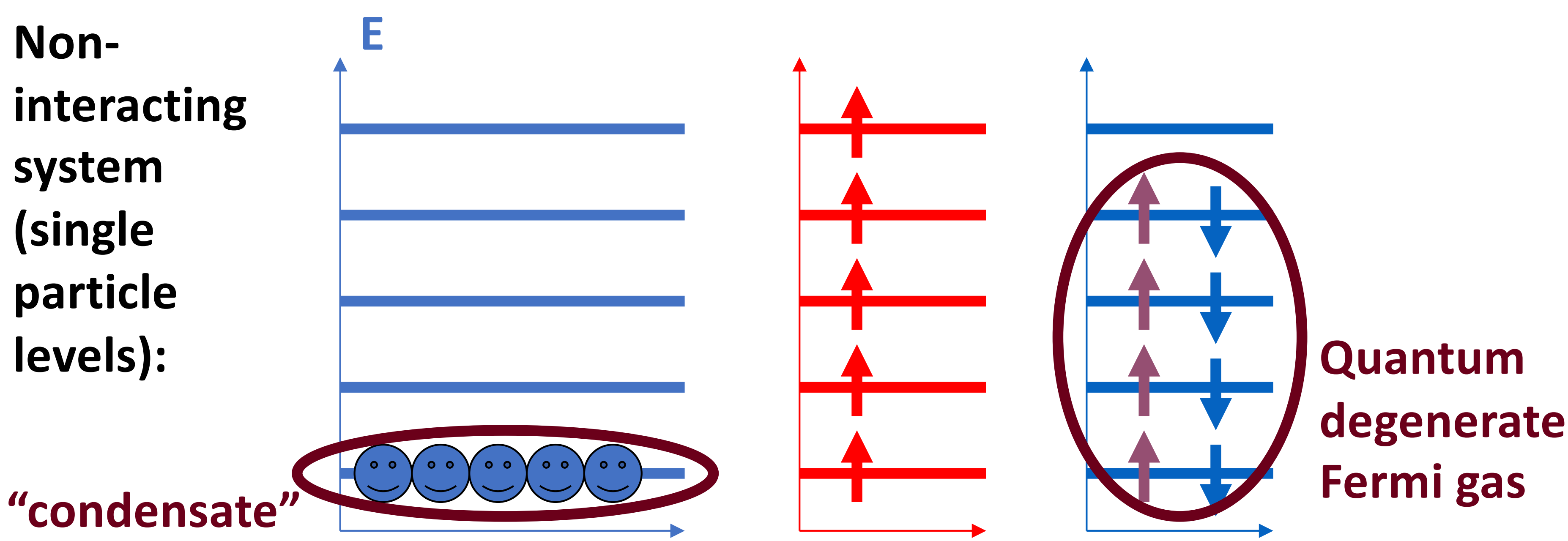
Bose Versus Fermi Statistics: Non-Interacting Particles

One-component Bose gas:

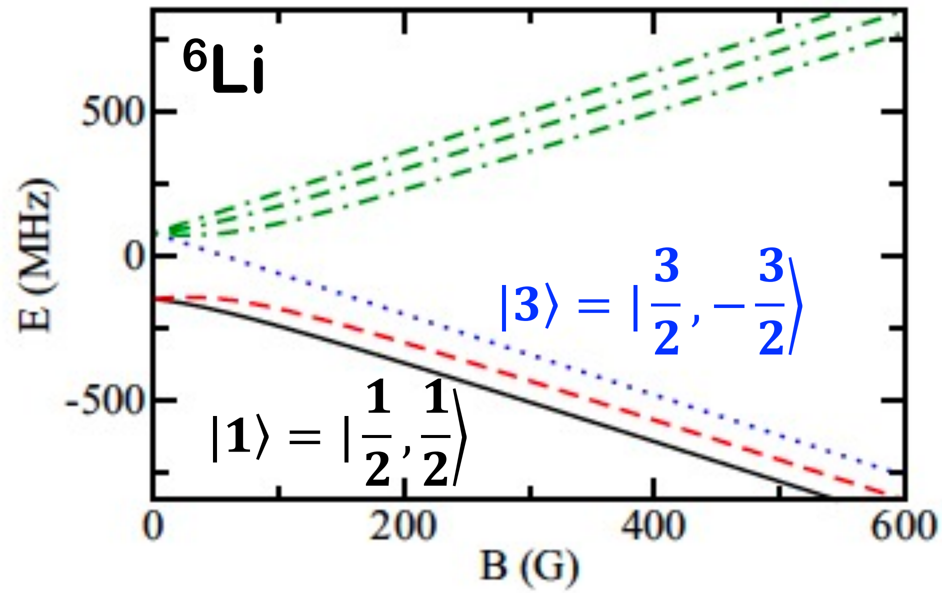
One-component spin-polarized Fermi gas:

Two-component Fermi gas:

Non-interacting system (single particle levels):



Back To Two-Particle System: Need Interactions



External magnetic field can be used to tune the interactions in the vicinity of a Feshbach resonance: B to a_{3D} mapping.

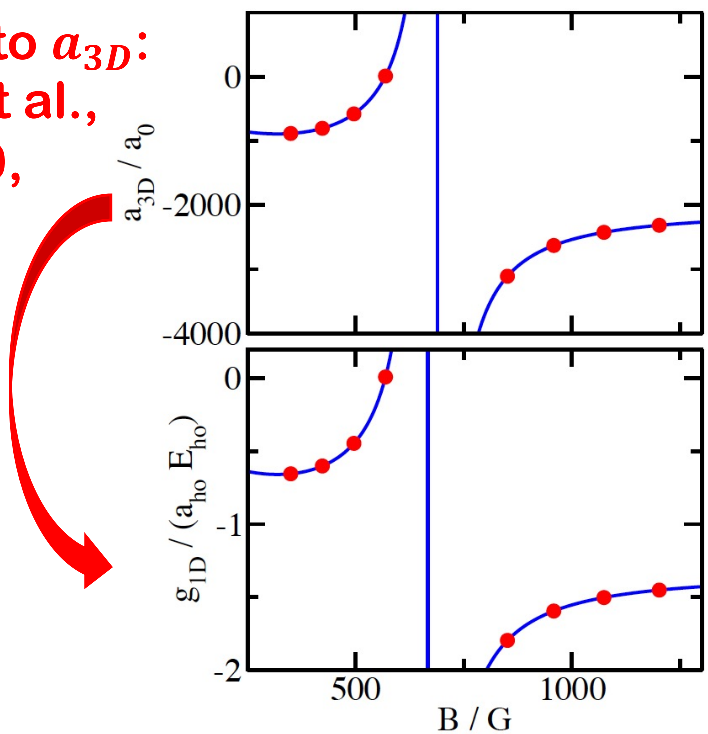
^{6}Li: Nuclear spin $I = 1$ and total electronic spin $J = 1/2$.
Total spin $F = 1/2$ and $F = 3/2$.
"Upper branch:" states $|1\rangle$ and $|2\rangle$.
"Molecular branch:" states $|1\rangle$ and $|3\rangle$.

Mapping Of Magnetic Field Strength To Coupling Strength

"Molecular branch:" states $|1\rangle$ and $|3\rangle$.

