Structure of Ultracold Trapped Fermi and Bose Gases

Robert Roth

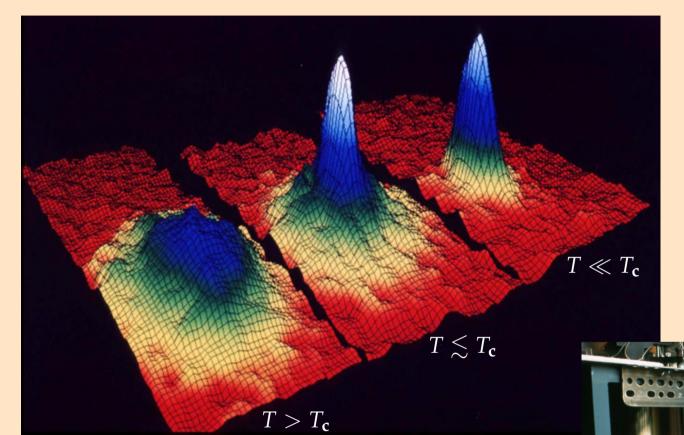
Gesellschaft für Schwerionenforschung
Darmstadt

12. November 2001 Universität Osnabrück

Overview

- The World of Trapped Ultracold Atomic Gases
- Theoretical Description of Trapped Ultracold Gases
 - The Many-Body Problem
 - Correlations & Effective Interaction
 - Mean-Field & Thomas-Fermi Approximation
 - Energy Functional
- Structure of a Trapped Degenerate Fermi Gas
 - Energy Landscapes & Density Profiles
 - Mean-Field Induced Collapse
 - Component Separation
 - Phase Diagram

BEC of Rubidium Atoms

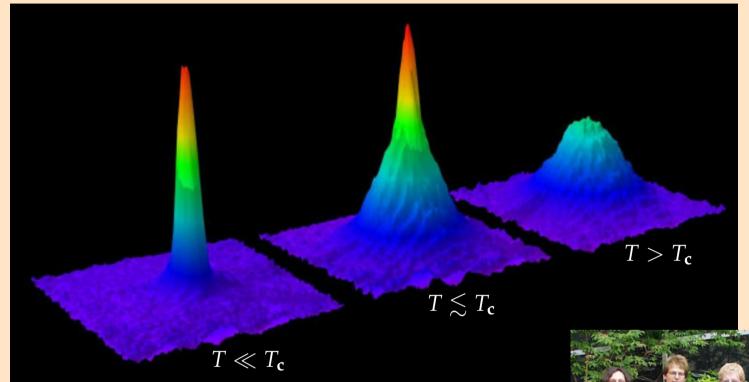


- 87 Rb $(F=2, m_F=2)$
- $N_{\rm initial} \approx 10^6$
- $N_{\rm BEC} \approx 2000$
- $T_{\rm c} \approx 170 {\rm nK}$
- absorption image after 60 ms expansion
- 0.2mm $\times 0.27$ mm

E. Cornell, C. Wieman, et al.(JILA, NIST, U of Colorado)Nobel Prize in Physics 2001

Cambridge / Massachusetts — September 1995

BEC with Sodium Atoms



- 23 Na $(F=1, m_F=-1)$
- $N_{\rm initial} \approx 10^9$
- $N_{\rm BEC} \approx 5 \times 10^5$
- $T_{\rm c} \approx 2 \,\mu{\rm K}$
- absorption image after 60 ms expansion
- 1mm × 1mm

W. Ketterle, et al. (MIT)

Nobel Prize in Physics 2001

Ultracold Atomic Gases

Why are they so Attractive...

a macroscopic system which exhibits quantum properties

large composite bosons/fermions



meta stable many-body state

interatomic interactions are "weak"

BE condensation $T_{\rm BEC} \sim \mu {\rm K}$

all relevant quantities are observable & tunable

size, density, particle number, mass, statistic, composition, temperature, distributions, interaction strength...

