Few-Body Aspects of Bose and Fermi Gases

Theoretical frameworks for treating cold

few-particle systems: Two-body scattering

and hyperspherical perspective



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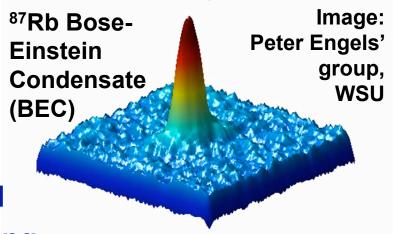
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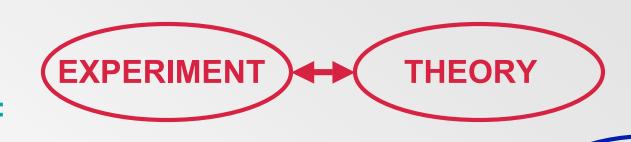
Outline of This Talk

- Broad introduction:
 - Cold atom physics.
 - Few-body physics.
 - Overview of lectures.



- Two-body interactions and scattering length.
- Connection between microscopic world and mean-field formulation.
- Microscopic understanding of stability of Bose and Fermi gases: Linear Schroedinger equation within hyperspherical framework.

The Field of Cold Atom Physics



Nobel Prizes:

Laser cooling (1997): Chu, Cohen-Tannoudji, Phillips.

Bose-Einstein condensation (2001): Cornell, Ketterle, Wieman.

Theory of superconductors and superfluids (2003): Abrikosov, Ginzberg, Leggett.

Quantum optics and frequency comb (2005): Glauber, Hall, Hansch.

molecular physics

nuclear physics

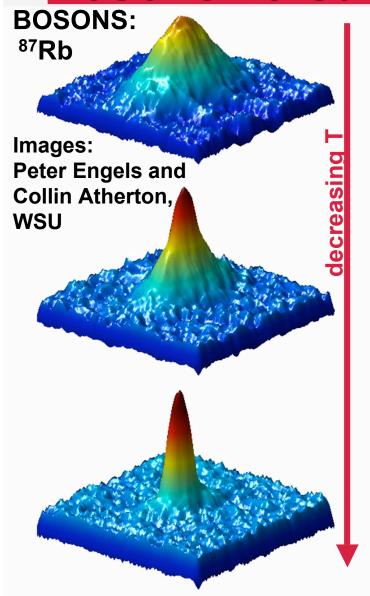
condensed matter

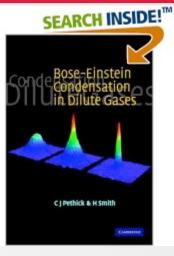
atomic physics

quantum information science

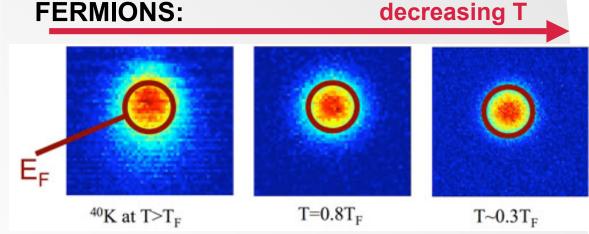
quantum optics

Reaching Quantum Degeneracy: Bosons versus Fermions





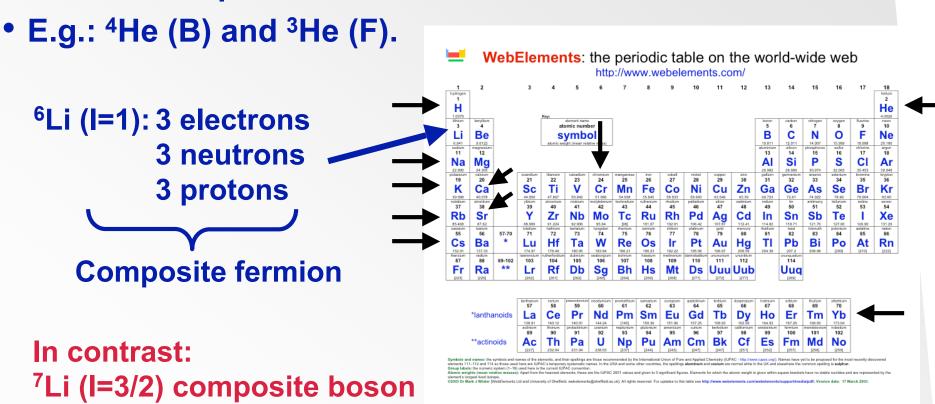
Transition temperature of bosons: a few 100nK (BEC: the coldest place in the known Universe)



Images: Thywissen group, University Toronto.

Composite Atomic Bosons versus Fermions.

- Boson: Integer spin; e.g., photon, mesons (q, anti-q).
- Fermion: Half-integer spin; e.g., electron, quarks, proton, neutron, baryons (q,q,q).
- Atoms: Composite bosons and fermions.