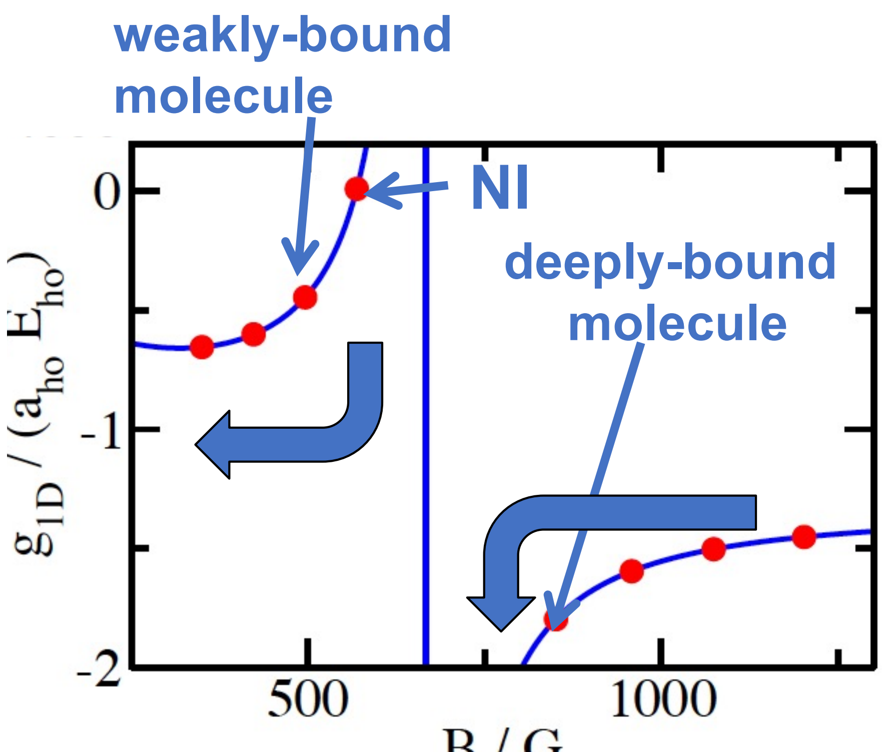
"Molecular branch" means that the interaction energy is negative. In free space, the 1D two-body system would form a molecule of size ~ $-2/g_{1D}$.

From B to a_{3D}: Zuern et al., PRL 110, 135301 (2013).



$$\frac{g_{1D}}{\hbar\omega_\rho a_\rho} = \frac{2a_{3D}}{a_\rho}\left[1 - \frac{|\zeta(1/2)|}{\sqrt{2}}\frac{a_{3D}}{a_\rho}\right]^{-1}$$

Olshanii, PRL 81, 938 (1998)



Effective One-Dimensional Interaction Potential

Contact or delta-function interaction

$$V(z_1 - z_2) = g_{1D}\delta^{(1)}(z_1 - z_2)$$

This approach works

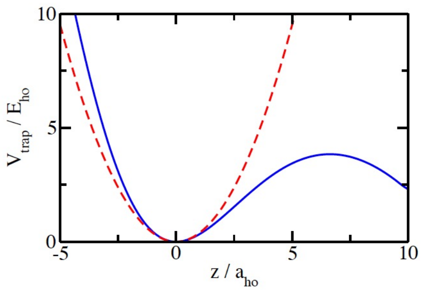
provided the s-wave scattering length, in magnitude, is larger than the effective range and

provided transverse degrees of freedom are frozen, i.e., interaction energy $\ll \hbar\omega_\rho$.

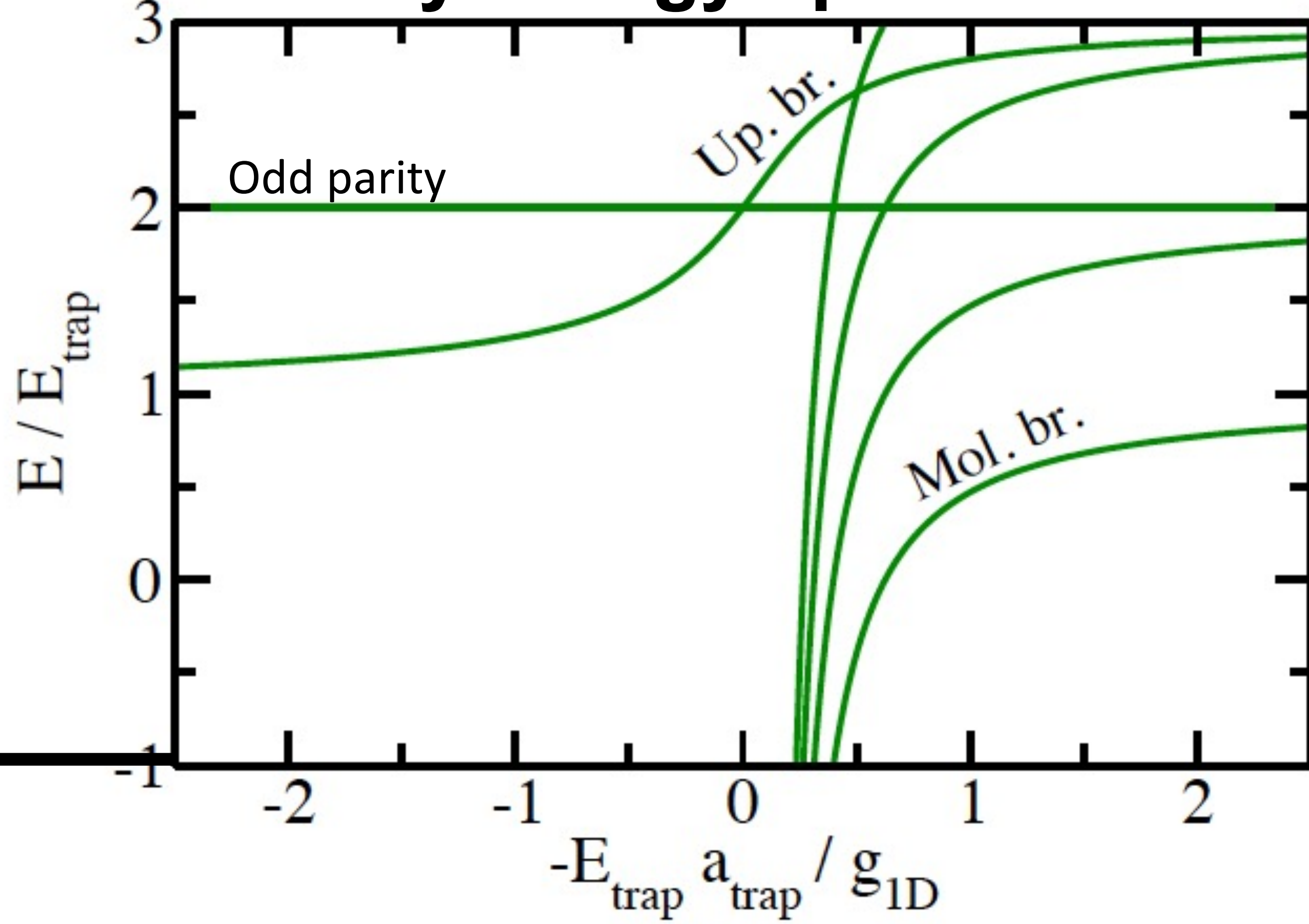
Question: What units does g_{1D} have?