realization of a dilute quantum gas

BCS transition $T_{\rm BCS} \sim {\rm nK}$

Experimentalists' Toolbox

Trapping

- magneto-optical trap: absorption of counterpropagating photons and reemission leads to net restoring force
- magnetic trap: inhomogeneous magnetic field couples to the magnetic moment of the atoms; trapped in field minimum
- optical traps

Cooling

- Doppler cooling: atom absorbs a red detuned photon and reemits an onresonance photon; energy difference is paid with kinetic energy
- **evaporative cooling**: selective removal of high-energy atoms and thermalization results in lower temperature of the remanent

Imaging

- resonance absorption: shine resonant laser onto the cloud and observe shadow
- phase-contrast: use off-resonant laser and observe interference of scattered and unscattered light
- **ballistic expansion**: momentum distribution can be determined

Manipulation

- Feshbach resonances allow tuning of the strength of inter-atomic interactions (scattering length) over a wide range
- **optical tools**: e.g. focused blue detuned lasers 'repel' the atoms and can be used to cut or stir the gas

Trapped Degenerate Fermi Gas

Science 285 (1999) 1703

Onset of Fermi Degeneracy in a Trapped Atomic Gas

B. DeMarco and D. S. Jin*†

An evaporative cooling strategy that uses a two-component Fermi gas was employed to cool a magnetically trapped gas of 7×10^5 ⁴⁰K atoms to 0.5 of the Fermi temperature $T_{\rm F}$. In this temperature regime, where the state occu-

the lowest energies has increased from essentially zero

cooling a cloud of neutral $^{40}{\rm K}$ atoms kept in a magnetic trap

tive cooling and as a modification of the total spin: fermion

$$F = 4 \pm 1/2 = \frac{9}{2}, \frac{7}{2}$$

two-component mixture

$$\left|F = \frac{9}{2}, m_F = \frac{9}{2}\right\rangle$$

 $\left|F = \frac{9}{2}, m_F = \frac{7}{2}\right\rangle$

 $N \approx 10^5 ... 10^6$

$$\rho \approx 10 \, \mu \text{m}^{-3}$$

$$\ell \approx 1 \,\mu\mathrm{m}$$

$$\tau \approx 300 \,\mathrm{s}$$

$$T \approx 300 \,\mathrm{nK}$$

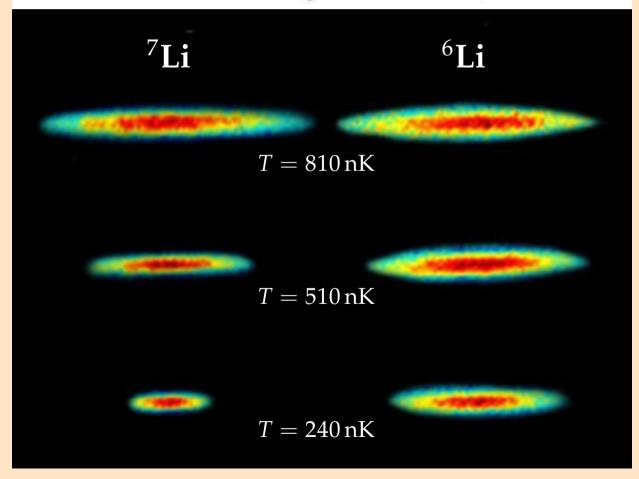
 $\approx 0.5 \,\varepsilon_F$

Degenerate Boson-Fermion Mixtures

Science 291 (2001) 2570

Observation of Fermi Pressure in a Gas of Trapped Atoms

Andrew G. Truscott, Kevin E. Strecker, William I. McAlexander,*
Guthrie B. Partridge, Randall G. Hulet†



simultaneous trapping of

⁷Li
$$(F = 2)$$
 ⇒ boson
⁶Li $(F = \frac{3}{2})$ ⇒ fermion

evaporative cooling of the bosons → sympathetic cooling of the fermions

$$N_{\rm B} \approx N_{\rm F} \approx 10^5 \dots 10^6$$

$$T \approx 240 \,\mathrm{nK}$$

 $\approx 0.25 \,\varepsilon_F$

Theoretical Description of Trapped Ultracold (Fermi) Gases

- The Many-Body Problem
- Correlations & Effective Interaction
- Mean-Field & Thomas-Fermi Approximation
- Energy Functional