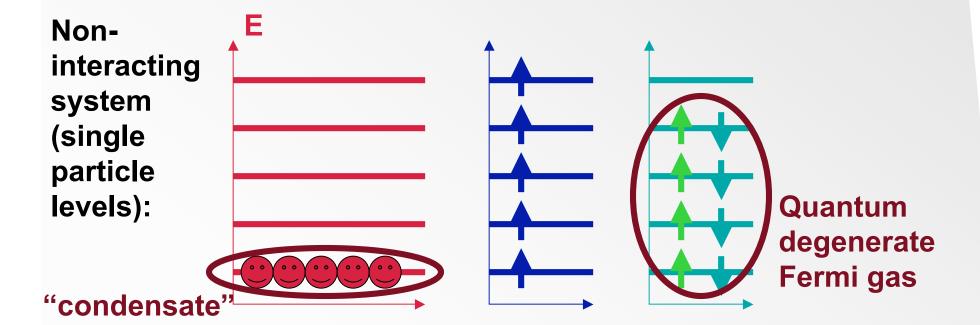


Bose versus Fermi Statistics: Gas at Low Temperature

One-component Bose gas:

One-component spin-polarized Fermi gas:

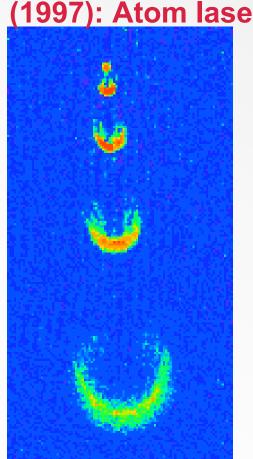
Two-component Fermi gas:

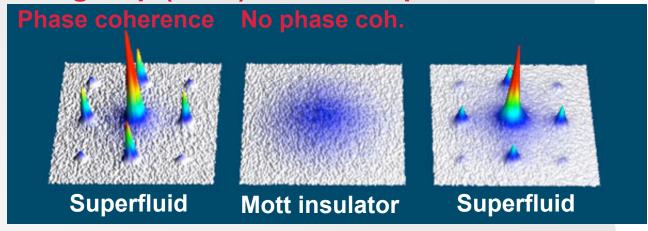


Selected Highlights from Cold Atom Experiments

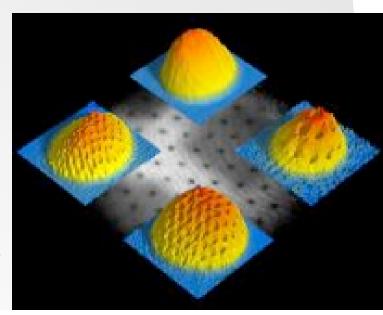
MPI, Hansch group (2002): Quantum phase transition:

MIT, Ketterle group (1997): Atom laser.

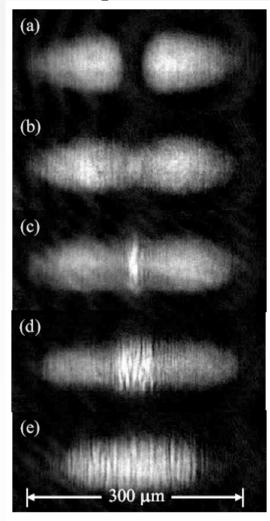




MIT, Ketterle group (2001): Vortex lattice in Na BEC.

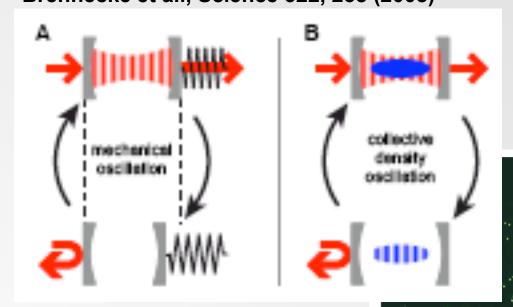


More Highlights from Cold Atom Experiments...



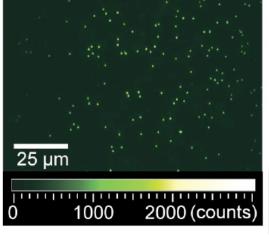
Quantum shock Chang et al., PRL (2008)

Cavity opto-mechanics with a BEC Brennecke et al., Science 322, 238 (2008)

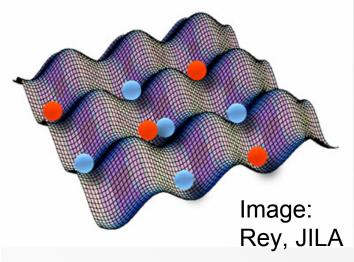


Quantum gas microscope Bakr et al.,

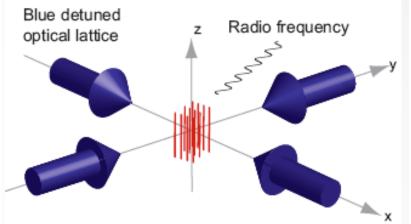
arXiv:0908.01744.



Few-Body Highlights: Optical Lattice



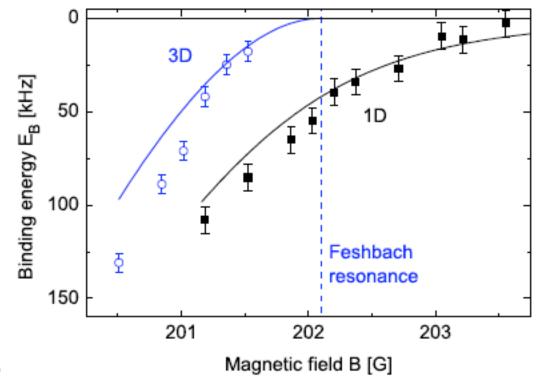
Designing effectively 1D and 2D confinement:



Palzer et al., PRL 103, 150601 (2009)