Overview: Upper Branch And Molecular Branch For Deep Trap

Harmonic approximation



Two-body energy spectrum:

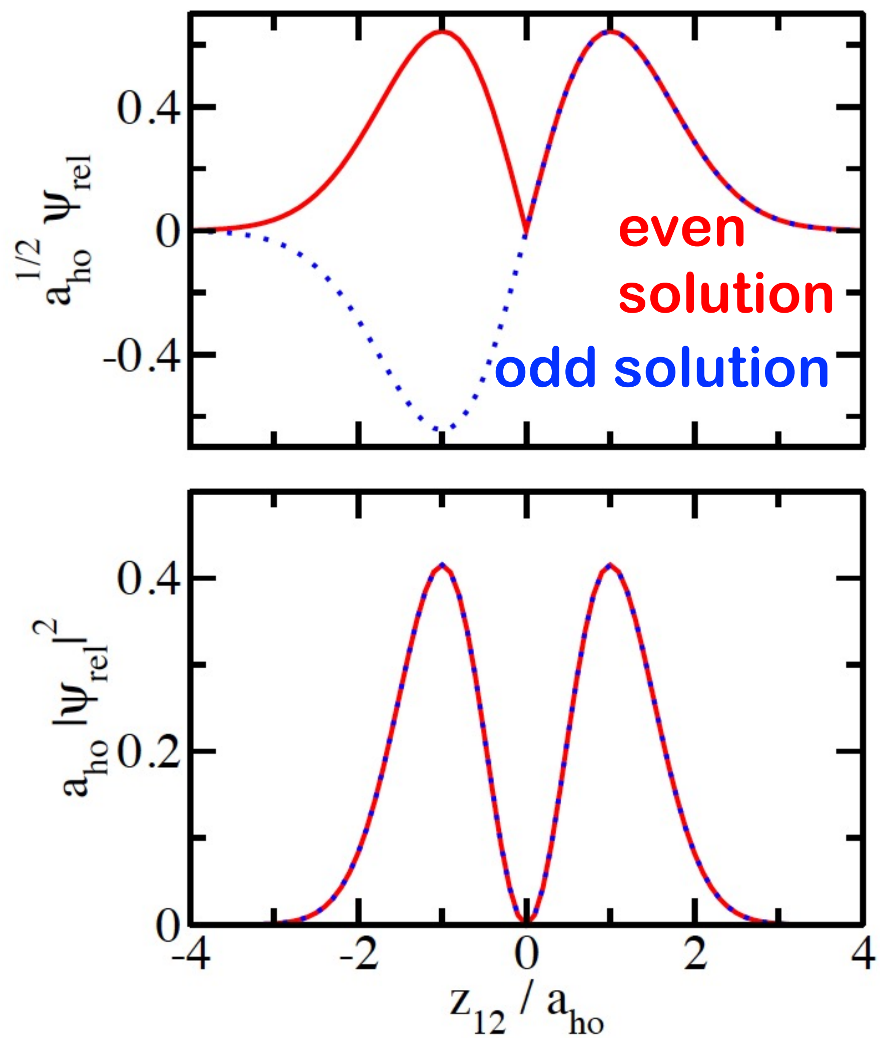


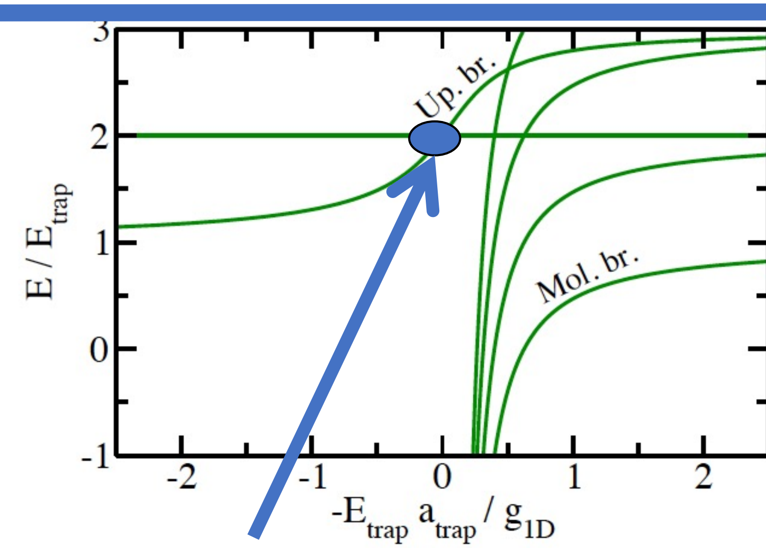
non-interacting (NI)

NI

1 / (two-body interaction strength)

Fermionization For Two Particles



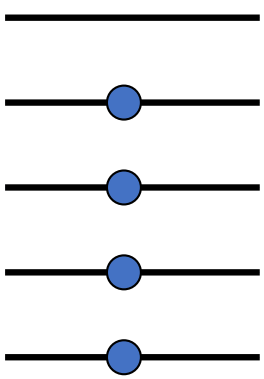


Fermionization:
If we flip the sign of half of the wave function, then the even parity solution looks like the (odd parity) wave function.
For two particles, this mapping holds for all g_{1D}:

$$g_{1D,even} \propto \frac{-1}{g_{1D,odd}}.$$

Fermionization For Larger Single-Component Systems

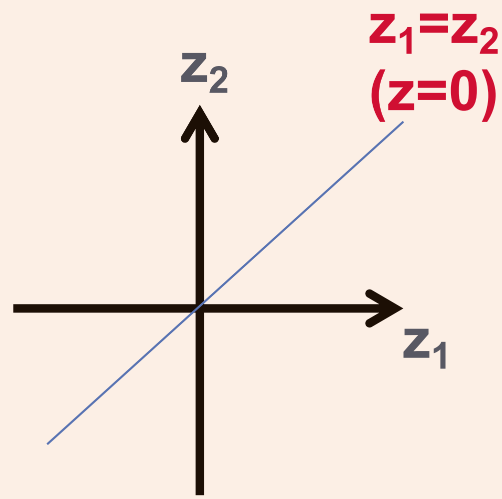
Bose-Fermi mapping (Girardeau):



$g_{1D}=\infty$
(bosonic wave fct.= Slater determinant with "different signs")

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

N=2:



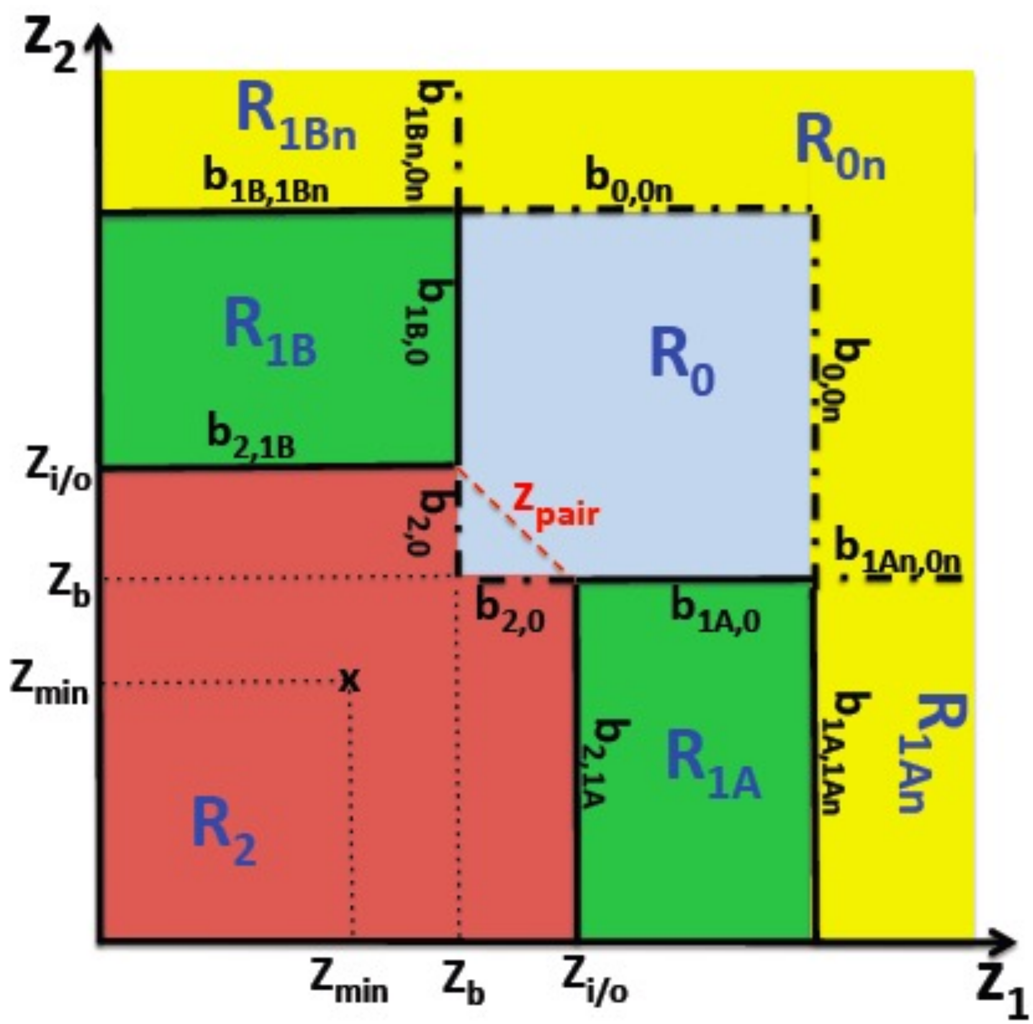
Node at $z_1=z_2$: Particles cannot penetrate.