Route Through the Many-Body Problem

Hamiltonian

$$\mathbf{H} = \sum_{i} U(\vec{\mathbf{x}}_i) + \frac{1}{2m} \sum_{i} \vec{\mathbf{p}}_i^2 + \sum_{i < j} \mathbf{V}_{ij}$$



Model Space

mean-field states: product of single-particle states

Energy Functional

energy expectation value as functional of the density

Thomas-Fermi Approx.

neglect all gradients of the density in the energy functional

Functional Variation

ground state density is obtained by energy minimization

Short-Range Correlations

Interaction

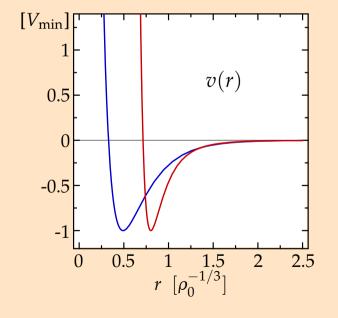
many realistic two-body interactions show a strong short-range repulsion (e.g. nucleon-nucleon & van der Waals interactions)

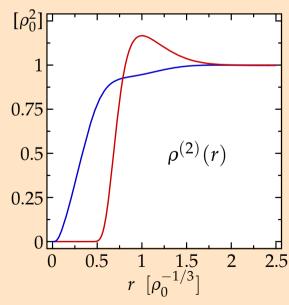
Correlations

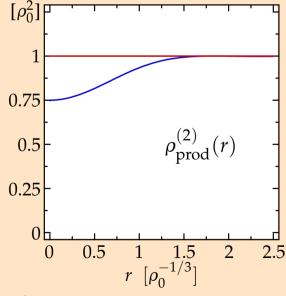
core induces strong short-range correlations in many-body state (e.g. correlation hole in two-body density)

Product States

short-range correlations cannot be described by product-type states (e.g. mean-field, superposition of few product states,...)







nuclear matter

$$\rho_0 = 0.17 \, \mathrm{fm}^{-3}$$

liquid ⁴He (bosonic)

$$\rho_0 = 0.022 \,\text{Å}^{-3}$$

The Problem

Short-Range Correlations

Interaction

many realistic two-body interactions show a strong short-range repulsion (e.g. nucleon-nucleon & van der Waals interactions)

Correlations

core induces strong short-range correlations in many-body state (e.g. correlation hole in two-body density)

Product States

short-range correlations cannot be described by product-type states (e.g. mean-field, superposition of few product states,...)

Effective Interaction

replace the full potential by a tamed effective interaction

Effective Contact Interaction

Correlated States

include correlations in many-body model-space

A Suitable Effective Interaction...

system is very dilute and cold

$$ho^{-1/3}\gg$$
 range of interaction $q^{-1}\gg$ range of interaction

treat the many-body problem in a restricted **model-space** that does not contain correlations

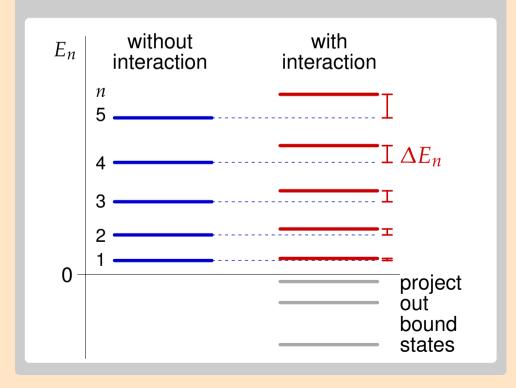
looking for the structure of **non-selfbound states** in an external potential

hermitean interaction operator that obeys standard symmetries (translation, rotation,...)

