~~Dynamics of Few-Body Systems~~

Dynamics of Two-Body Systems

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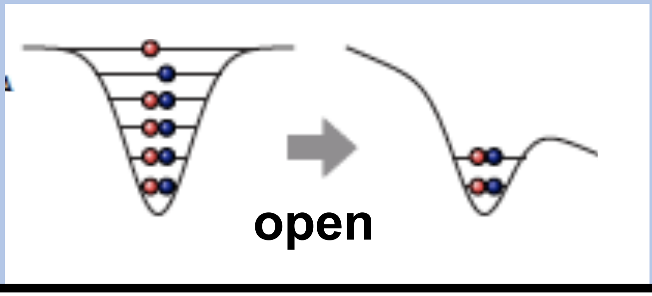
This Lecture: Motivation, How To, and Two Examples

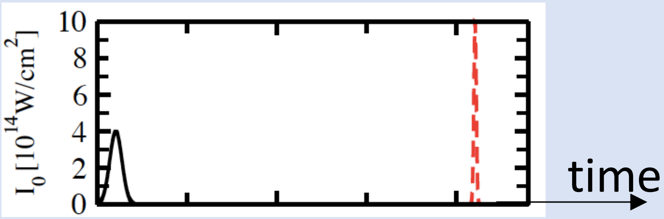
Dynamic properties of one-dimensional few-atom gases:

Tunneling dynamics in the presence of short-range interactions.

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



Dissociative dynamics: pump-probe (something different but related):



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.

- Conditions for thermalization.
- Time scale separation.

Things to Keep in Mind

Time-independent Hamiltonian:

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.

Time-dependent Hamiltonian:

Energy is not, in general, conserved.

How Do We Perform Time-Dynamics?

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

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

$U(t - t_0) = exp\left(-\frac{\imath H(t - t_0)}{\hbar}\right)$.

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

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

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

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

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

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

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

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

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

Use Trotter formula:

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

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

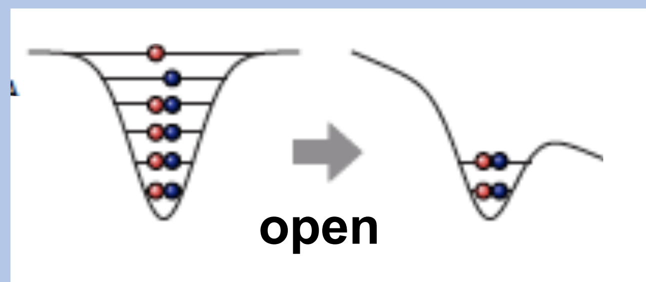
Requires small Δt. Integrand oscillates with frequency $\propto (\Delta t)^{-1}$.

Example 1: Simplest Non-Trivial Open Quantum System

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 cold atom context:
Tunneling as spectroscopy.

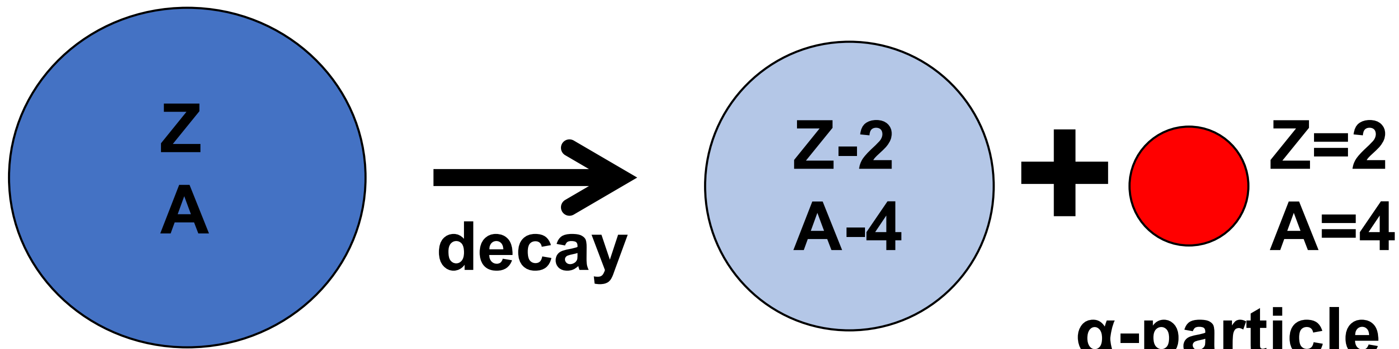
More generally:
Weird quantum mechanical phenomenon.

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

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

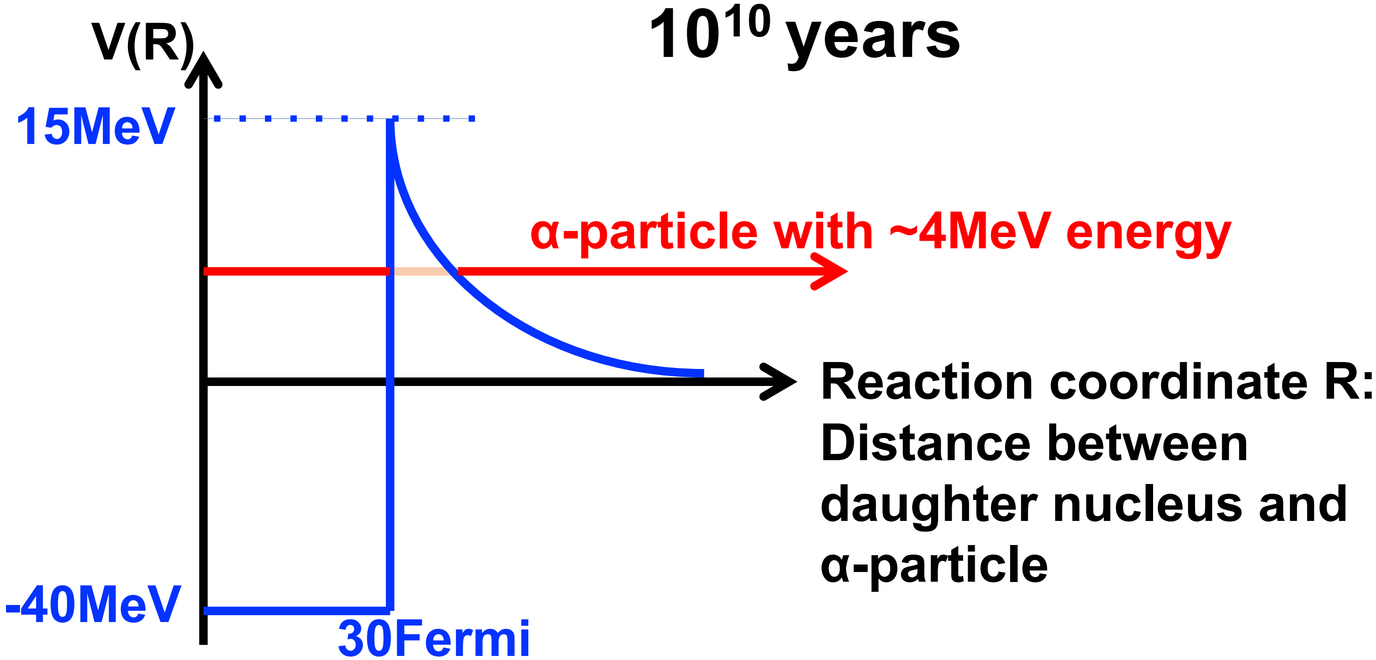
α-Decay (Textbook Example). E.g.: $^{232}Th \rightarrow {}^{228}U + {}^{4}He$

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



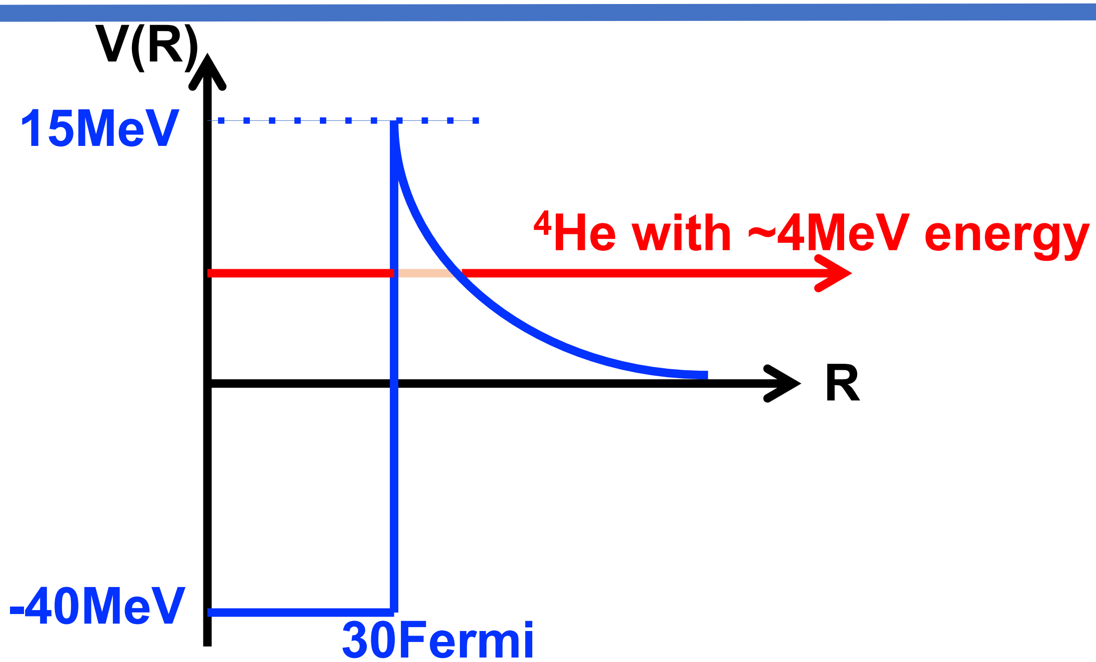
Lifetime of 10^{10} years

α-particle has ~4MeV energy



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

Alpha Decay Through Tunneling



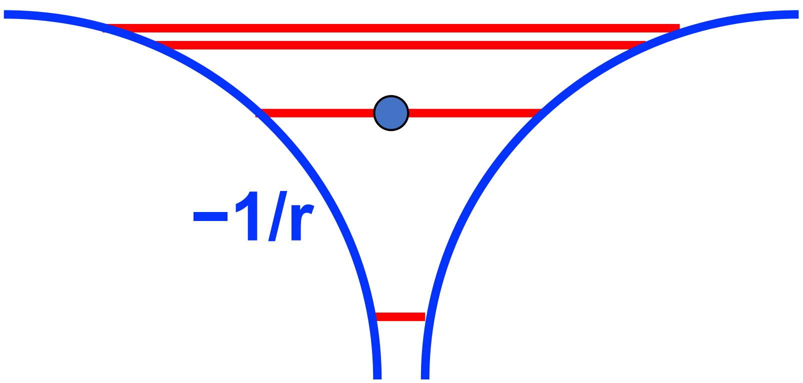
Explanation:
α-particle repeatedly hits the barrier and each time there is a probability to get out.