Non-symmetrized states:

For $z_1<z_2$: $\mathrm{Det}(\phi_0(z_1),\phi_1(z_2))\Theta_{z1<z2}$

For $z_1>z_2$: $\mathrm{Det}(\phi_0(z_1),\phi_1(z_2))\Theta_{z2<z1}$

2D Numerics: Three Different Lengths ($z_0 \ll a_{ho} \ll \mathrm{Num.\,Box}\ L$)



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

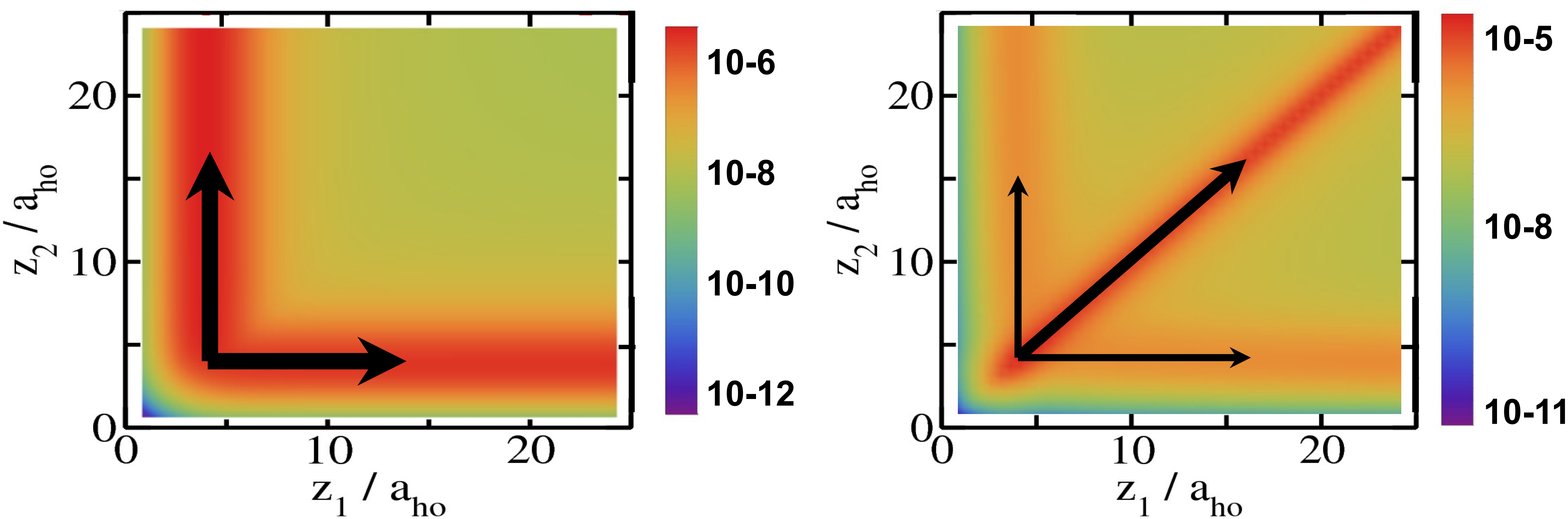
To get average number of particles in trap, we monitor flux through $b_{2,1A}$, $b_{2,1B}$, $b_{2,0}$.

"Numerical" region (yellow): Apply damping so as to avoid reflection from edge of box.

Molecular Branch: Magnitude of the Flux

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

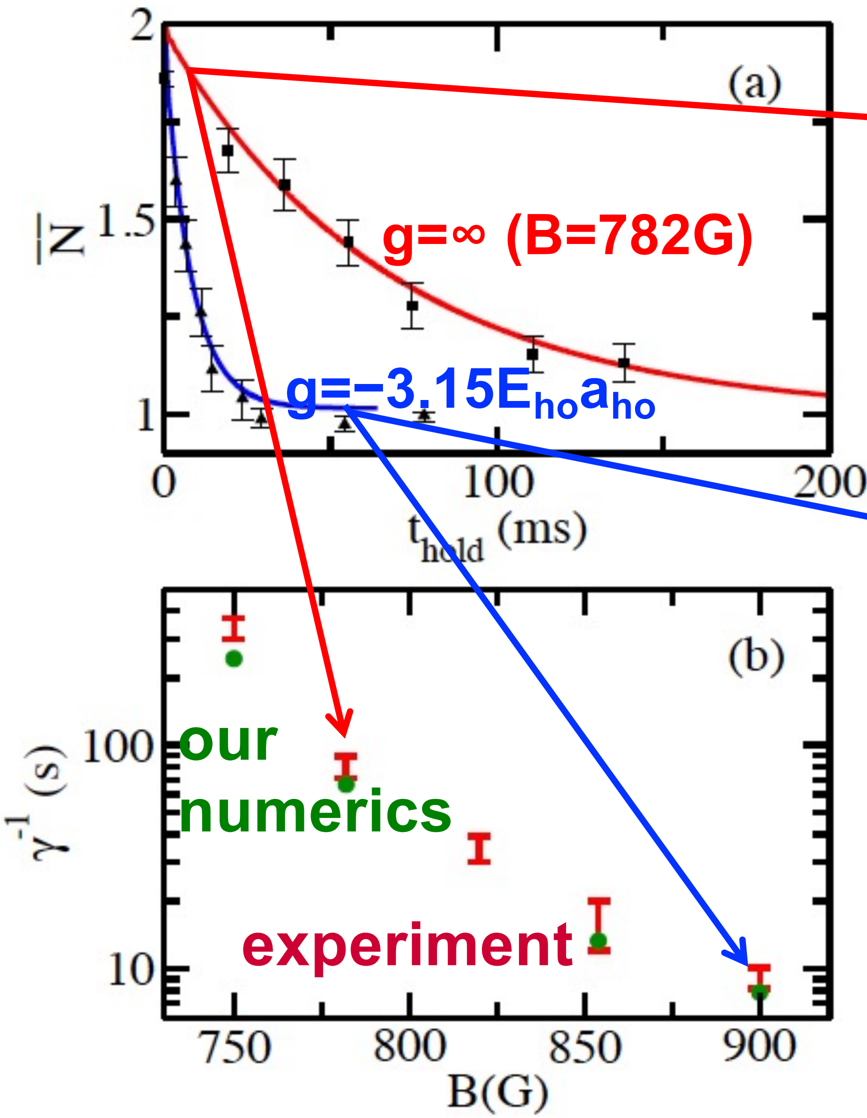
Attractive interaction (a_{1D}=1.38a_{ho}, g <0): Pair tunneling.