Effective Contact Interaction (ECI)

- zero-range potential (for each partial wave)
- expectation value in two-body modelstates equals the energy shift induced by the full interaction

$$\langle \phi_n^{\text{mod}} | \mathbf{v}^{\text{ECI}} | \phi_n^{\text{mod}} \rangle \stackrel{!}{=} \Delta E_n$$



Construction of the ECI

Energy Shift

• relative two-body wave function w/o and with interaction for r > range of v(r)

$$\phi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\vartheta, \varphi)$$

$$R_{nl}(r) \propto j_l(q_{nl}r)$$

$$\bar{R}_{nl}(r) \propto j_l(\bar{q}_{nl}r) - \tan \eta_l(\bar{q}_{nl}) n_l(\bar{q}_{nl}r)$$

• auxiliary boundary condition $R_{nl}(\Lambda) = 0$ to obtain discrete momentum spectrum

$$q_{nl}\Lambda = \pi(n + \frac{l}{2})$$

 $\bar{q}_{nl}\Lambda = \pi(n + \frac{l}{2}) - [\eta_l(\bar{q}_{nl}) - \pi n_l^{\text{bound}}]$

momentum shift

$$\Delta q_{nl} \Lambda = (\bar{q}_{nl} - q_{nl}) \Lambda$$

$$= -[\eta_l(q_{nl}) - \pi n_l^{\text{bound}}] =: -\hat{\eta}_l(q_{nl})$$

• relative energy shift

$$\frac{\Delta E_{nl}}{E_{nl}} = -\frac{2}{q_{nl}\Lambda} \,\,\hat{\eta}_l(q_{nl})$$

Interaction Operator

 ansatz for a nonlocal contact interaction for the lth partial wave

$$\mathbf{v}_{l}^{\text{ECI}} = (\vec{\mathbf{q}} \cdot \frac{\vec{\mathbf{r}}}{\mathbf{r}})^{l} g_{l} \delta^{(3)}(\vec{\mathbf{r}}) (\frac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}})^{l}$$

$$= \int d^{3}r |\vec{r}\rangle \frac{\overleftarrow{\partial}^{l}}{\partial r^{l}} g_{l} \delta^{(3)}(\vec{r}) \frac{\overleftarrow{\partial}^{l}}{\partial r^{l}} \langle \vec{r}|$$

 expectation value in non-interacting twobody states

$$\langle \phi_{nlm} | \mathbf{v}_l^{\text{ECI}} | \phi_{nlm} \rangle \stackrel{!}{=} \Delta E_{nl}$$

• interaction strengths g_l determined by $\hat{\eta}_l(q)$

$$g_l = -\frac{4\pi}{2\mu} \left[\frac{(2l+1)!!}{l!} \right]^2 \frac{\hat{\eta}_l(q)}{q^{2l+1}}$$

• parametrization of $\hat{\eta}_l(q)$ in terms of the scattering lengths a_l for $|q \, a_l| \ll 1$

$$g_l = \frac{4\pi}{2\mu} \frac{(2l+1)}{(l!)^2} a_l^{2l+1} + \mathcal{O}(q^2)$$

Trapped Degenerate Fermi Gas

- trapped gas of Ξ distinguishable fermionic species ($\xi = 1,...,\Xi$) interacting via the sand p-wave contact interaction
- for simplicity: equal trapping potentials and s- and p-wave scattering lengths, a_0 and a_1 , for all components

Hamiltonian

$$\mathbf{H} = \sum_{i} U(\vec{\mathbf{x}}_{i}) + \frac{1}{2m} \sum_{i} \vec{\mathbf{p}}_{i}^{2} + \frac{4\pi a_{0}}{m} \sum_{i < j} \delta^{(3)}(\vec{\mathbf{r}}_{ij}) + \frac{12\pi a_{1}^{3}}{m} \sum_{i < j} \left(\vec{\mathbf{q}}_{ij} \cdot \frac{\vec{\mathbf{r}}_{ij}}{\mathbf{r}_{ij}}\right) \delta^{(3)}(\vec{\mathbf{r}}_{ij}) \left(\frac{\vec{\mathbf{r}}_{ij}}{\mathbf{r}_{ij}} \cdot \vec{\mathbf{q}}_{ij}\right)$$
trap kinetic s-wave p-wave