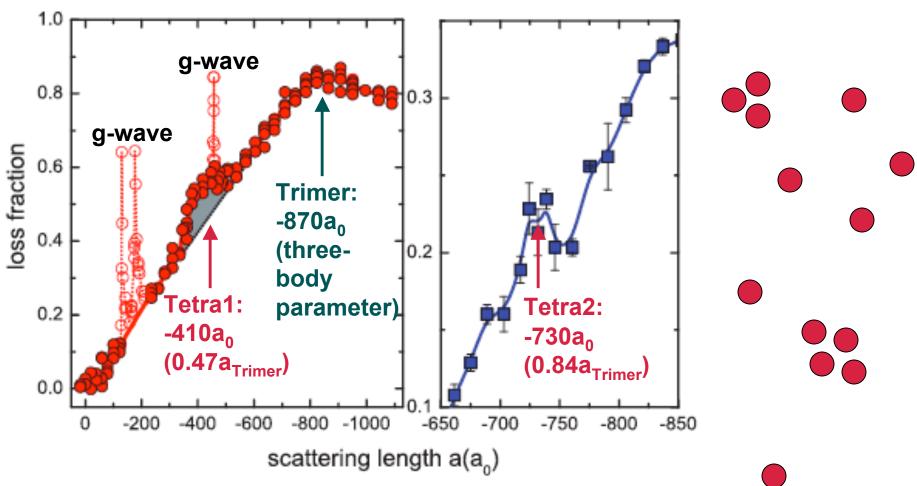
Measurement of two-body binding energy in 3D and 1D

Moritz et al.,PRL 94, 210401 (2005)



Measurement of Loss Rate for Non-Degenerate Bosonic ¹³³Cs Sample

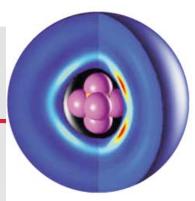
First measurement of universal 4-body physics (probe of Efimov physics) Ferlaino et al., PRL 102, 140401 (2009).



How to stabilize these delicate trimers and tetramers?

Few-Body Physics: Bridge to Macroscopic World

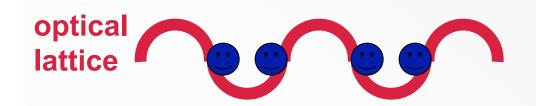
Toennies et al.,
Physics
Today 54,
31 (2001).

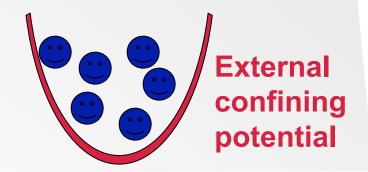


Microscopic to macroscopic:



- Other examples:
 - Doped helium clusters: Molecular rotations, microscopic superfluidity,...
 - Metal clusters: conductivity, designing materials,...
- What is special about cold atomic Bose and Fermi systems?
 - Universal behavior.
 - Much experimental progress!





Topics to be Covered

equal-mass Fermi gas unequal-mass Fermi gas Bose gas

dipolar Bose gas

Scattering theory

Monte Carlo techniques

hyperspherical framework

Stochastic variational approach

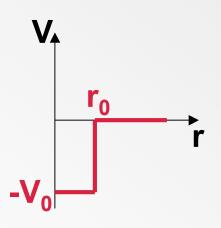
Virial expansion

Mean-field theory

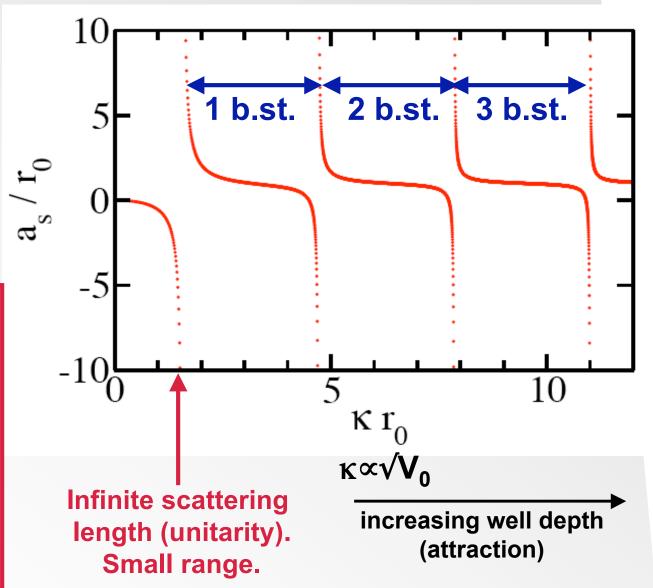
Generalized Scattering Length: Central Two-Body Interaction V(r)

- Two-particle system: Separate off CM degrees of freedom.
- Partial wave decomposition of wave function in relative coordinates: $\psi(r,\theta,\phi) = \Sigma_{lm} R_l(kr) Y_{lm}(\theta,\phi)$.
- Scaling: $u_l(kr) = kr R_l(kr)$.
- Outside: Radial solution defines phase shifts $\delta_l(k)$. $R_l(kr) = A_l(k)[j_l(kr) tan(\delta_l(k)) n_l(kr)]$.
- Generalized energy-dependent scattering lengths (SR) $a_l(k) = -tan(\delta_l(k)) / k^{2l+1}$.
- Generalized energy-independent scattering lengths $a_1 = \lim_{k\to 0} a_1(k)$.
- Inside solution: Same as bound state solution.