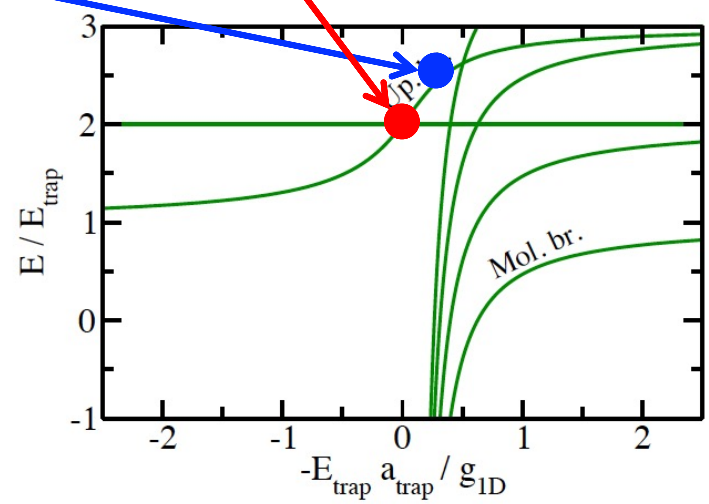


Upper Branch: Comparison With Experimental Data

Very good agreement with experimental results!!!

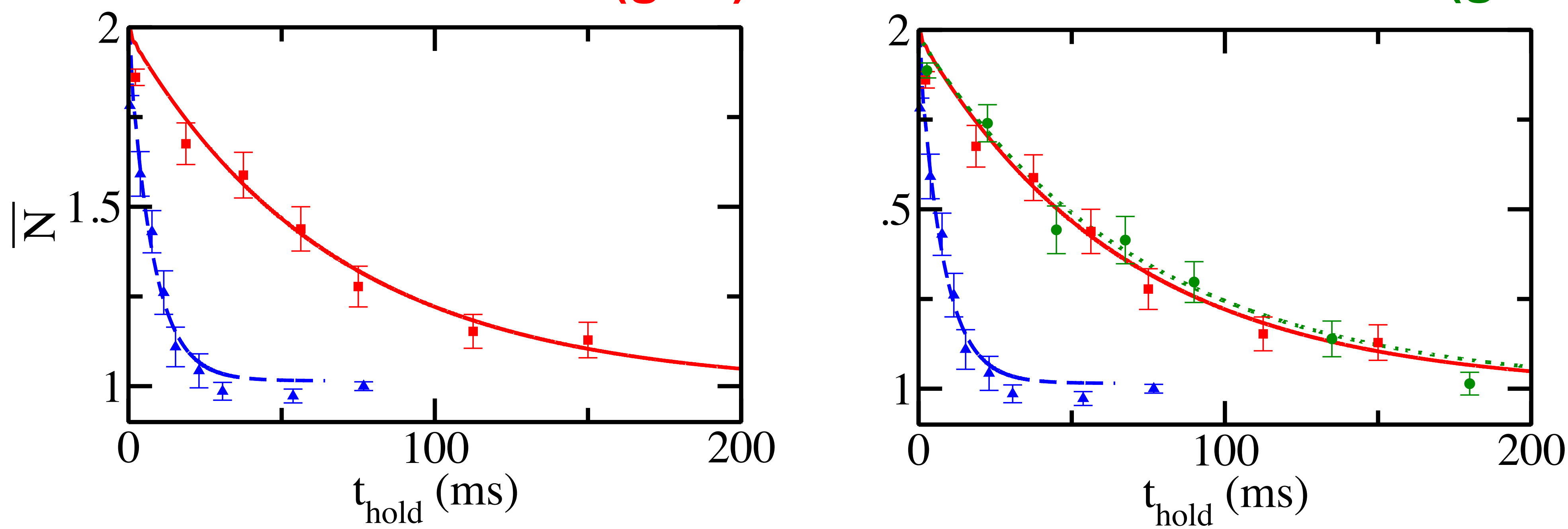
The "further up" the upper branch the system is, the faster the decay.





Fermionization Of Two-Particle System: Effect On Tunneling

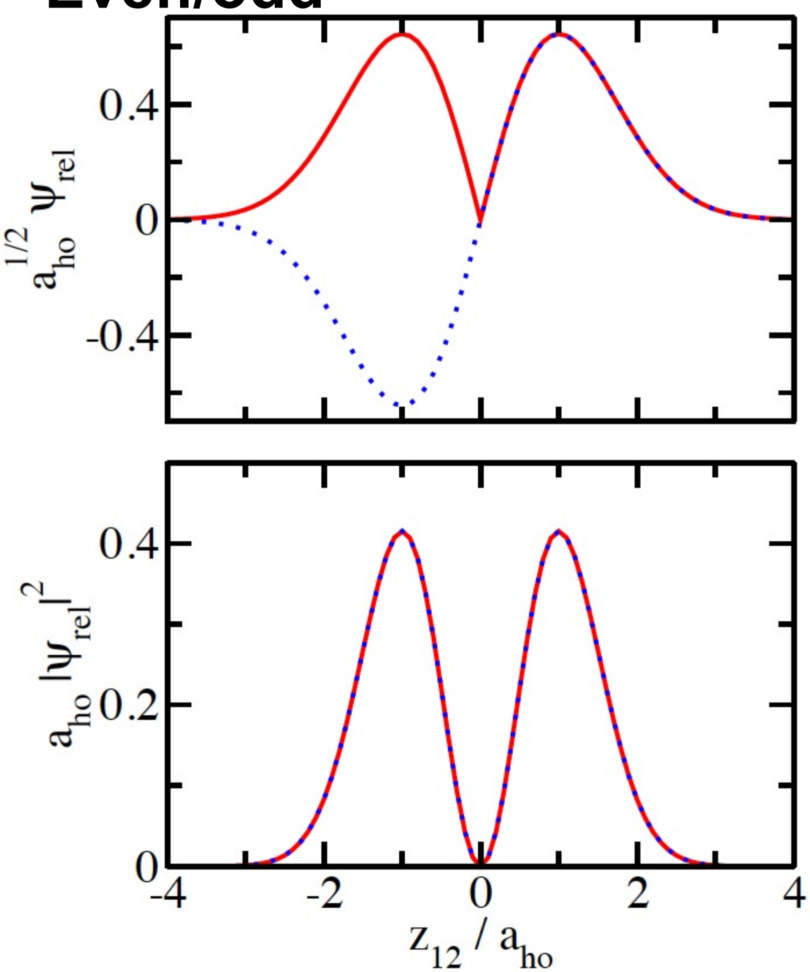
Two different HF states (g=∞): **Two identical HF states (g=∞):**



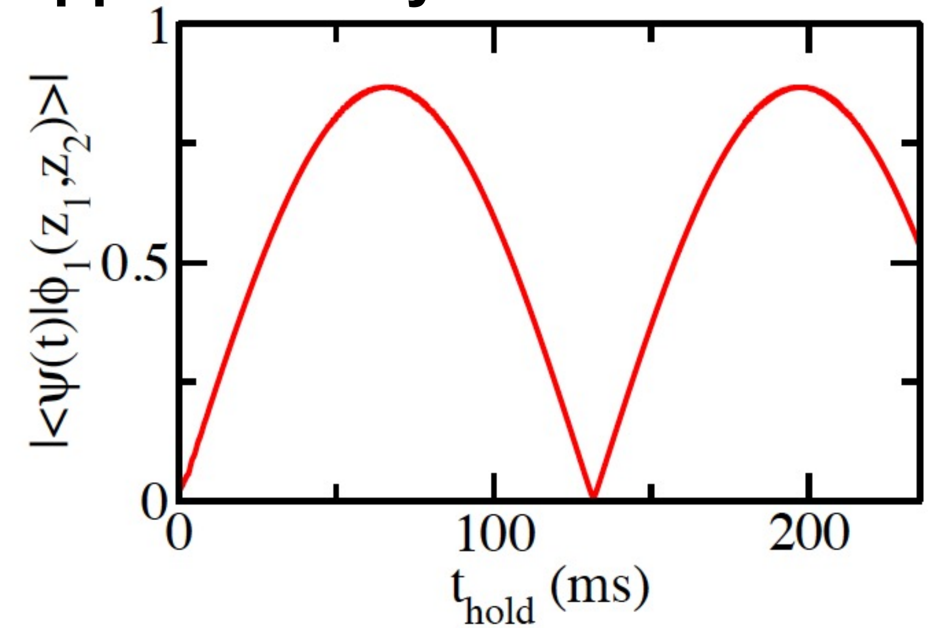
There is a small difference since the trapping potential depends on the hyperfine state.
Also, the two distinguishable particle system exhibits dynamics that reflects the near degeneracy of two states.