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.**

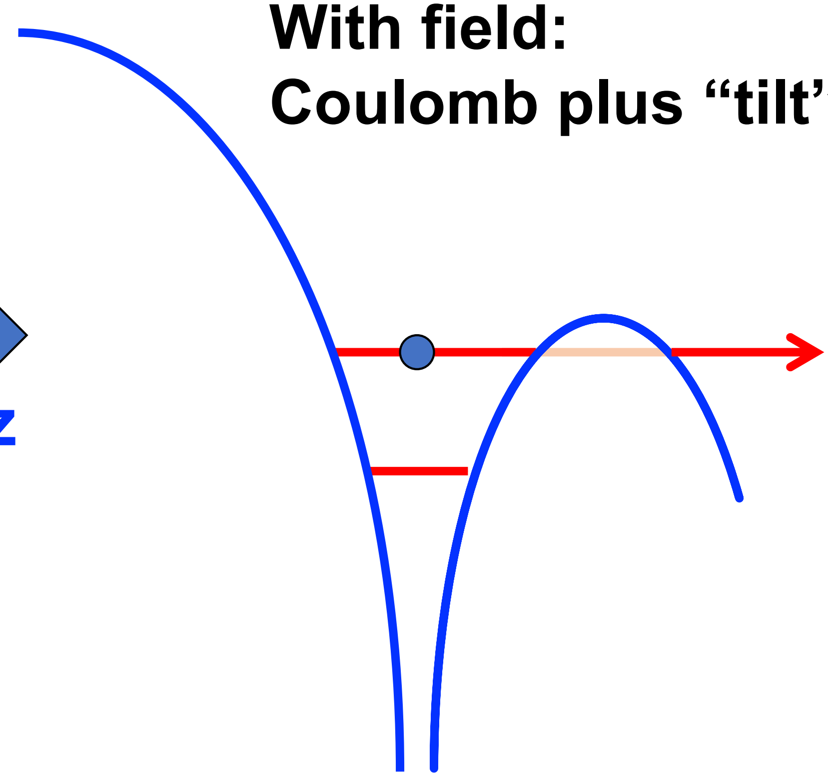
Different Example:
H-Atom In External Field

No field: just Coulomb



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

With field:
Coulomb plus "tilt"

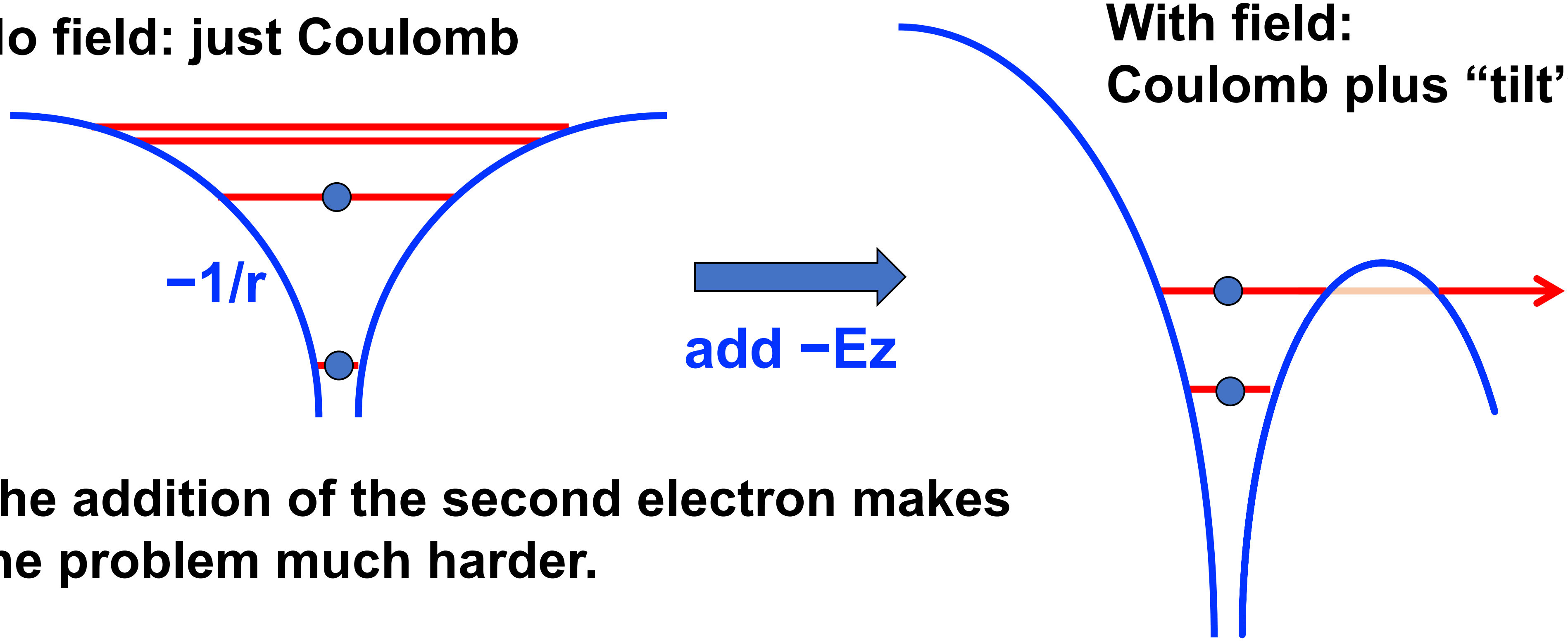


Relatively simple single-electron problem.
What happens when we go to He-atom? Two electrons…

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

No field: just Coulomb

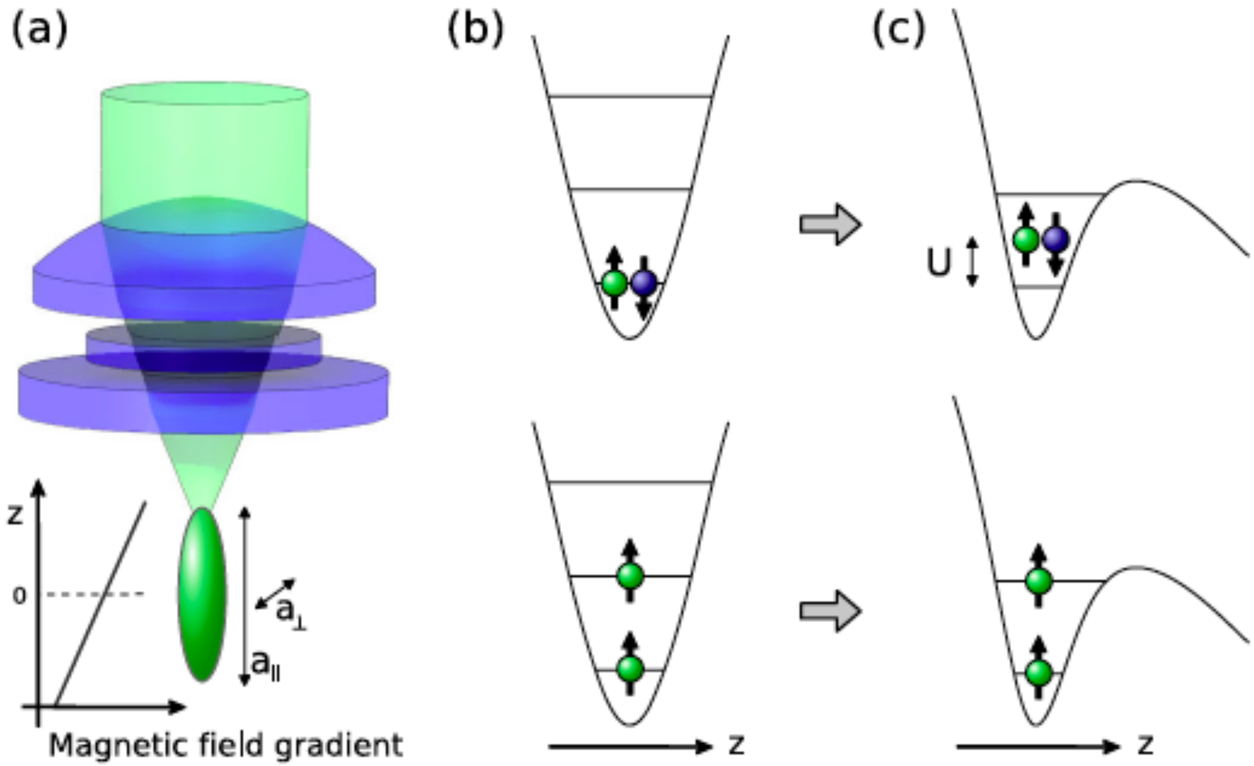
With field: Coulomb plus “tilt”



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 microscope 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.

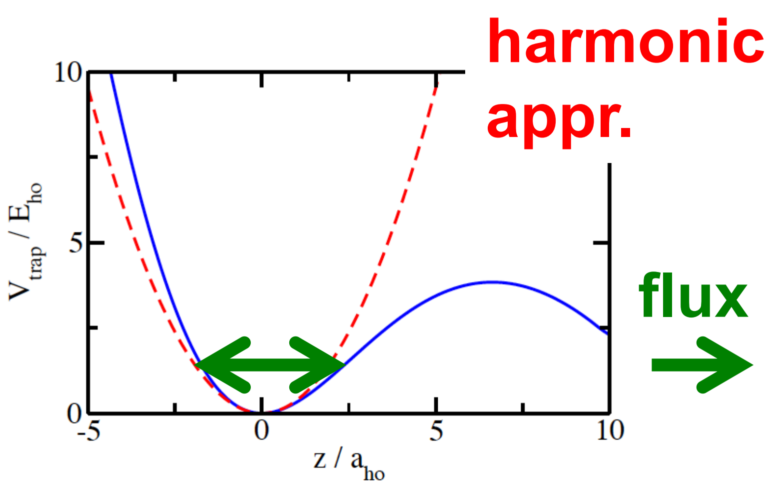
Electrons: **Atoms in particular hyperfine state.**
Electron-electron Coulomb potential: **Zero-range contact potential.**
Electron-nucleus Coulomb potential: **External harmonic trap.**

Some 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).

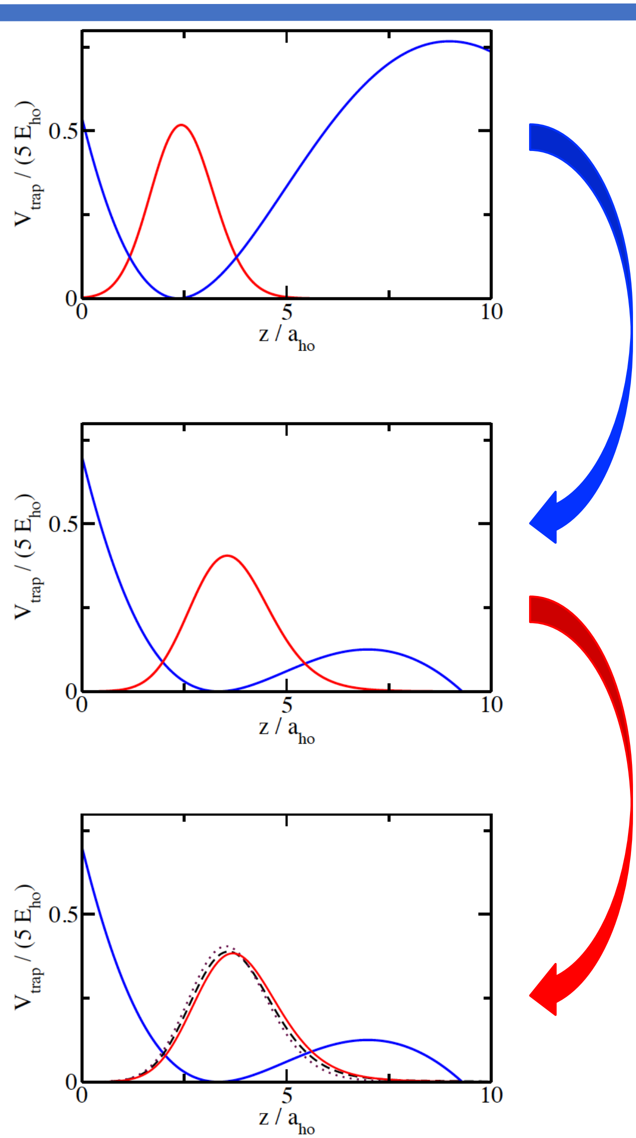


Trap time scale: $T_{ho}=\omega^{-1}$.

"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?