Mean-Field States (homogeneous)

• N-body state $|\Psi\rangle$ is an antisymmetrized product of single-particle momentum eigenstates $|\vec{k}_i, \xi_i\rangle$

$$|\Psi\rangle = \mathcal{A} \left(|\vec{k}_1, \xi_1\rangle \otimes \cdots \otimes |\vec{k}_N, \xi_N\rangle \right)$$

• for each component ξ all momenta $|\vec{k}|$ up to the **Fermi momentum** κ_{ξ} appear

Thomas-Fermi Approximation

 energy density of the trapped gas is locally given by the energy density of the homogeneous system

$$\mathcal{E}_{\text{hom}}(\kappa_1,...,\kappa_{\Xi}) = \frac{1}{V} \langle \Psi | \mathbf{H}_{\text{hom}} | \Psi \rangle$$

• i.e. the Fermi momenta κ_{ξ} are replaced by local Fermi momenta $\kappa_{\xi}(\vec{x})$

Energy-Density for Trapped Fermions

Single-Component System

$$\mathcal{E}_{1}[\kappa](\vec{x}) =$$

$$= \frac{1}{6\pi^{2}} U(\vec{x}) \kappa^{3}(\vec{x})$$

$$+ \frac{1}{20\pi^{2}m} \kappa^{5}(\vec{x})$$

$$\star$$

$$+ \frac{a_{1}^{3}}{30\pi^{3}m} \kappa^{8}(\vec{x})$$

Two-Component System

$$\mathcal{E}_{2}[\kappa_{1},\kappa_{2}](\vec{x}) =$$

$$= \frac{1}{6\pi^{2}}U(\vec{x})\left[\kappa_{1}^{3}(\vec{x}) + \kappa_{2}^{3}(\vec{x})\right]$$

$$- \text{kinetic} - \frac{1}{20\pi^{2}m}\left[\kappa_{1}^{5}(\vec{x}) + \kappa_{2}^{5}(\vec{x})\right]$$

$$- \text{s-wave} - \frac{a_{0}}{9\pi^{3}m} \kappa_{1}^{3}(\vec{x}) \kappa_{2}^{3}(\vec{x})$$

$$- \text{p-wave} - \frac{a_{1}^{3}}{30\pi^{3}m} \left[\kappa_{1}^{8}(\vec{x}) + \kappa_{2}^{8}(\vec{x}) + \kappa_{2}^{8}(\vec{x}) + \frac{1}{2}\kappa_{1}^{3}(\vec{x}) \kappa_{2}^{5}(\vec{x}) + \frac{1}{2}\kappa_{1}^{5}(\vec{x}) \kappa_{2}^{3}(\vec{x})\right]$$

energy expectation value

$$E[\kappa_1, ..., \kappa_{\Xi}] = \int d^3x \ \mathcal{E}_{\Xi}[\kappa_1, ..., \kappa_{\Xi}](\vec{x}) \qquad \qquad \rho_{\xi}(\vec{x}) = \frac{1}{6\pi^2} \kappa_{\xi}^3(\vec{x})$$

density

—— trap ——

$$\rho_{\xi}(\vec{x}) = \frac{1}{6\pi^2} \kappa_{\xi}^3(\vec{x})$$

particle number

$$N_{\xi}[\kappa_{\xi}] = \int \!\! \mathrm{d}^3 x \; \rho_{\xi}(\vec{x})$$

Ground State — Variationally

Functional Variation

minimization of the energy $E[\kappa_1, ..., \kappa_{\Xi}]$ for fixed numbers of particles $N_1, ..., N_{\Xi}$ gives the ground state density profile