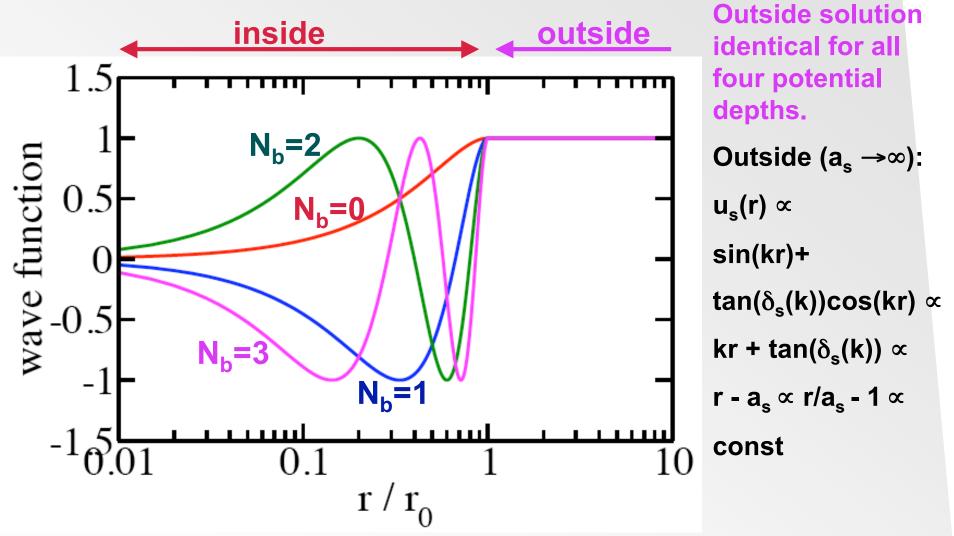
Example: Square-Well Interaction Potential



In contrast:
Hardcore potential: $a_s = r_0$ V_{\uparrow} r_0

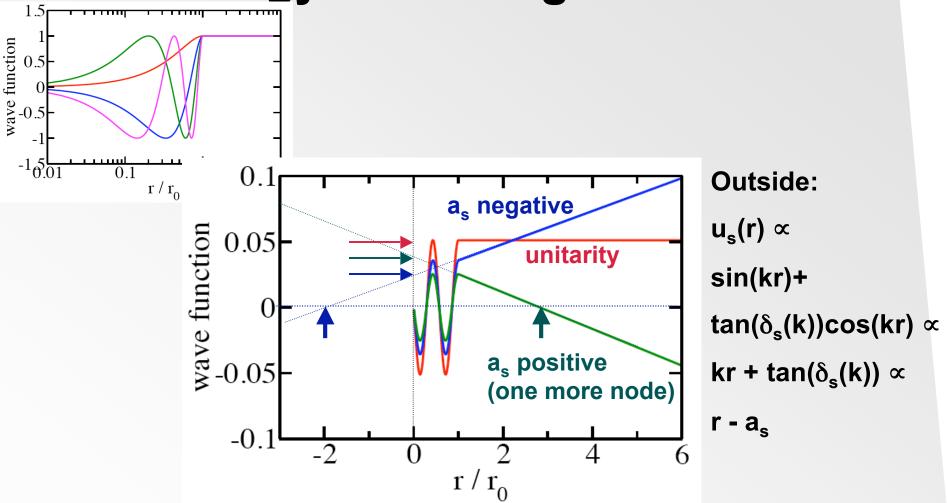


Zero-Energy Scattering Wave Function at Unitarity



Inside solution depends on details of interaction potential.

Zero-Energy Scattering Wave Function



Inside solution depends on details of interaction potential.

These details are not being probed at low temperature because...

deBroglie Wave Length: Degeneracy and Resolution

$$\lambda$$
 = h / (2 π m k_BT)^{1/2}

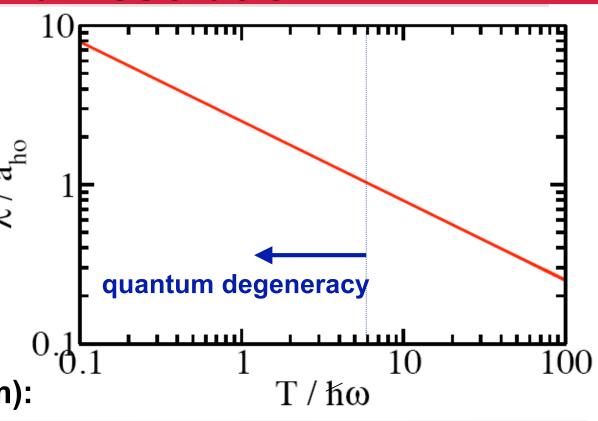
Assuming a trapped system with osc. length a_{ho} :

$$\lambda / a_{ho} = (2\pi \ hv / k_BT)^{1/2}$$

Quantum degeneracy (homogeneous system):

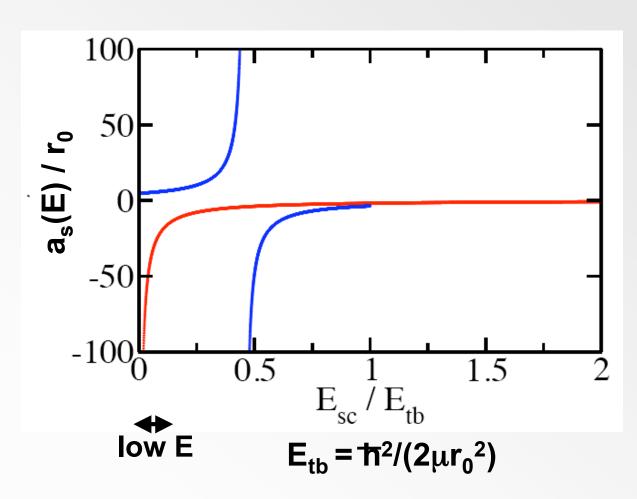
$$\lambda / < r_{ij} > > (2.6)^{1/3} \approx 1.38$$

Resolution is set by λ ($r_0 << a_{ho}, \lambda$).