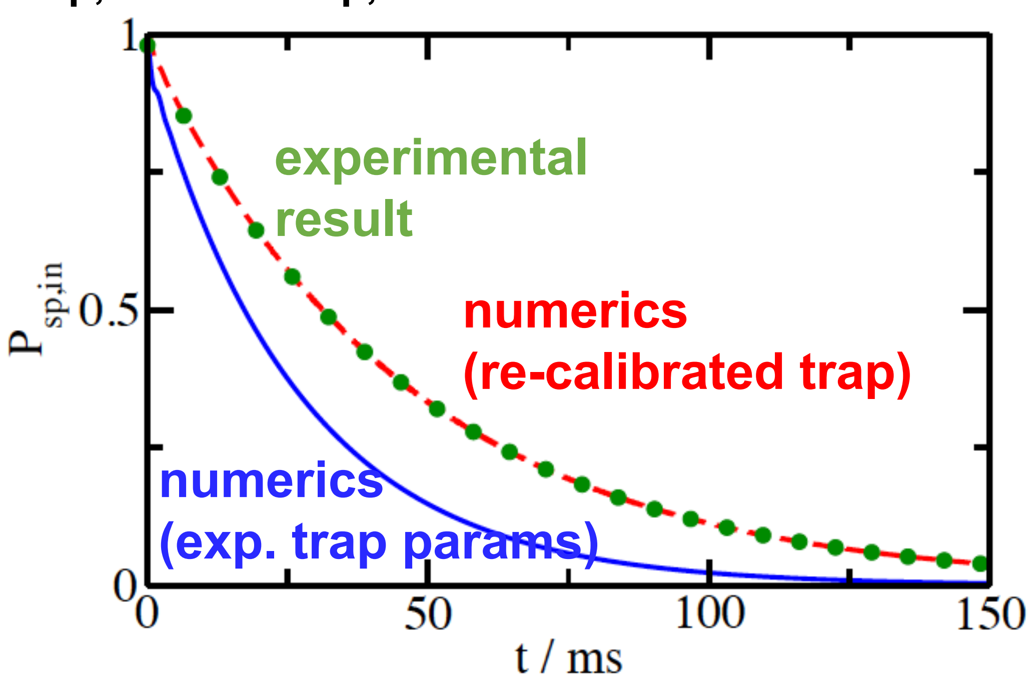
Look at upper branch.

Single-Particle Dynamics: Experiment vs. Theory

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.

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

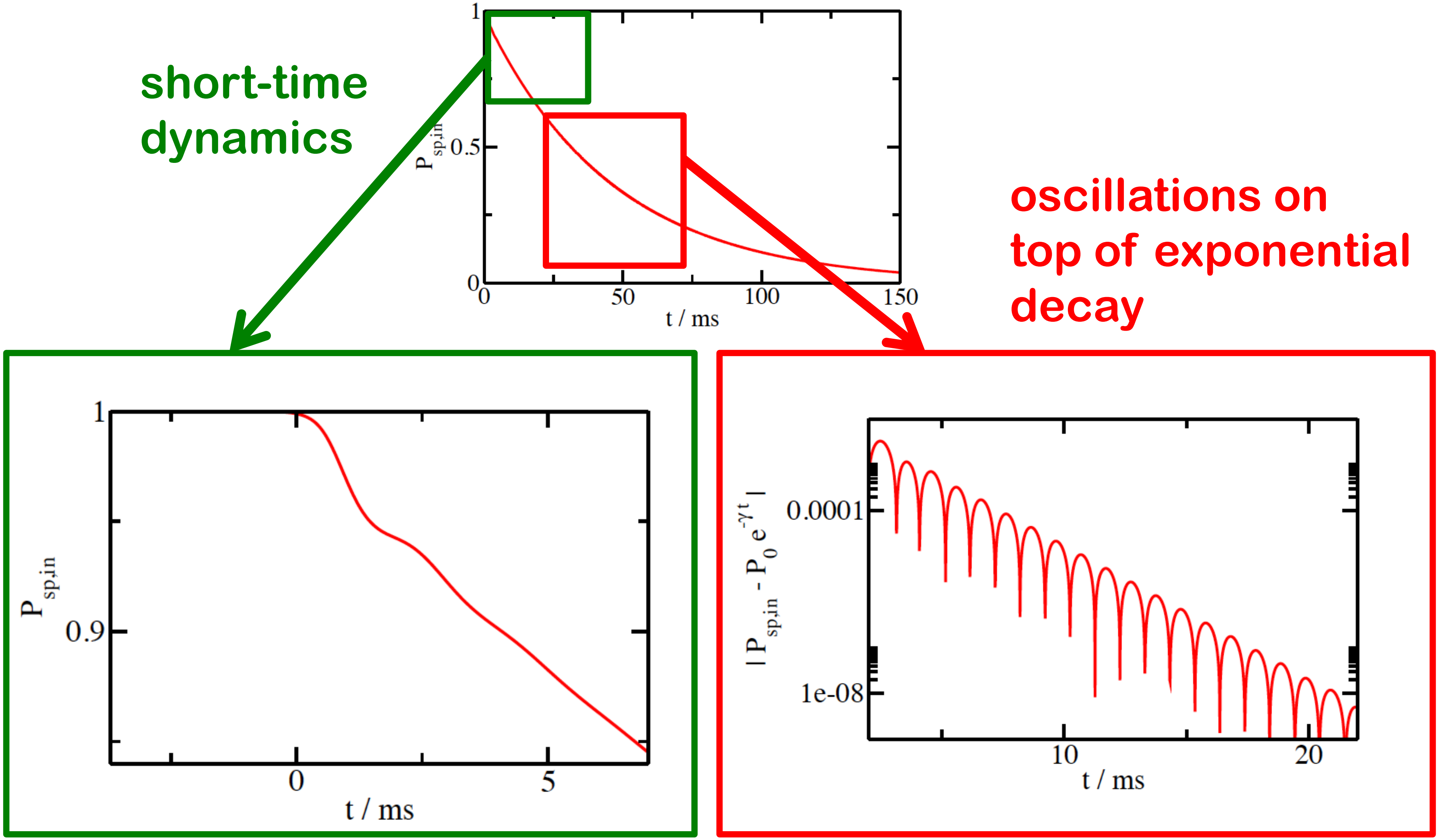


Why? Trap parameters p and $c_{|j>}B'$ are calibrated using semi-classical WKB approximation. WKB tunneling rate is inaccurate.

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

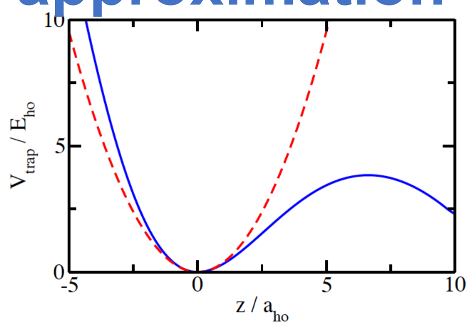
Re-parameterize trap: Find parameters such that our γ agrees with experimental γ.

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



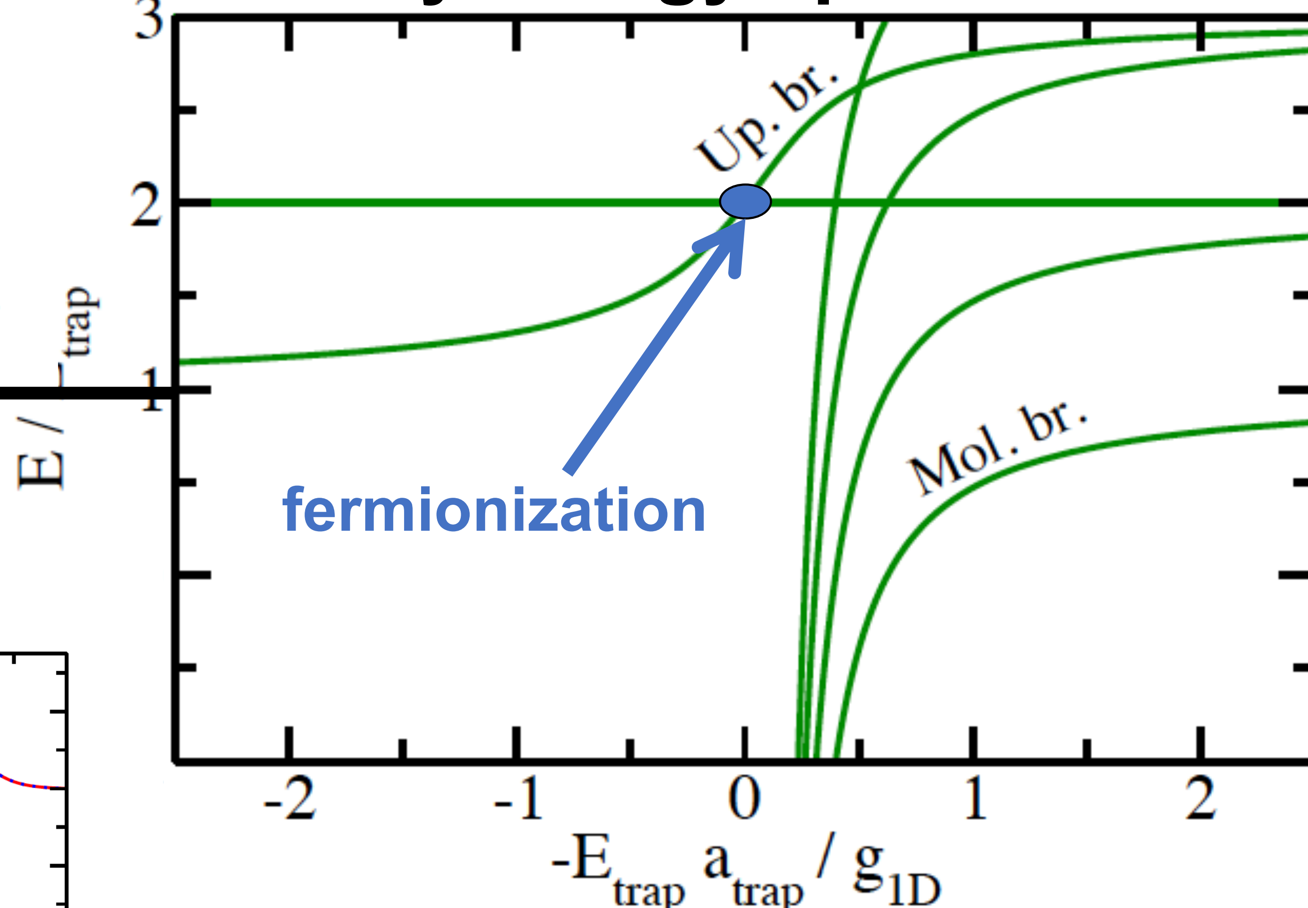
Overview: Upper Branch And Molecular Branch For Deep Trap

Harmonic approximation



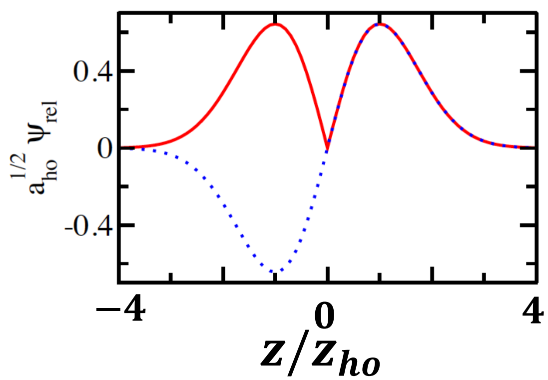
non-interacting (NI)

Two-body energy spectrum:

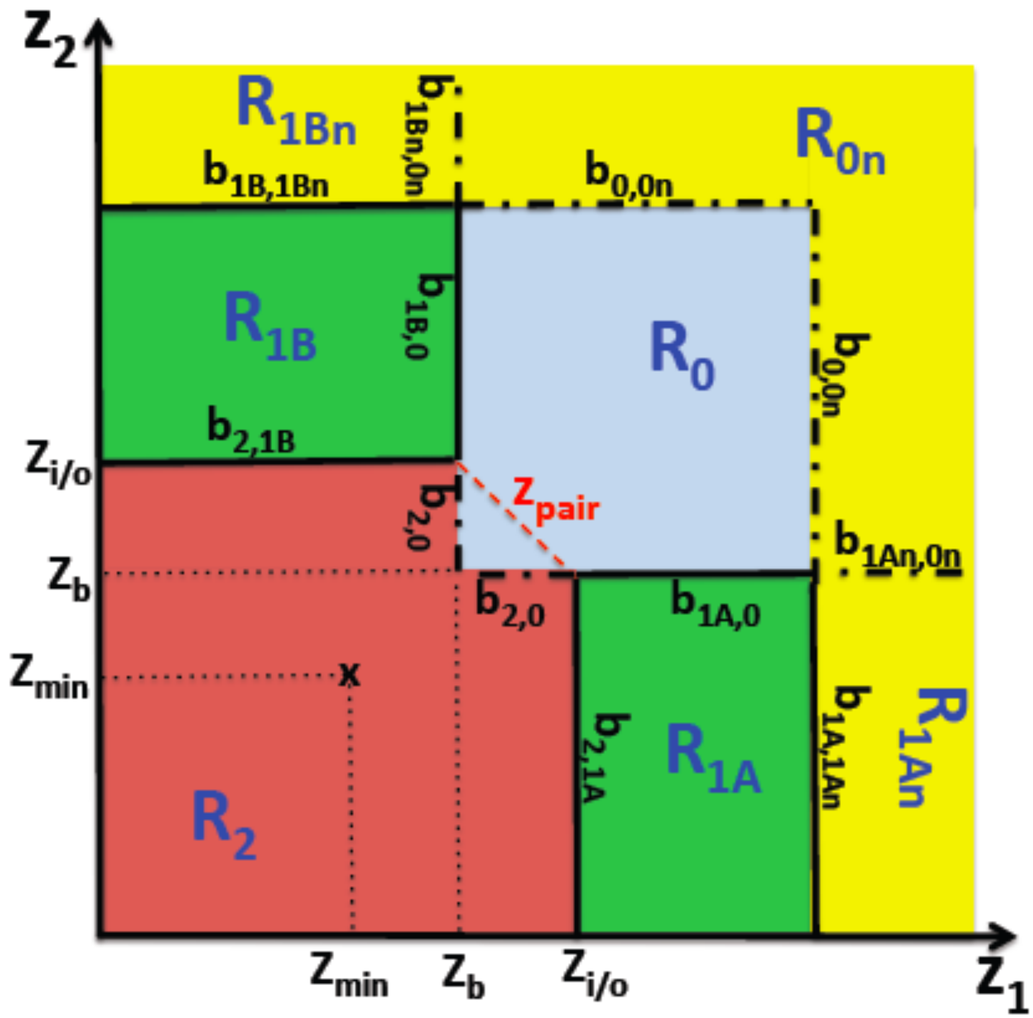


NI

1 / (two-body interaction strength)



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

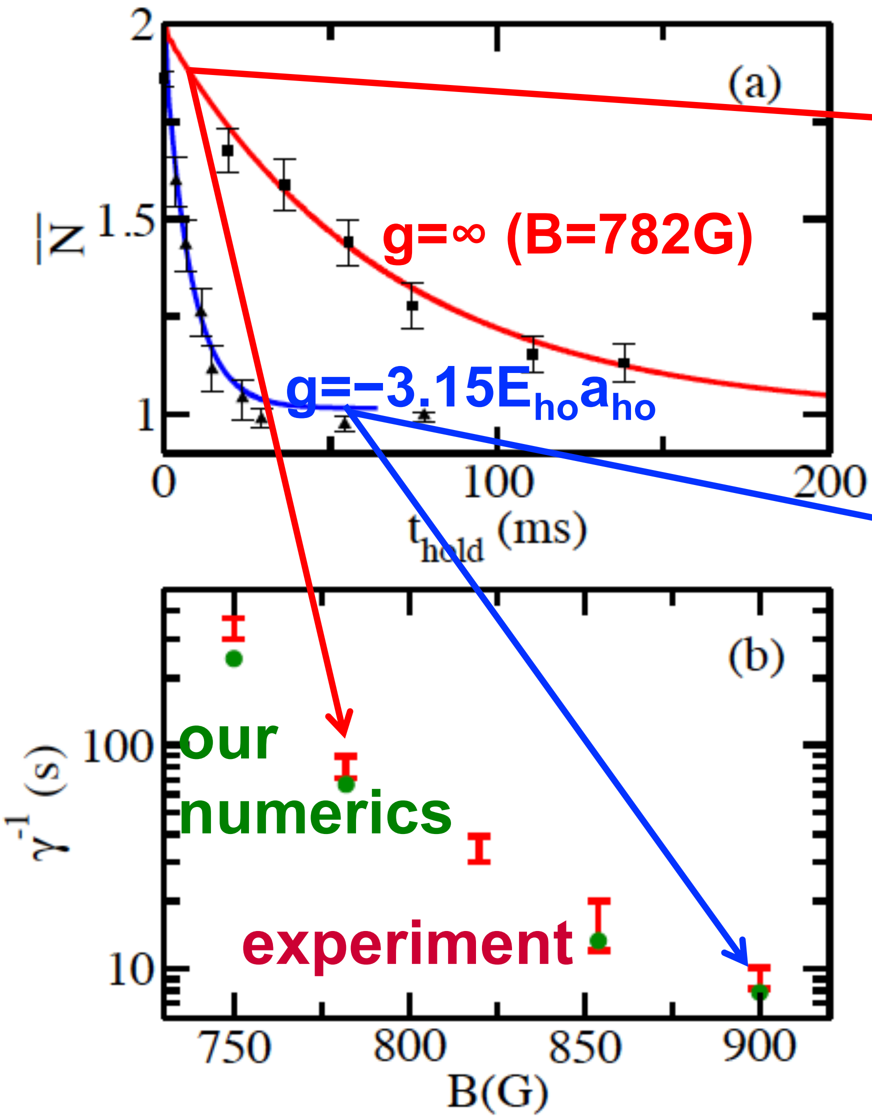


Region with two trapped particles (R_2).
Regions with one trapped particle (R_{1A} and R_{1B}).
Region with zero trapped particles (R_0).

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

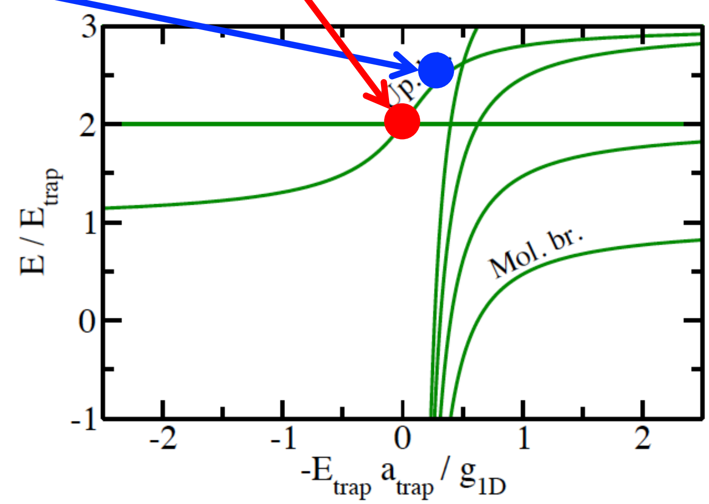
"Numerical" region (yellow): Apply damping so as to avoid reflection from edge of box.

Upper Branch: Comparison With Experimental Data



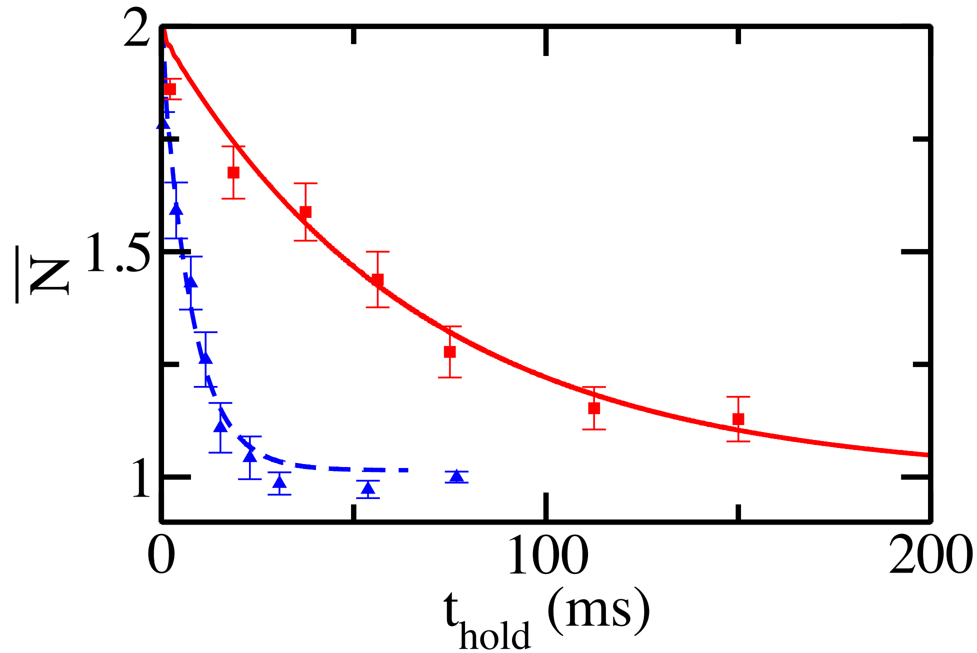
Very good agreement with experimental results!!!

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

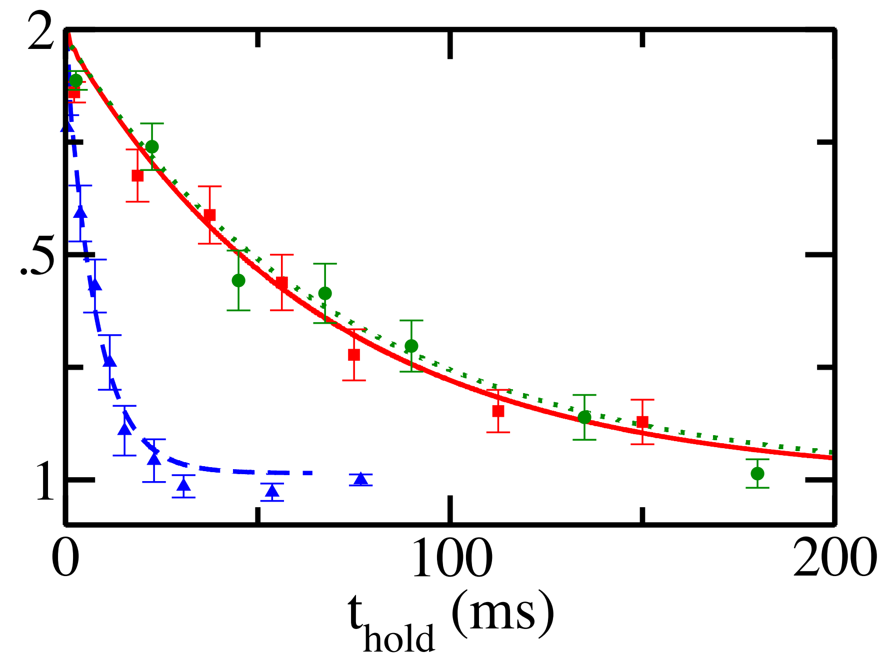


Fermionization Of Two-Particle System: Effect On Tunneling

Two different HF states (g=∞):



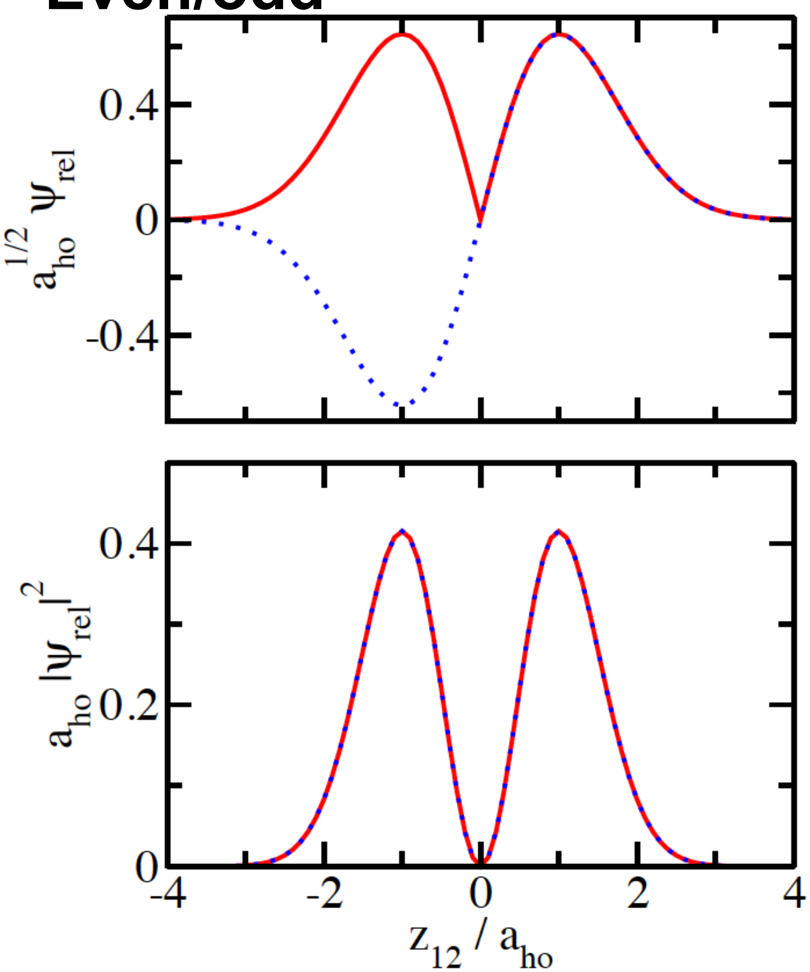
Two identical HF states (g=∞):