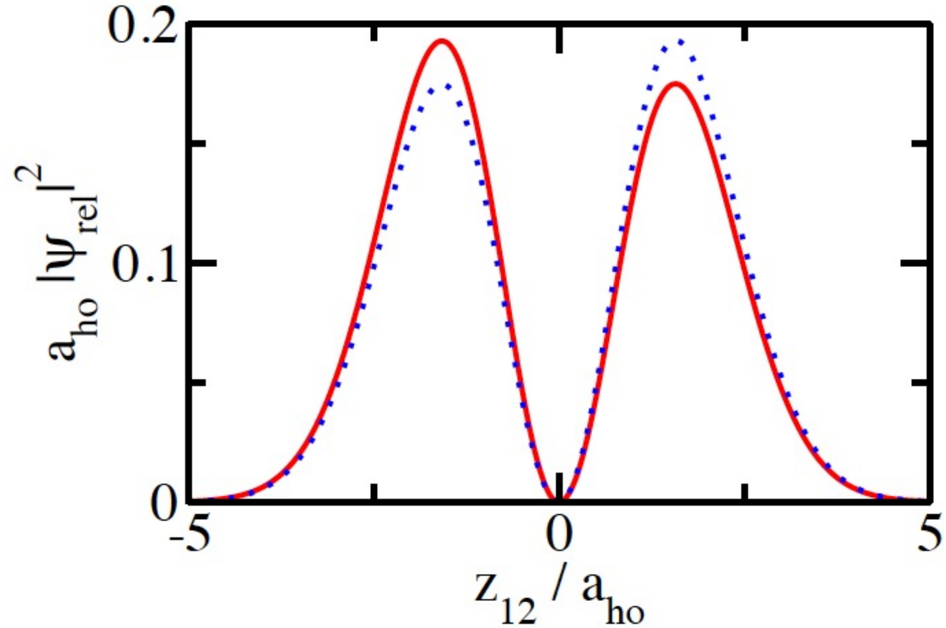
Fermionization

Two identical particles:
Even/odd



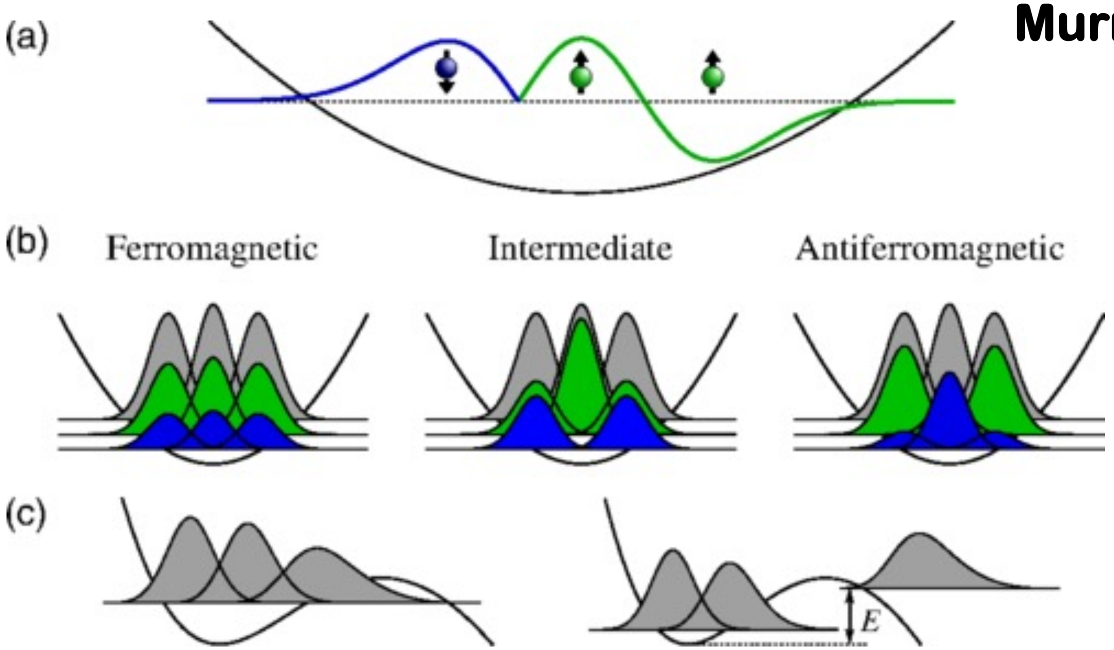
Two distinguishable particles:
Approximately even/odd

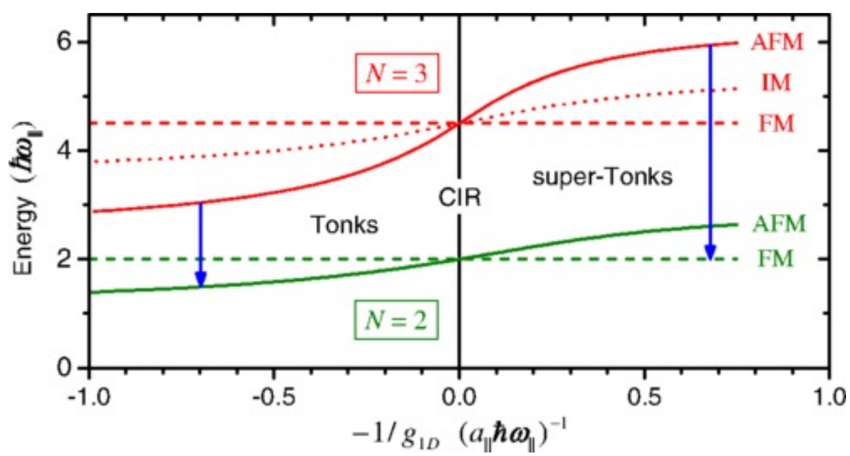


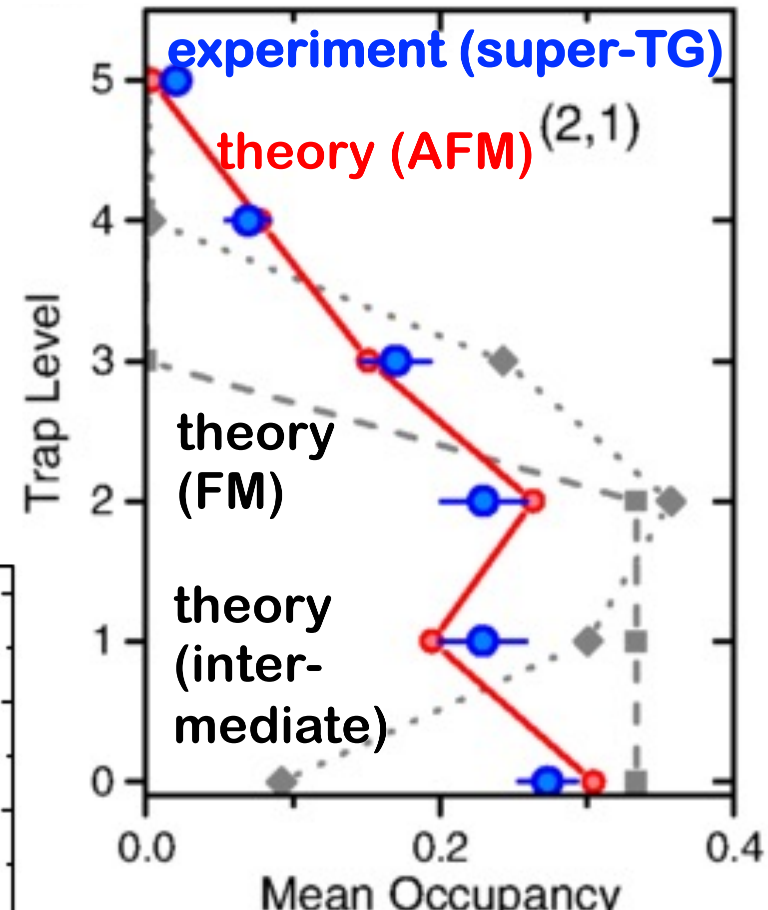


Beyond Two Particles

Murmann et al., PRL 115, 215301 (2015)







What Did We Learn?