Low T: Collisions are too slow to probe small r piece (high momentum piece) of wave fct. High T: Can probe small r piece of wave fct.

Temperature Determines Collision Energy



Low energy physics implies:

$$E_{sc} \ll E_{tb}$$

 $E_{bound} << E_{tb}$ (dimer size larger than range r_0)

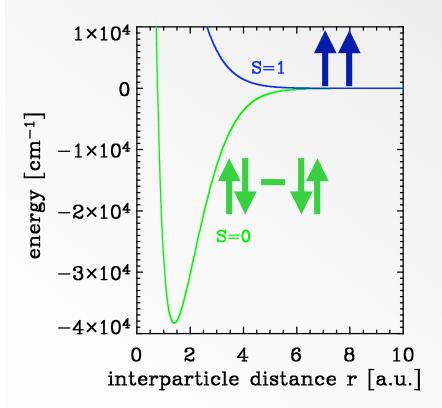
Weak binding: E_{bound} ≈ -h²/ma_s²

But: Scattering Length Determined by Coupled Channel Interaction

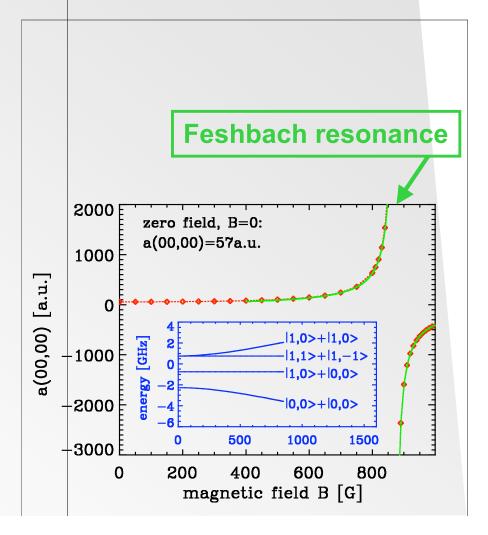
Hyperfine Hamiltonian couples singlet and triplet potential curves.

In the vicinity of Fano-Feshbach resonance, scattering length tunable

(here, tritium-tritium system).

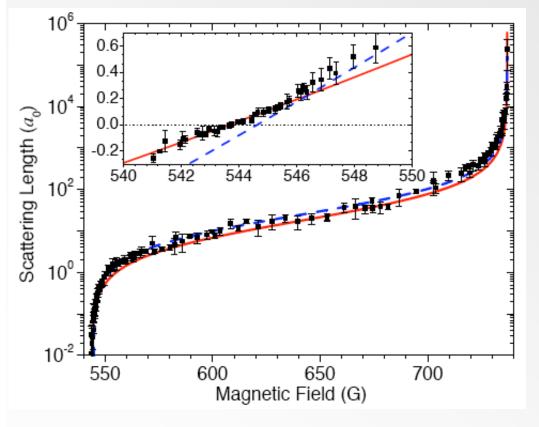


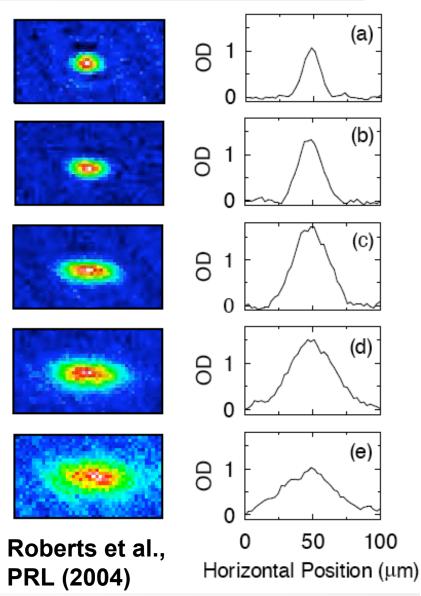
See Blume et al., PRL 89, 163402 (2002).



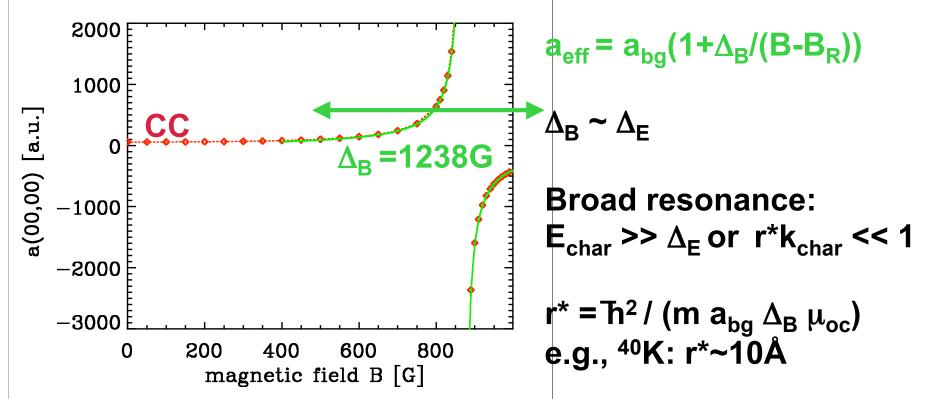
Experimental Feshbach Resonance Tuning

Extreme tunability of ⁷Li Bose gas Pollack et al., PRL 102, 090402 (2009)





Broad and Narrow Resonance: Can We Get Away With Single Channel Model?