- **chemical potentials**: implement constraints on the particle numbers via a set of Lagrange multipliers $\mu_1, ..., \mu_{\Xi}$
- unconstraint minimization of the transformed energy functional

$$F[\kappa_1, ..., \kappa_{\Xi}] = E[\kappa_1, ..., \kappa_{\Xi}] - \sum_{\xi=1}^{\Xi} \mu_{\xi} N_{\xi} [\kappa_{\xi}]$$
$$= \int d^3 x \, \mathcal{F}_{\Xi}[\kappa_1, ..., \kappa_{\Xi}](\vec{x})$$

 stationary points of the energy density are solutions of the Euler-Lagrange equations

$$\frac{\partial}{\partial \kappa_{\xi}(\vec{x})} \mathcal{F}_{\Xi}[\kappa_1,...,\kappa_{\Xi}](\vec{x}) = 0$$
, $\forall \xi$

• since \mathcal{F}_{Ξ} is local (does not depend on gradients) the ground state has to minimize \mathcal{F}_{Ξ} for each \vec{x}

Recipe

ground-state densities at some \vec{x} are given by the minimum of the transformed energy density $\mathcal{F}[\kappa_1,...\kappa_{\Xi}](\vec{x})$ for this \vec{x}

Structure of a Trapped Degenerate Two-Component Fermi Gas

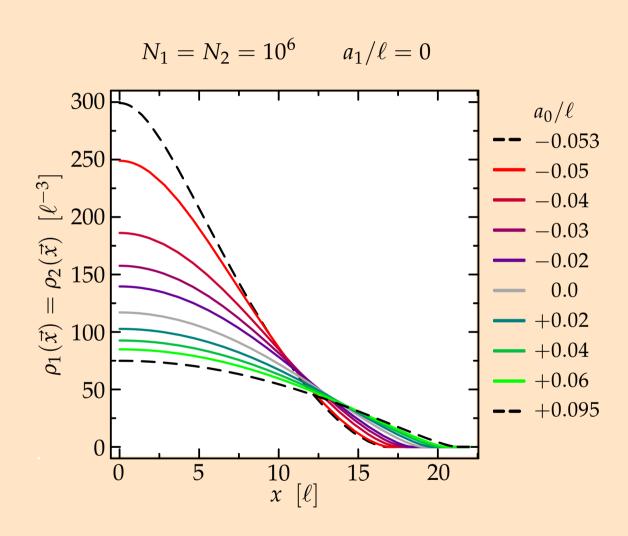
- Energy Landscapes & Density Profiles
- Mean-Field Induced Collapse
- Component Separation
- Phase Diagram

Two-Component Fermi Gas Density Profiles

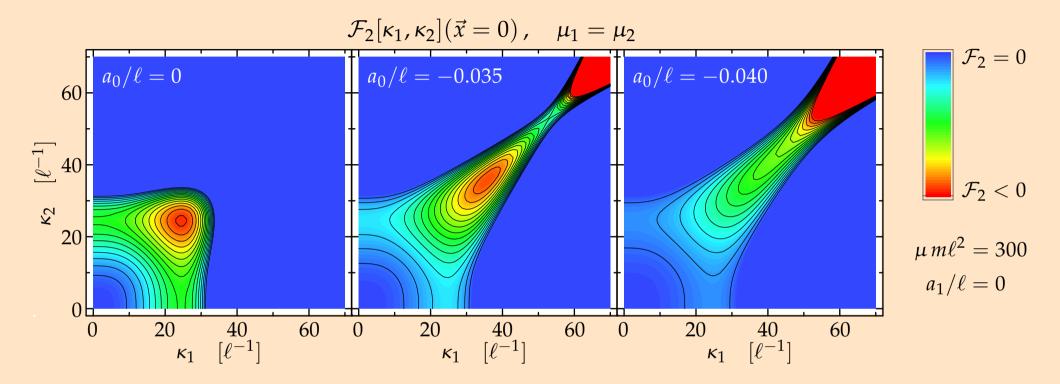
 assume a spherical symmetric parabolic trapping potential

$$U(\vec{x}) = \frac{m\omega^2}{2} \ x^2 = \frac{1}{2m\ell^4} \ x^2$$

- determine the densities for μ_1 , μ_2 chosen such that the desired particle numbers are reproduced
- $a_0 > 0$: repulsive interactions flatten the density profile
- $a_0 < 0$: attractive interactions enhance the central density
- outside a certain range of scattering lengths a_0 no solutions of this type exist anymore