Tunneling is exponentially sensitive (well, we knew this…): Accurate trap parametrization is crucial.

Two-particle system in 1D: Flexible, “simple” toy model that allows for direct contact between theory and experiment.

Access to single-particle and pair tunneling dynamics.

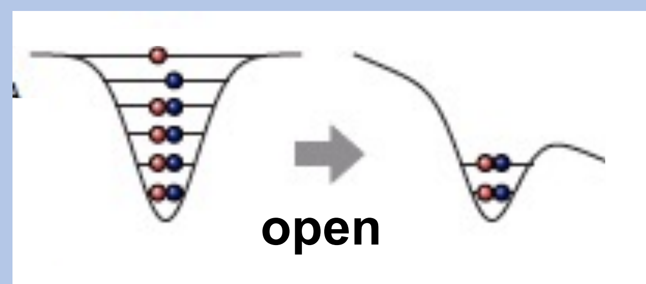
Outcome can be used to analyze “ordering” of three- and higher-particle systems.

Magnetic ordering and spin chain models:
Cui, Ho, Zinner, Gharashi/Blume, Parish, Levinsen, Massignan, Santos, Deuretzbacher, Pu, Guan,…

Today, Just Two Particles. But Want To Treat More…

Dynamic properties of one-dimensional few-atom gases:

Tunneling dynamics in the presence of short-range interactions.

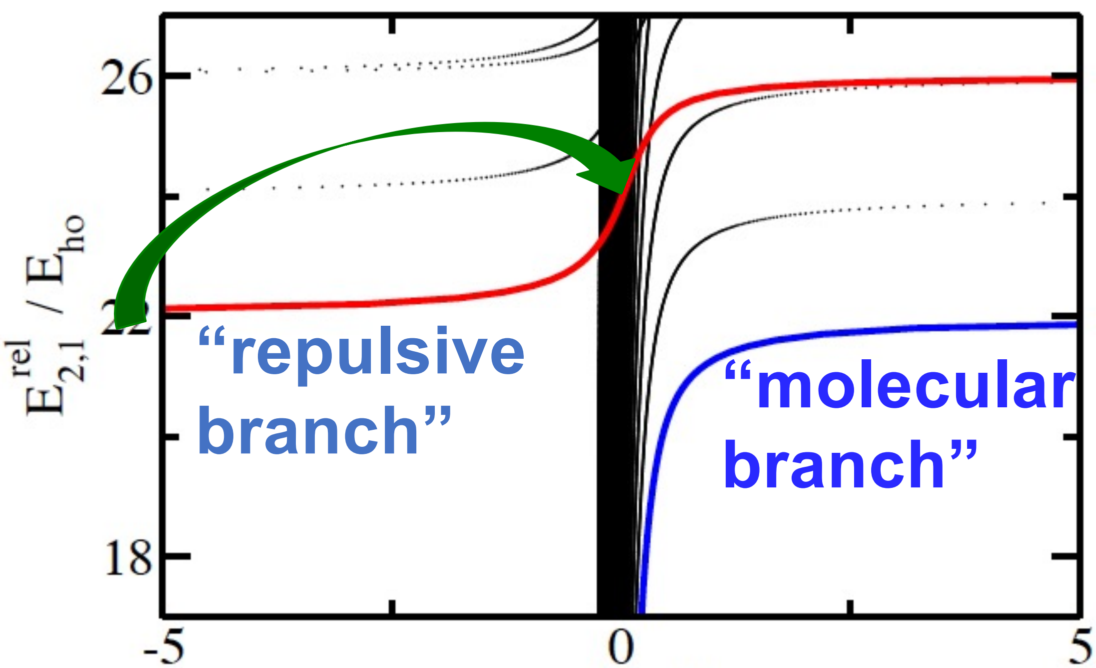


Serwane et al., Science 332, 6027 (2011)

In the remaining slides:
A few static results for more than two particles….

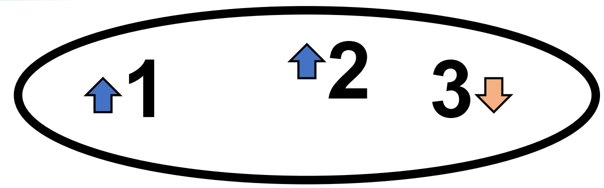
Three-Particle Spectrum In Tight Harmonic Trap

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

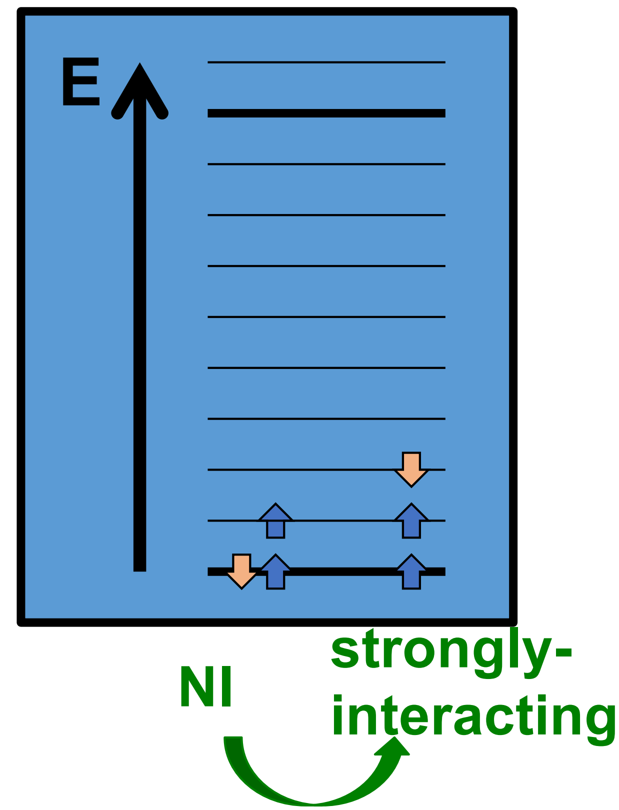


$-(a_{ho}E_{ho})/g_{1D}$

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

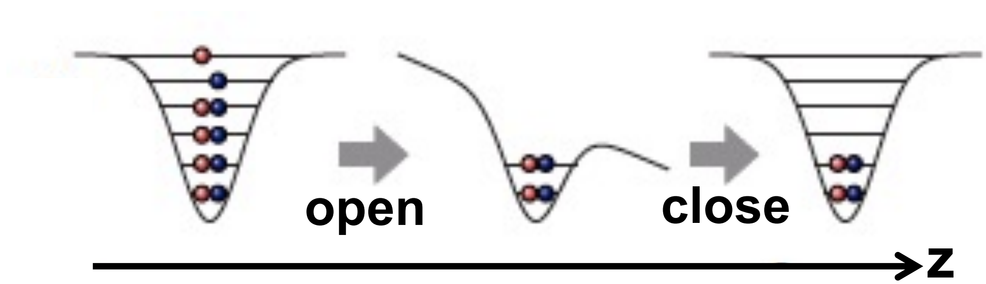


1 and 3 interact.
2 and 3 interact.