Fermi gas in strongly-interacting regime:

k_{char} = k_F (negligible occupation of closed channel molecule)

Composite molecular Bose gas:

$$E_{char} = E_{bind}$$
, $k_{char} = 1/a_{s}$

Physics Determined by s-Wave Scattering Length

- Reaching quantum degeneracy requires thermalization.
- Efficient thermalization requires finite a_s.
- No thermalization for single-component Fermi gas.

Three examples:

- 1. Gas-like states of trapped two-particle system are determined by s-wave scattering length a_s.
- 2. Stability/instability of Bose gas determined by scattering length.
- 3. Stability/instability of multi-component Fermi gas determined by scattering length plus Fermi pressure (Pauli exclusion principle).

1. Two-Particle System: Replace Atom-Atom Interaction by ZR Interaction

- Start with ab initio atom-atom potential.
- Coupled channel calculation provides phase shifts $\delta_l(k)$.
- Construct zero-range pseudo-potential with same a_s (outside solution):

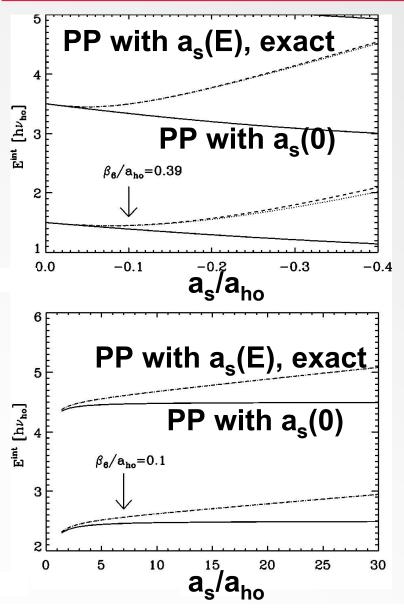
$$V(\vec{r}) = \frac{4\pi \, \hbar^2 \, \operatorname{a_s}}{m} \delta^{(3)}(\vec{r}) \frac{\partial}{\partial r} r$$

Cures 1/r divergence of radial function (specific to 3D)

Analytical treatments

[Huang and Yang, PR 105, 767 (1957)]

1. Two Particles under External Harmonic Confinement



- Two-particle energy spectrum known semi-analytically: Simple transcendental equation [Busch et al., Found. of Physics (1998)].
- Self-consistent solution when a_s=a_s(E) [Blume and Greene, PRA 65,043613 (2002); see also Bolda et al. (PRA, 2002)].
- Energy-independent pseudopotential, I.e., use of $a_s(0)$, works if $|a_s| << a_{ho}$.
- Energy-dependent pseudopotential, I.e., use of a_s(E), works if r_{vdW}<<a_{ho}.

2. Stability of Bose Gas Under Harmonic Confinement

N bosons in a box. Constant density. Periodic boundary conditions. Positive scattering length: Stable gas (not self-bound).

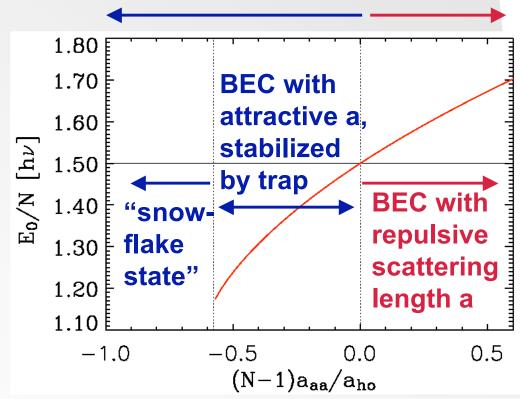
Negative scattering length: Gas not stable; collapse toward solid or liquid (self-bound).

Bosonic atoms in harmonic trap (mean-field GP treatment):

Positive scattering length: Effectively repulsive interaction.

Negative scattering length: Effectively attractive interaction.

Dodd et al., PRA 54, 661 (1996)

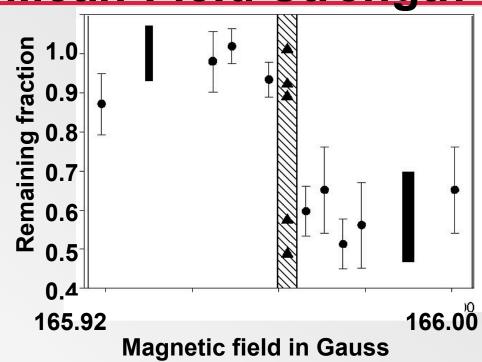


2. Experiments with Bosonic 85Rb: Probing Critical Mean-Field Strength

Roberts et al., PRL 86, 4211 (2001)

- Mean-field prediction confirmed by experiment.
- Underlying physical mechanism? Threebody recombination.