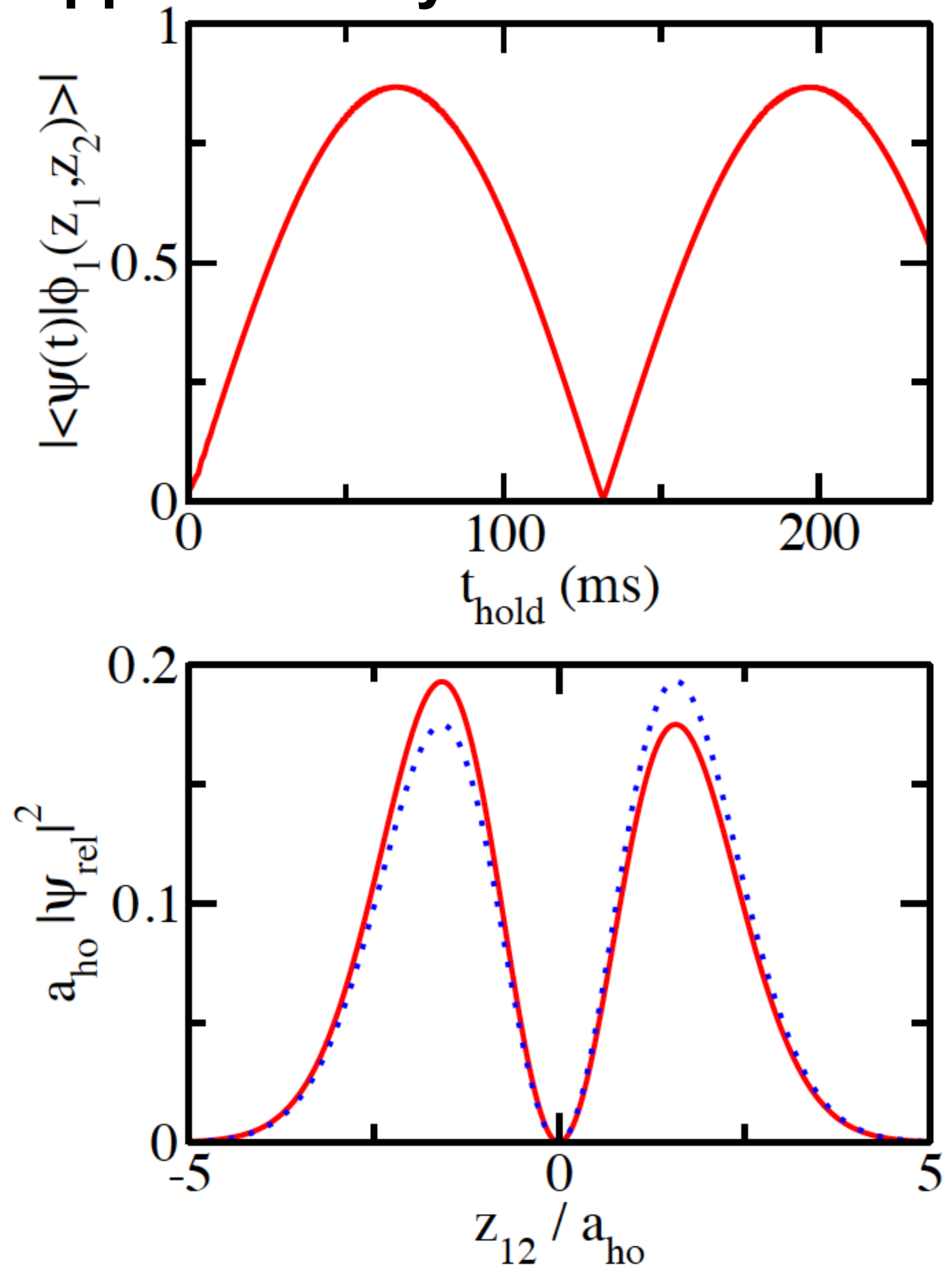
There is a small difference since the trapping potential depends on the hyperfine state.
Also, the two distinguishable particle system exhibits dynamics that reflects the near degeneracy of two states.

Fermionization

Two identical particles: Even/odd



Two distinguishable particles: Approximately even/odd



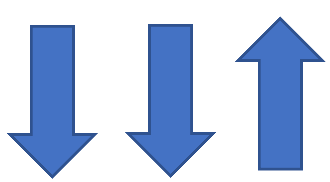
Example 1:
What Did We Learn?

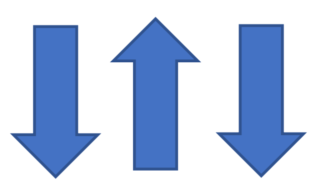
Tunneling is exponentially sensitive (well, we knew this…): Accurate trap parametrization is crucial.

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.

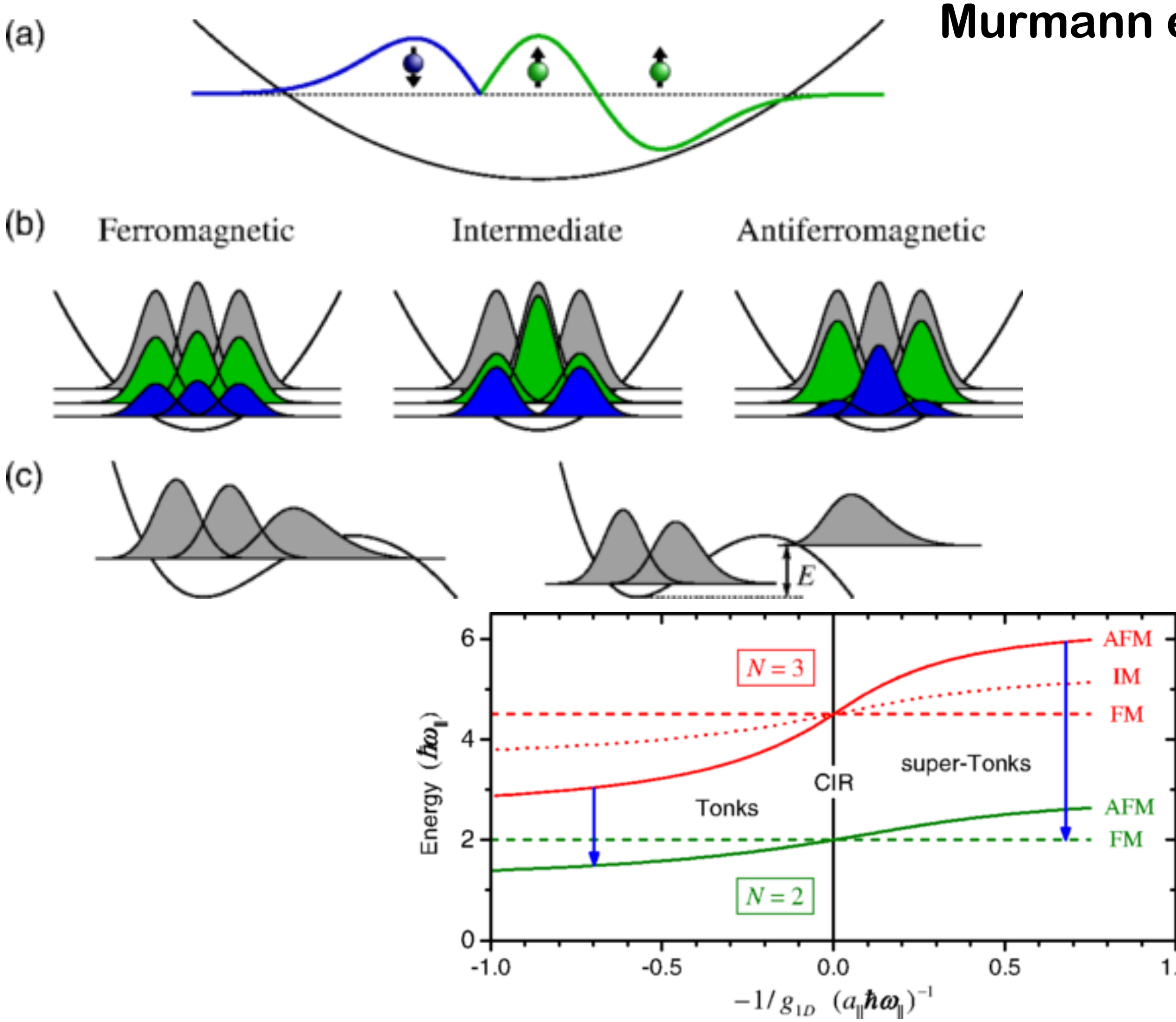


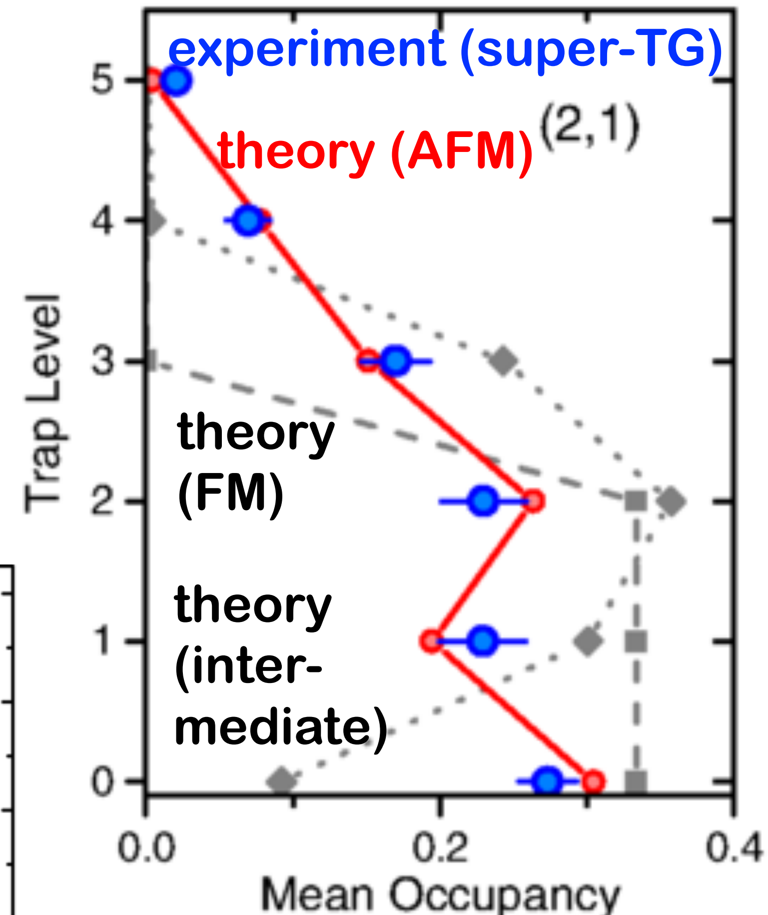


Magnetic ordering and spin chain models:
Cui, Ho, Zinner, Gharashi/Blume, Parish, Levinsen, Massignan, Santos, Deuretzbacher, Pu, Guan,…