Rf Spectroscopy Data Versus 3D And 1D Theory

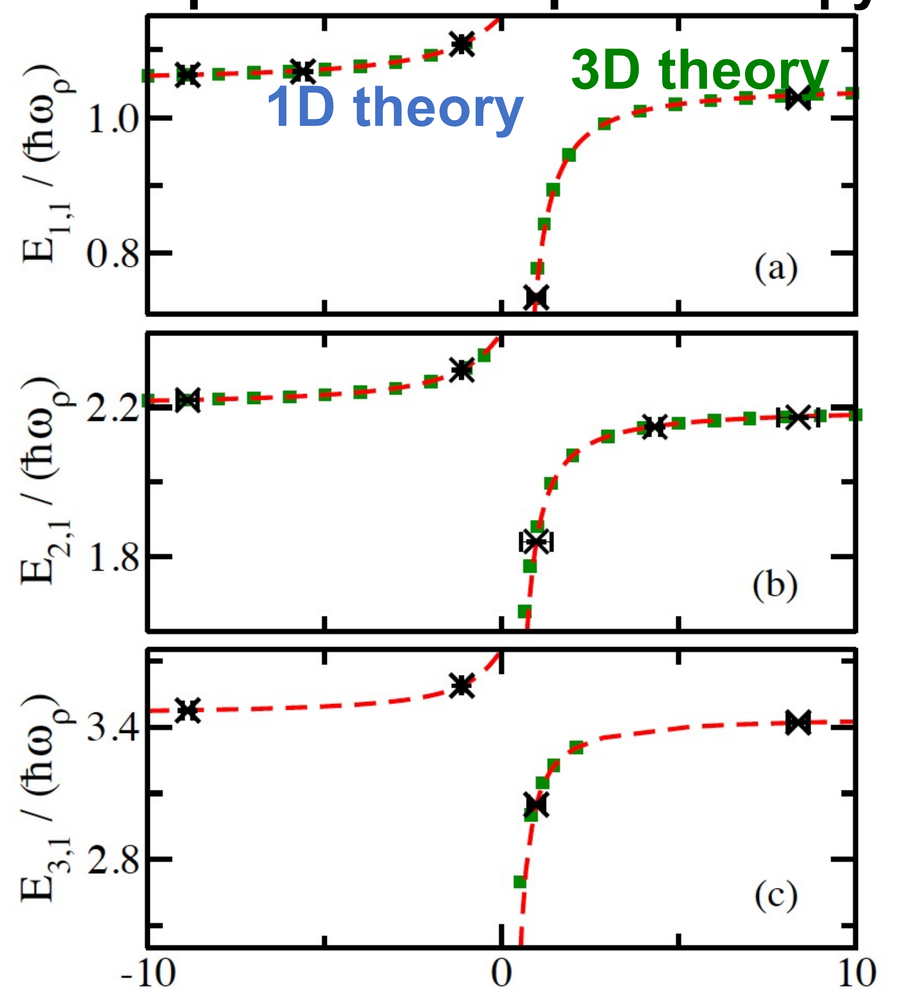
In the tight xy-directions, the confinement is approximately harmonic. Tunneling in z allows for preparation of (1,1), (2,1), (3,1), (2,2),… systems:



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

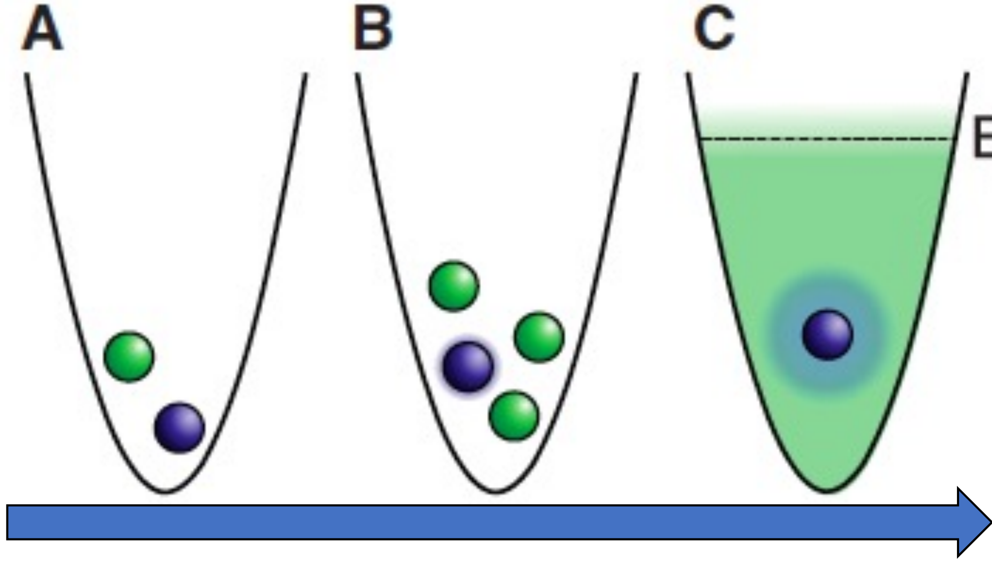
Experimental data: G. Zuern, Ph.D. thesis, Heidelberg (2012).
Theory: Gharashi, Yin, Blume, PRA 89, 023603 (2014).

Experiment: rf spectroscopy



1 / (two-body interaction strength)

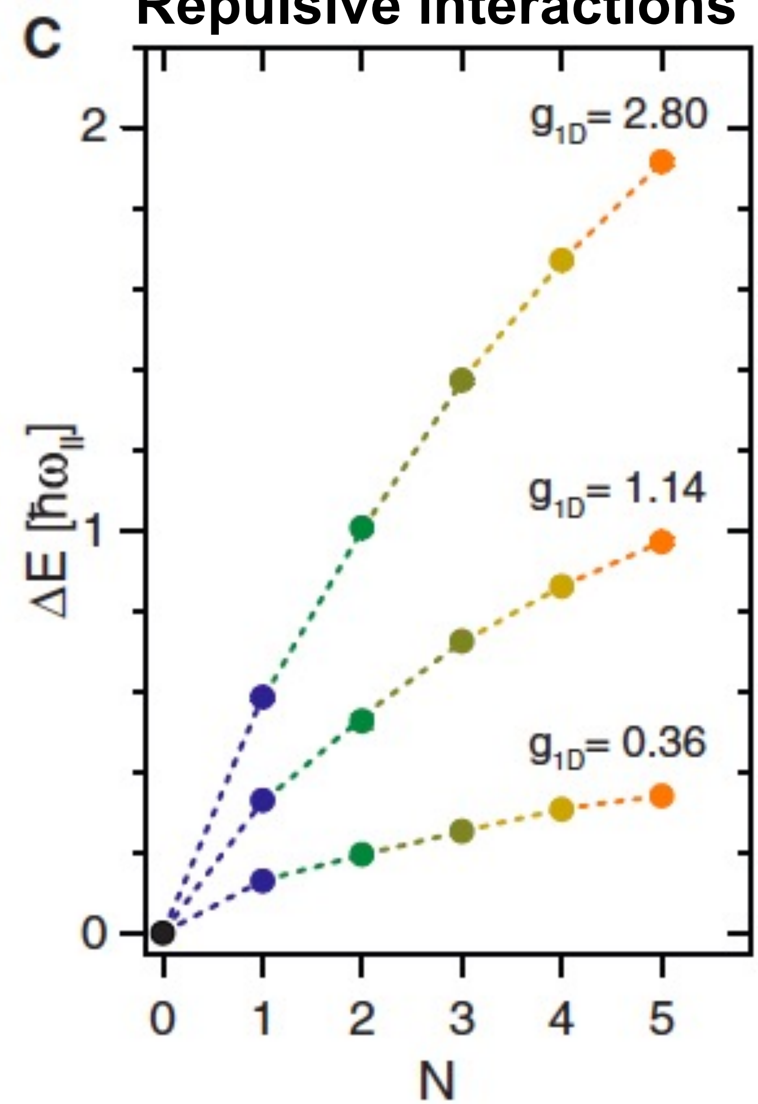
From Few To Many: Building Up The Fermi Sea



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).

Repulsive interactions



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