Physical picture?
 Connection between
 MF GP eq. and many-body Hamiltonian?



more negative a_s

$$\uparrow$$
 (N-1)a_s/a_{ho} ~ -0.58

2. Mean-Field Equation Derived from Many-Body Hartree Wave Function

Many-body Hamiltonian for N bosons under confinement:

$$H = \sum_{j=1}^{N} \left[\frac{-\hbar^2}{2m} \nabla_{\vec{r}_j}^2 + \frac{1}{2} m \omega^2 \vec{r}_j^2 \right] + \sum_{j < k}^{N} V_{aa} (\vec{r}_j - \vec{r}_k)$$
SW, HS,...

Hartree product (restricted Hilbert space):

$$\psi(\vec{r}_1, \dots, \vec{r}_N) = \prod_{i=1}^{N} \phi_a(\vec{r}_i)$$

ZR atom-atom potential:

$$V_{aa}(\vec{r}) = \frac{4\pi \hbar^2 a_{aa}}{m} \delta^{(3)}(\vec{r}) \propto U_{aa} \delta^{(3)}(\vec{r})$$

Gross-Pitaevskii (GP) equation for "single atom":

$$\left(-\frac{1}{2}\nabla_{\vec{r}}^2 + \frac{1}{2}\vec{r}^2 + U_{aa}(N-1)|\phi_a(\vec{r})|^2\right)\phi_a(\vec{r}) = \epsilon_a\phi_a(\vec{r})$$

Single atom feels effective potential/mean-field created by the other N-1 atoms.

2. Mechanical Instability or Collapse of Trapped Bose Gas

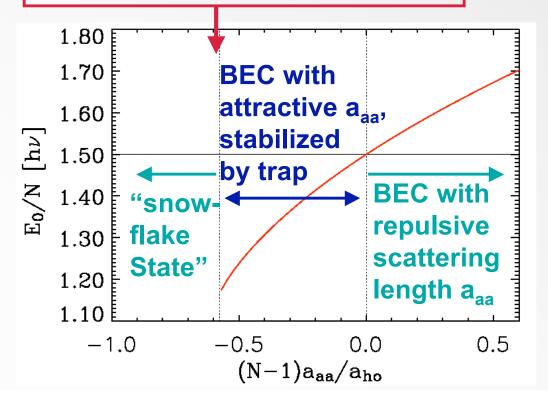
$$\left(-\frac{1}{2}\nabla_{\vec{r}}^2 + \frac{1}{2}\vec{r}^2 + U_{aa}(N-1)|\phi_a(\vec{r})|^2\right)\phi_a(\vec{r}) = \epsilon_a\phi_a(\vec{r})$$

1 parameter

Single particle orbital

Non-linearity





Why does ZR potential work?

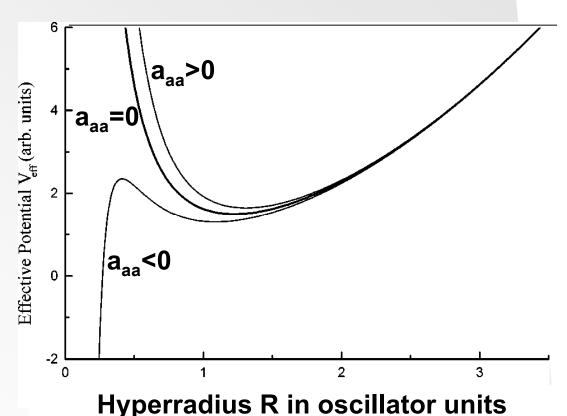
At collapse point, $n(0)|a_{aa}|^3 <<1$ (small parameter; long wave length approximation justified).

2. Interpretation within Hyperspherical Framework: Linear Schroedinger Eq.

- Coordinates: 1 hyperradius R, (3N-4) hyperangles Ω .
- Many-body symmetrized variational wave function: $F(R)\Phi(\Omega)$.
- Sum of two-body delta-function interactions.
- Effective potential: $V_{eff}(R) = c_1/R^2 + c_2R^2 + c_3a_{aa}/R^3$

Collapse prediction within ~20% of GP equation and experiment.

Bohn, Esry and Greene, PRA 58, 584 (1998)



2. Hyperspherical Coordinates: Three Step Approach

$$M=Nm \ \Psi_{NI}(ec{r}_1,\ldots,ec{r}_N)= G(ec{R}_{CM})F(R)\Phi(ec{\Omega}) \ R^2=rac{1}{N}\sum_{i=1}^N (ec{r}_i-ec{R}_{CM})^2$$

$$H_{NI} = H_{CM} - rac{\hbar^2}{2M} \left(rac{\partial^2}{\partial R^2} + rac{3N - 4}{R}rac{\partial}{\partial R}
ight) + rac{\Lambda^2}{2MR^2} + rac{1}{2}M\omega^2R^2$$

$$H_{CM}=rac{-\hbar^2}{2M}ec
abla^2_{CM}+rac{1}{2}M\omega^2R_{CM}^2$$
 1: Remove CM degrees of freedom.

2: Solve hyperangular equation (gives $V_{eff}(R)$).

$$\Lambda^2\Phi_{\lambda,\mu}(ec\Omega)=\hbar^2\lambda(\lambda+3N\!\!-\!\!5)\Phi_{\lambda,\mu}(ec\Omega)$$

3: Solve hyperradial equation.

With interactions: delta-function interactions can be treated analytically for **lowest hyperspherical** harmonic.

3. Similarly: Analyze Stability of Multi-Component Fermi Gases

- Simple variational wave function (ideal gas nodal surface) applied to multi-component Fermi gas with "bare" zero-range interactions (all s-wave scattering lengths equal) predicts collapse at:
 - 2-component gas: $(k_F a_{aa})^3 \sim -1.81$ (not small compared to 1)
 - 3-component gas: $(k_F a_{aa})^3 \sim -0.23$
 - 4-component gas: $(k_F a_{aa})^3 \sim -0.067$ (small compared to 1)
- However: Two-component Fermi gas is found to be stable (experiment plus Monte Carlo).