Example 1: Beyond Two Particles

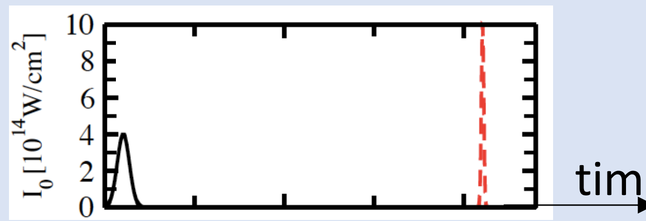
Murmann et al., PRL 115, 215301 (2015)





Example 2: Only Cold And Not Ultracold…

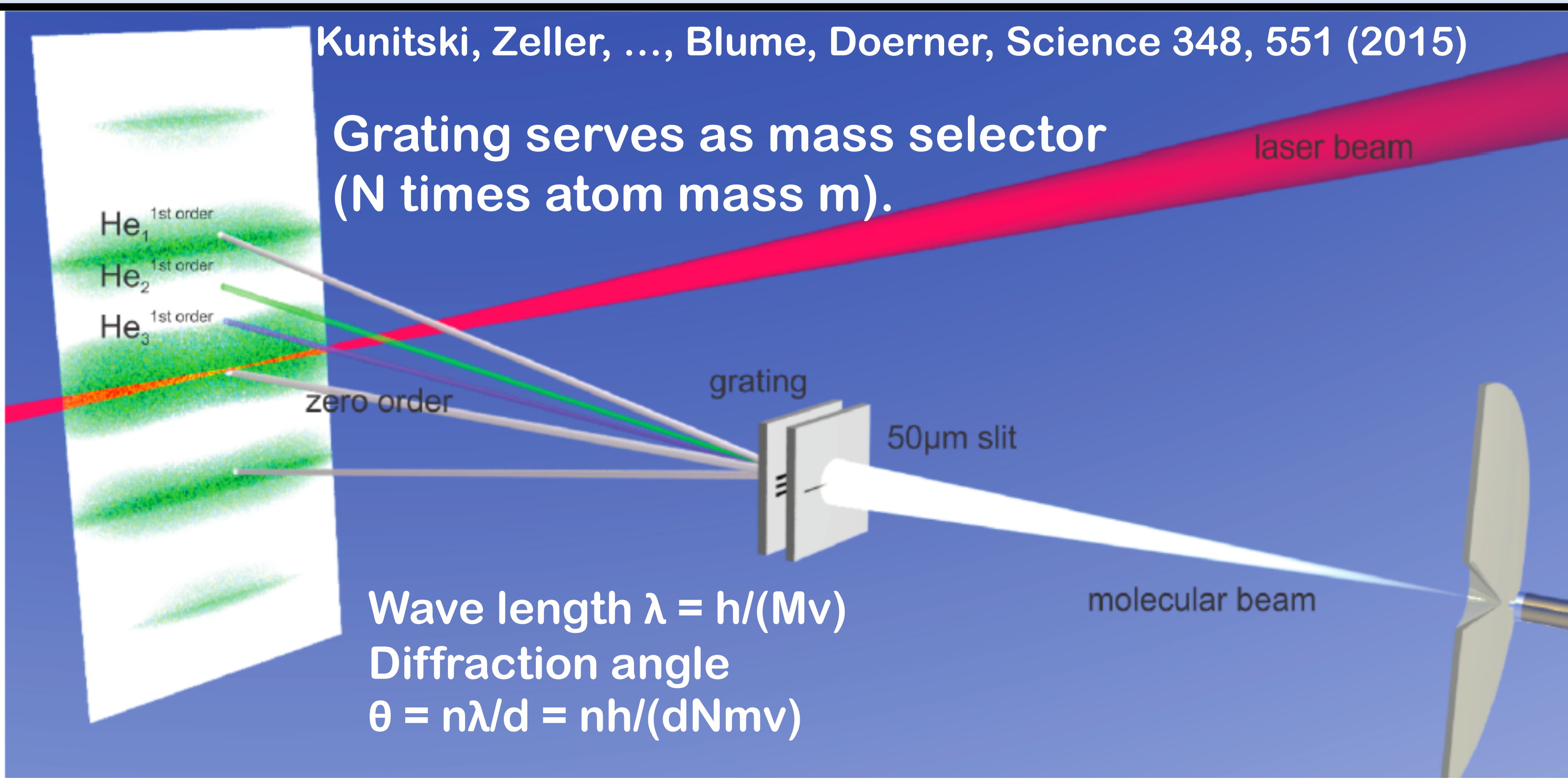
Dissociative dynamics:
pump-probe
(something different but related):



time (order of ps)

Kunitski, Zeller, …, Blume, Doerner, Science 348, 551 (2015)

Grating serves as mass selector
(N times atom mass m).



Wave length $\lambda = h/(Mv)$
Diffraction angle
$\theta = n\lambda/d = nh/(dNmv)$

Cold And Not Ultracold Samples

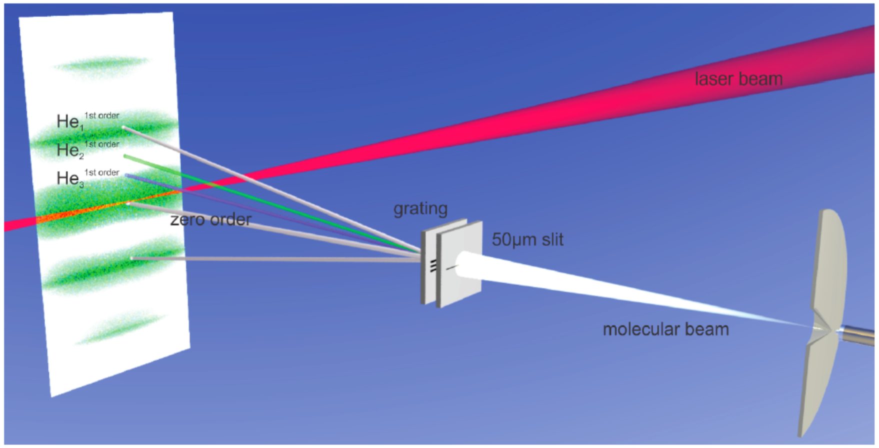
Cold ^{4}He atoms (sub-Kelvin temperatures):

Three-body (three-body Efimov state; no real-time dynamics)

Two-body (real-time dynamics)

In collaboration with Reinhard Doerner's group at Frankfurt University (lead postdoc Maksim Kunitski)

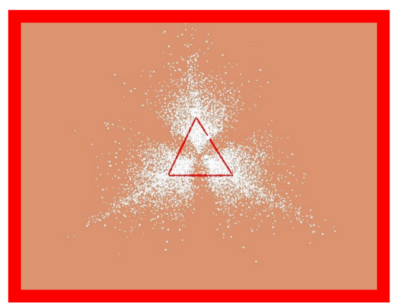
Size-selected nozzle beam expansion experiments and theory

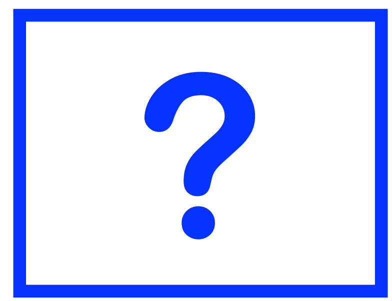


Some Background on the Helium System…

$1\ \text{K} = 8.6 \times 10^{-5}\ \text{eV}$

- Dimer:
  - ^{4}He-^{4}He bound state energy $E_{dimer} = -1.3$mK.
  - No $J > 0$ bound states.
  - Two-body s-wave scattering length $a_s = 171a_0$.
  - Two-body effective range $r_{eff} = 15.2a_0$ (alternatively, two-body van der Waals length $r_{vdW} = 5.1a_0$).
- Trimer:
  - Two $J = 0$ bound states with $E_{trimer} = -131.8$mK and -2.65mK.
  - No $J > 0$ bound states.



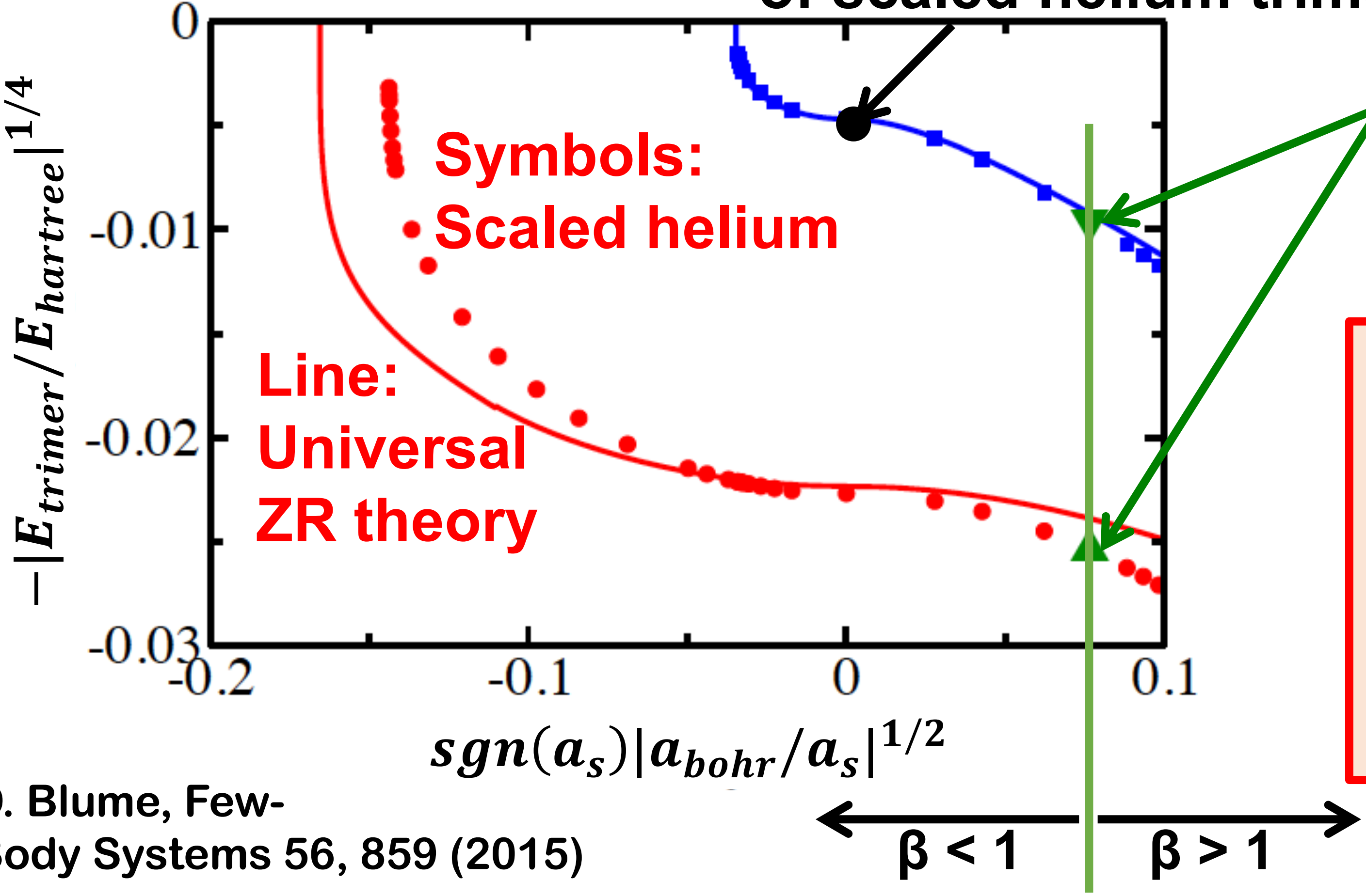


- Binding energy of liquid helium is $E/N = -7$K.

Helium Trimer Excited State is an Efimov State

$\beta V_{He\text{-}He}(r_{12}) + \beta V_{He\text{-}He}(r_{23}) + \beta V_{He\text{-}He}(r_{31})$.

Three-body parameter is chosen such that ZR energy agrees with energy of scaled helium trimer excited state.

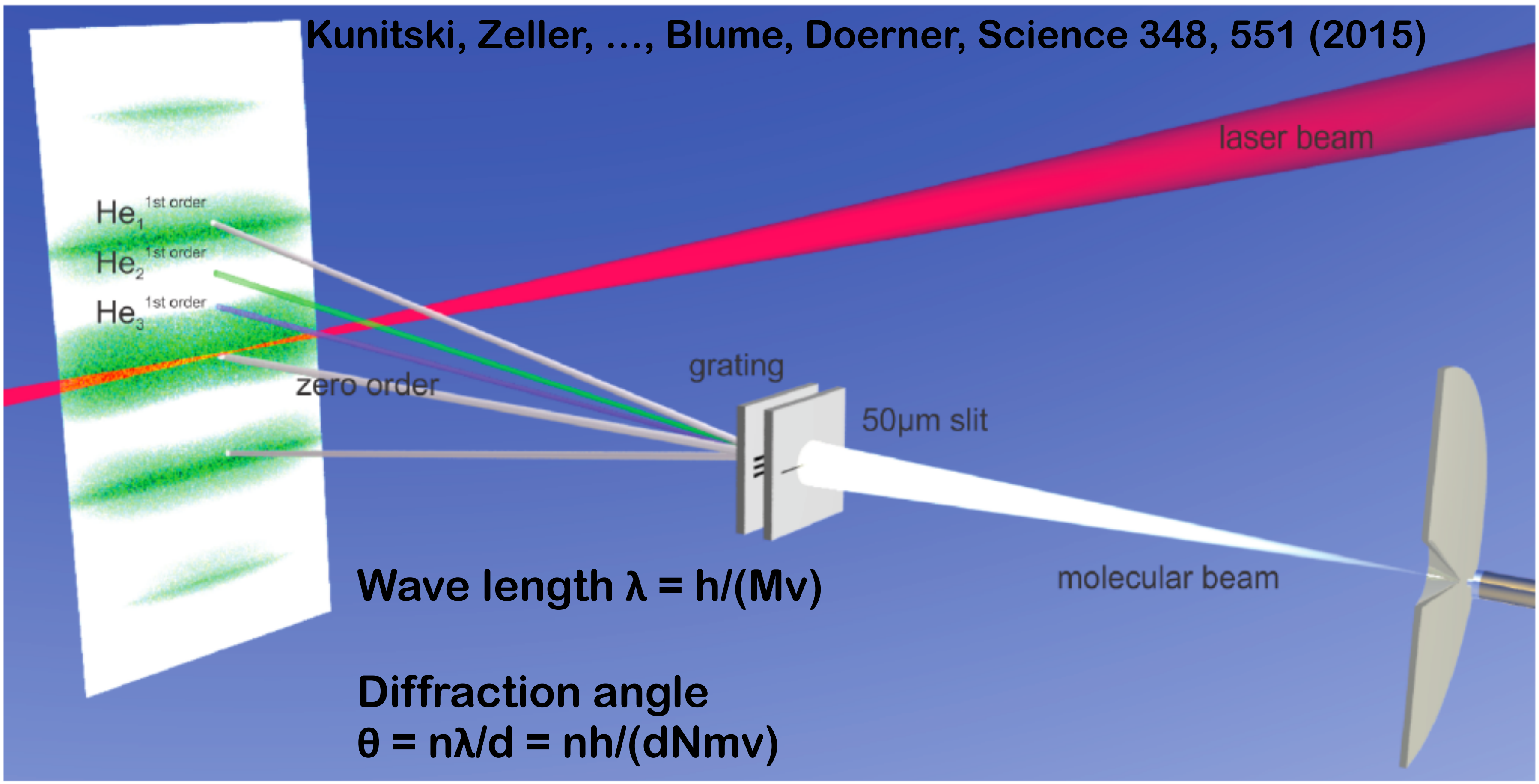


True helium (ground and excited states)

For the excited state, symbols agree with line! Molecular system follows predicted Efimov behavior.

D. Blume, Few-Body Systems 56, 859 (2015)

How to Prepare/Probe Helium Trimer Excited Efimov State?



Kunitski, Zeller, ..., Blume, Doerner, Science 348, 551 (2015)

Wave length $\lambda = h/(Mv)$

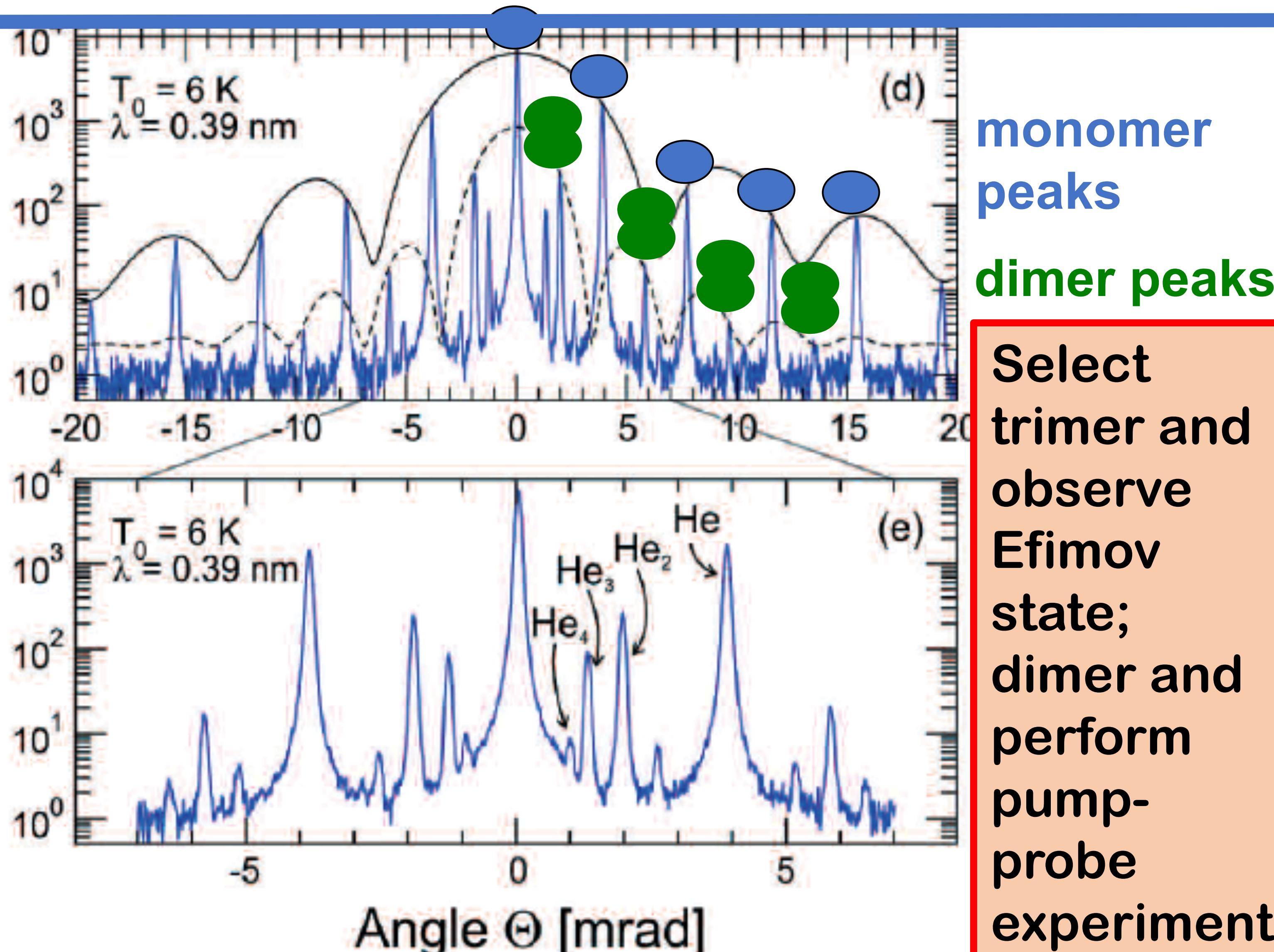
Diffraction angle
$\theta = n\lambda/d = nh/(dNmv)$

Grating serves as mass selector (N times atom mass m).

Matter Wave Diffraction Experiment

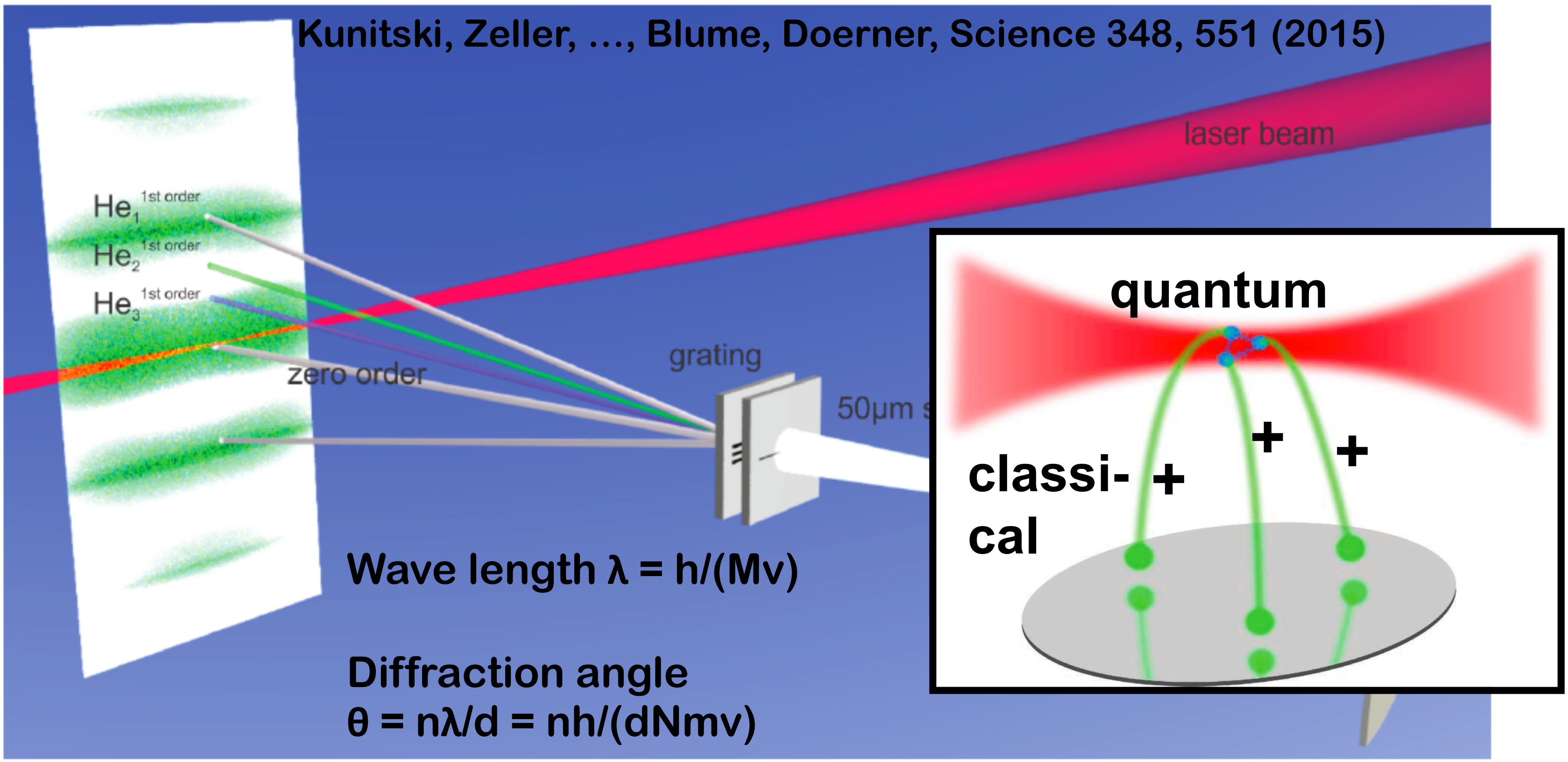
Kornilov, Toennies, 10.1051/ epn:2007003

Nozzle temperature and pressure can be adjusted.



Select trimer and observe Efimov state; dimer and perform pump-probe experiment

How to Prepare/Probe Helium Trimer Excited Efimov State?