How many components are needed to get instability? Proper theoretical framework?

Multi-component Fermi gas with one atom per component (Bose gas): Unstable at unitarity.

3. Two-Component Fermi Gas: Renormalization of Interaction

- Many-body anti-symmetrized wave function: $F(R)\Phi(\Omega)$.
- Effective potential: $V_{eff}(R) = c_1/R^2 + c_2R^2 + c_3k_Fa_{aa}/R^3$

At collapse point, $k_F|a_{aa}|\sim 1$. ZR potential no longer applicable.

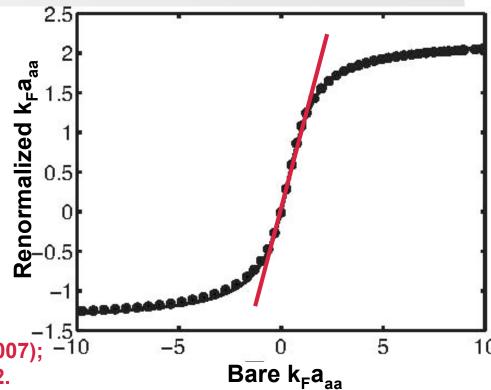
Renormalize $k_F|a_{aa}|$ so as to reproduce two-particle spectrum.

Use renormalized $k_F|a_{aa}|$ in hyperspherical framework.

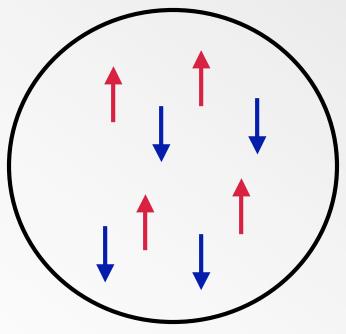
Rittenhouse, Cavagnero, von Stecher and Greene, PRA 74, 053624 (2006);

von Stecher and Greene, PRA 75, 022716 (2007) Rittenhouse and Greene, physics/0702161v2.

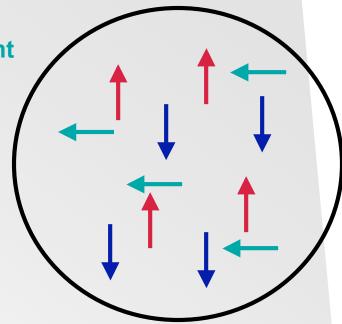
Renormalized ZR potential: For $|a_{aa}| \rightarrow \infty$: const/R²



3. Why Collapse for More Components? "Counting Argument"



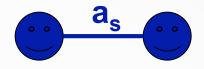
Add a third component (equal spins: non-interacting; unequal spins: attractive interaction)



Fermi statistics (repulsion): 12 equal spin pairs.

Attraction:

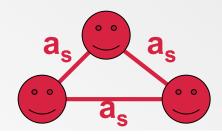
16 unequal spin pairs.



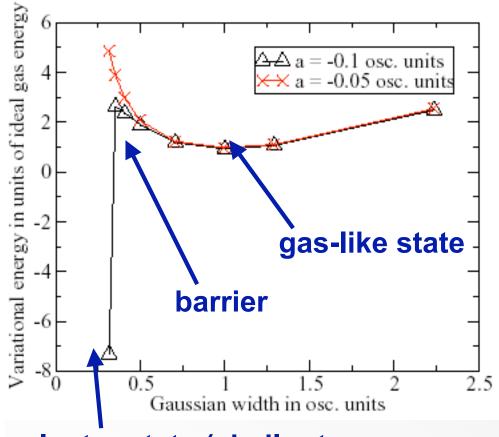
Fermi statistics (repulsion): 18 equal spin pairs.

Attraction:

48 unequal spin pairs.

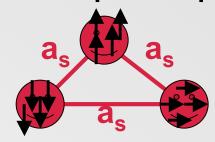


3. Many-Body Variational MC Treatment of Three-Component Fermi System



cluster state (similar to Bose gas with negative scattering length)

Four fermions per component:



- Square well interaction potential with range r₀=0.01a_{ho}.
- Variational wave function with one parameter b that determines size: exp(-0.5(r/b)²)
- Negative energy state exists if |a_{aa}| "large".
- Peak of barrier at length scale a few times |a_{aa}|, |a_{aa}|<<r₀.

Blume, Rittenhouse, von Stecher, Greene, PRA 77, 032703 (2008).

Summary and Outlook

- Broad introduction to cold atom physics: Many experiments and strong interactions among people from different communities.
- Revival of few-body physics: Largely due to Efimov physics (fourth lecture).
- Connections between microscopic and macroscopic worlds: Stability of Bose and Fermi gases within manybody framework.
- Next lecture:
 - Few-body techniques and calculations.

General Summary of Field of Cold Atom Physics

- Interaction strengths can be controlled (Fano-Feshbach resonance).
- Confinement can be designed (lattice, quasi-1d,...).
- Fundamental physics question:
 - Strongly-interacting system.
 - Multi-component systems.
 - Equal- and unequal-mass systems.
 - Efimov physics.
 - Dipolar systems.

Applications:

- High precision measurements of fundamental constants.
- Navigational devices.
- Quantum computation and quantum simulation.