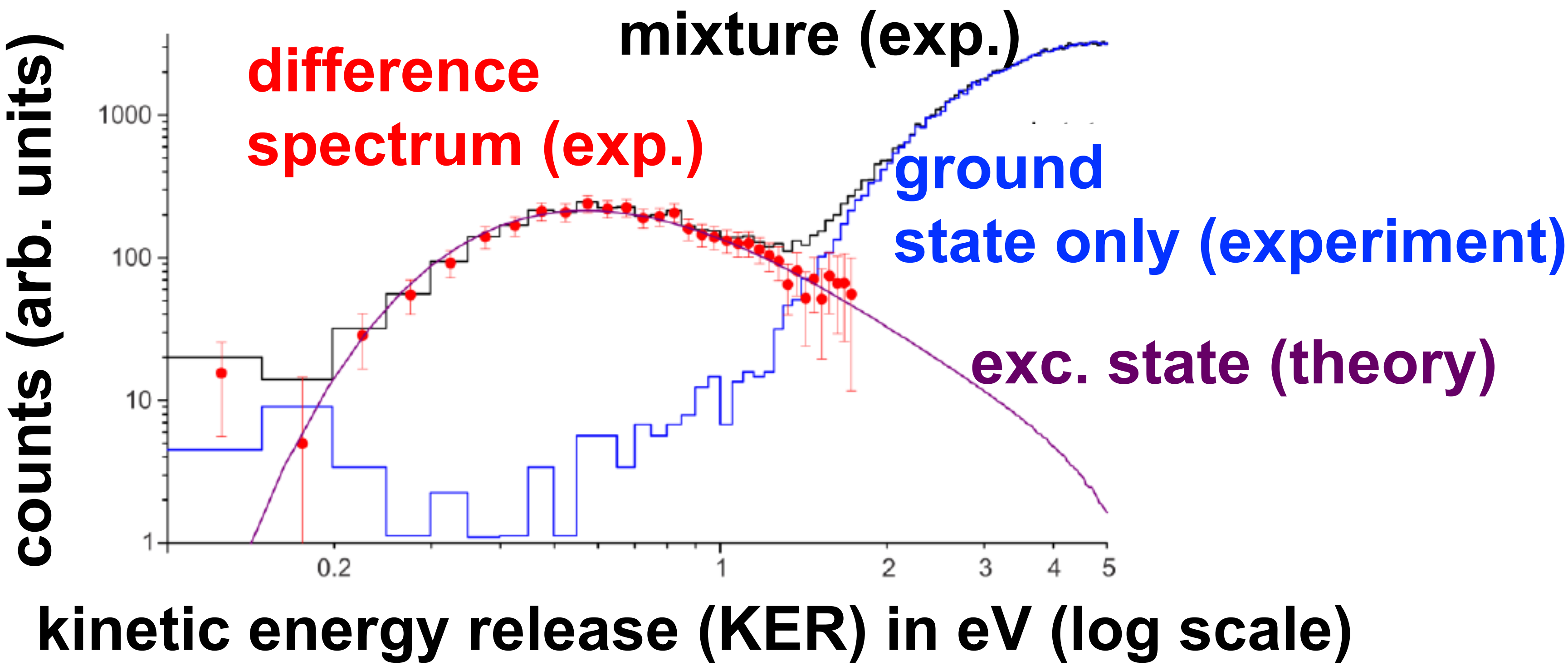


Grating serves as mass selector (N times atom mass m):

He$_3$ signal contains ground state trimer *and* excited state trimer.

Laser beam ionizes trimer: Coulomb explosion of $^4He_3$ (3 ions).

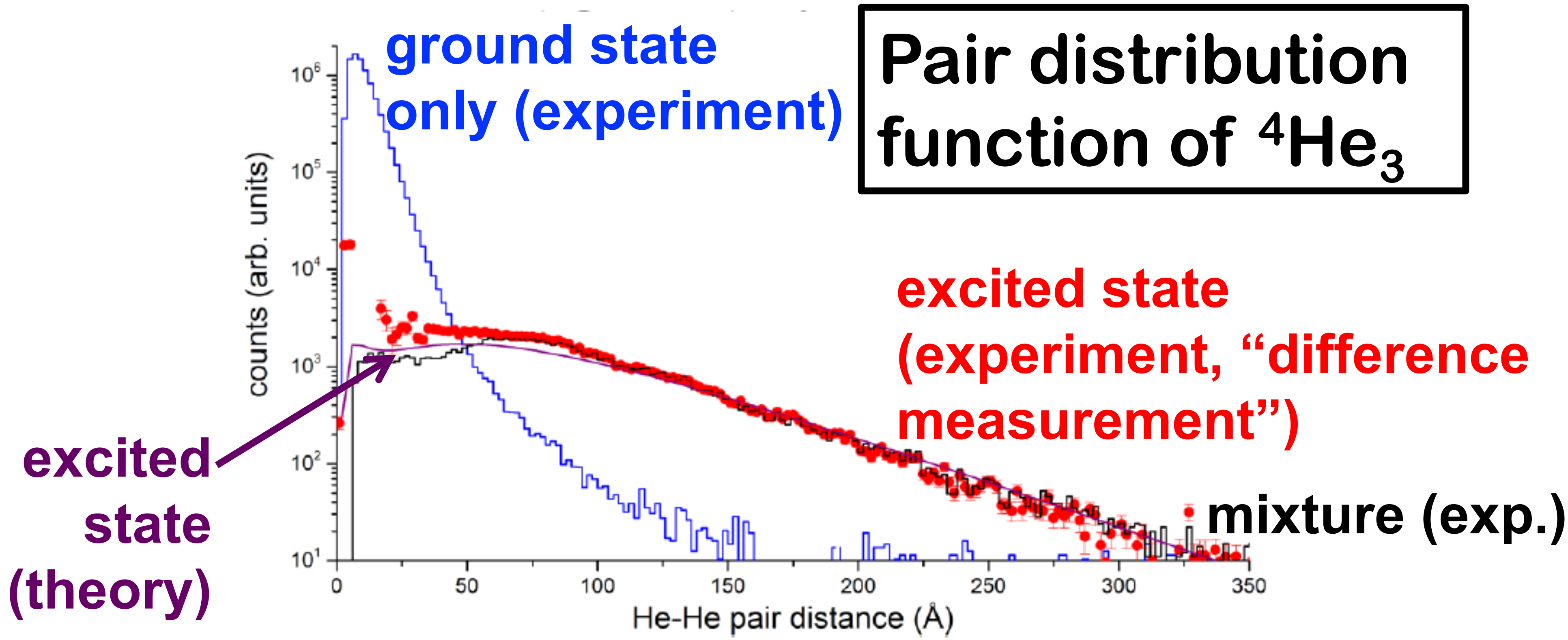
Kinetic Energy Release Measurement



The ionization is instantaneous and the He-ions are distributed according to the quantum mechanical eigen states of the ground and excited helium trimers.

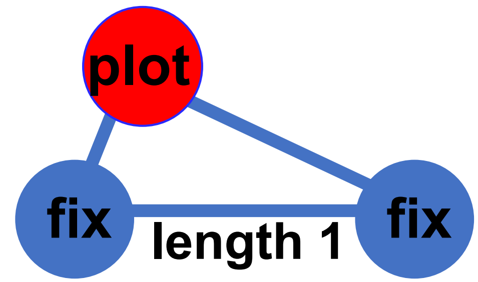
Large r_{12}, r_{23} and r_{31} correspond to small $KER=1/r_{12}+1/r_{23}+1/r_{31}$.

Reconstructing Real Space Properties

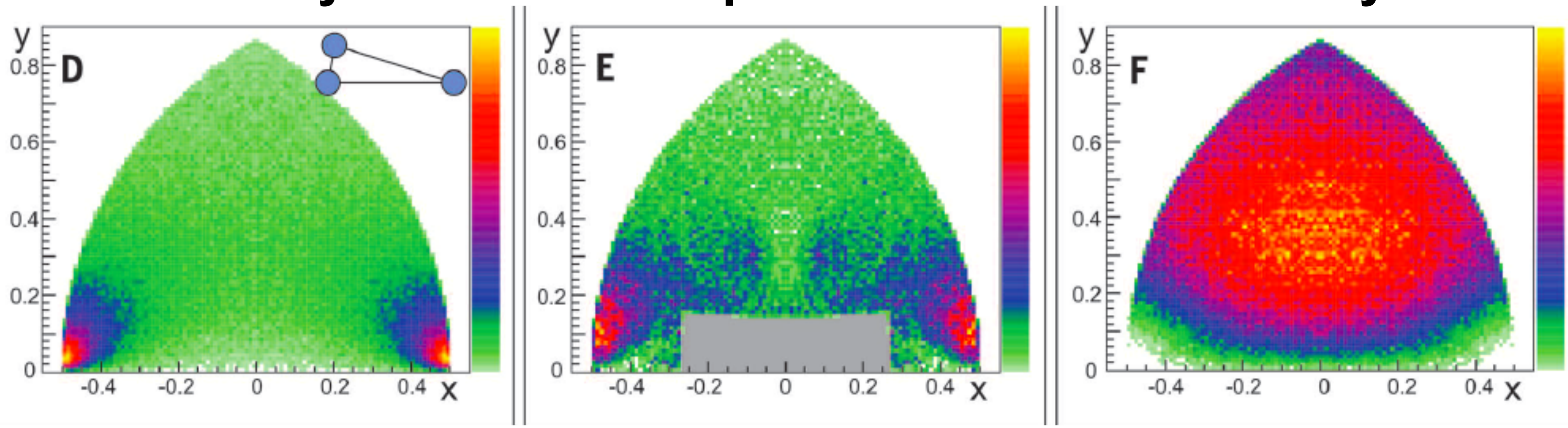


The excited state is eight times larger than the ground state. Assuming an "atom-dimer geometry", the tail can be fit to extract the binding energy of the excited helium trimer. Fit to experimental data yields 2.6(2)mK. Theory 2.65mK.

Normalized Structural Properties of $^4He_3$



excited state: theory | **excited state: experiment** | **ground state: theory**



Divide all three interparticle distances by largest r_{ij} and plot k^{th} atom (positive y): Corresponds to placing atoms i and j at (−1/2,0) and (1/2,0).

Ground state and excited states have distinct characteristics!!!

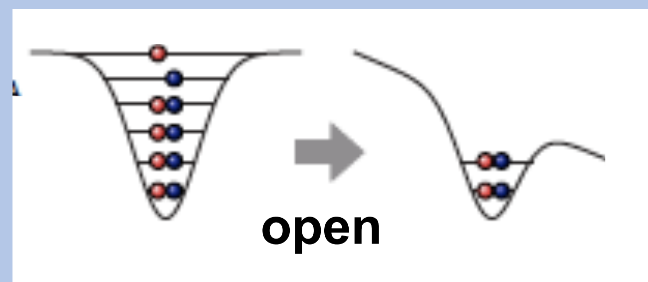
Message: Reconstruction of quantum mechanical trimer density.

Summary: Today, Just Two Particles. Want to Treat More…

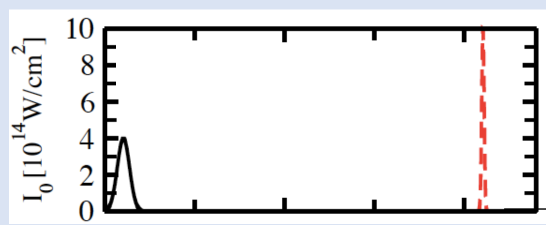
Dynamic properties of one-dimensional few-atom gases:

Tunneling dynamics in the presence of short-range interactions.

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



Dissociative dynamics:
pump-probe
(something different but related):



time (order of ps)

Thanks To Collaborators

Lecture 3:

Ebrahim Gharashi:
Tunneling dynamics.

Selim Jochim and his team:
Two-fermion experiments.

Reinhard Doerner and his team, especially Maksim Kunitski:
Helium trimer and dimer experiments.

Qingze Guan:
Expansion dynamics and helium dimer theory.

Lecture 2:

Debraj Rakshit, Xiangyu (Desmond) Yin:
ECG approach.

John Bohn, Michelle Sze:
Trapped bosons.

Qingze Guan:
Generalized radial scaling law, ECG approach.

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Brian Granger:
Effective odd-z coupling constant, frame transformation.

Krittika Kanjilal:
p-wave and odd-z pseudopotentials.

Grigori Astrakharchik, Stefano Giorgini:
Quasi-1D Bose and Fermi gases.

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