Energy-Density Landscape: $a_0 < 0$

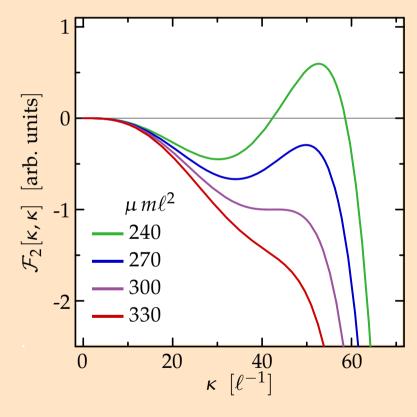


- minimum of \mathcal{F}_2 is only local for attractive interactions ($a_0 < 0$ or $a_1 < 0$)
- NB: physically the state is only metastable for all signs of the scattering lengths
- local minimum vanishes if the attractive s-wave interaction exceeds a critical strength

attractive interactions can induce a **collapse** of the Fermi gas towards high densities

Collapse — Stability Condition

$$\mathcal{F}_{2}[\kappa,\kappa](\vec{x}) = \frac{1}{3\pi^{2}} \left[U(\vec{x}) - \mu \right] \kappa^{3}(\vec{x}) + \frac{1}{10\pi^{2}m} \kappa^{5}(\vec{x}) + \frac{a_{0}}{9\pi^{3}m} \kappa^{6}(\vec{x}) + \frac{a_{1}^{3}}{10\pi^{3}m} \kappa^{8}(\vec{x}) \right]$$



$$a_0/\ell = -0.037$$
, $a_1/\ell = 0$, $\vec{x} = 0$

- onset of instability is indicated by the appearance of a saddle point in the energy density,
 i.e., a vanishing first and second derivative
- stability condition: metastable states exist only for

$$\mu < \mu_{\rm cr}(a_0, a_1)$$
 and $\kappa(\vec{x}) < \kappa_{\rm cr}(a_0, a_1)$

 the critical Fermi momentum and the critical chemical potential are given by

$$-2 a_0 \kappa_{\rm cr} - 4 (a_1 \kappa_{\rm cr})^3 = \pi$$

$$m \,\mu_{\rm cr} = \frac{1}{2} \,\kappa_{\rm cr}^2 + \frac{2 \,a_0}{3\pi} \,\kappa_{\rm cr}^3 + \frac{8 \,a_1^3}{15\pi} \,\kappa_{\rm cr}^5$$

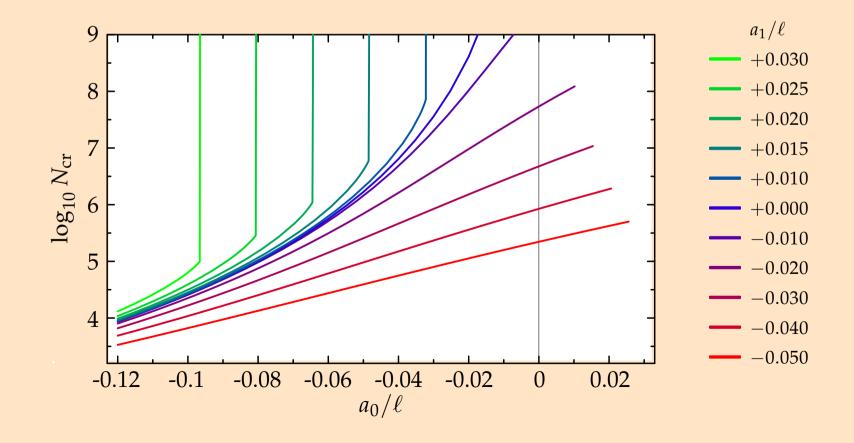
Collapse — Critical Particle Number

- ullet assume parabolic trapping potential with mean oscillator length ℓ
- obtain the density profile for the critical chemical potential $\mu_{\rm cr}$ and calculate $N_{\rm cr}$

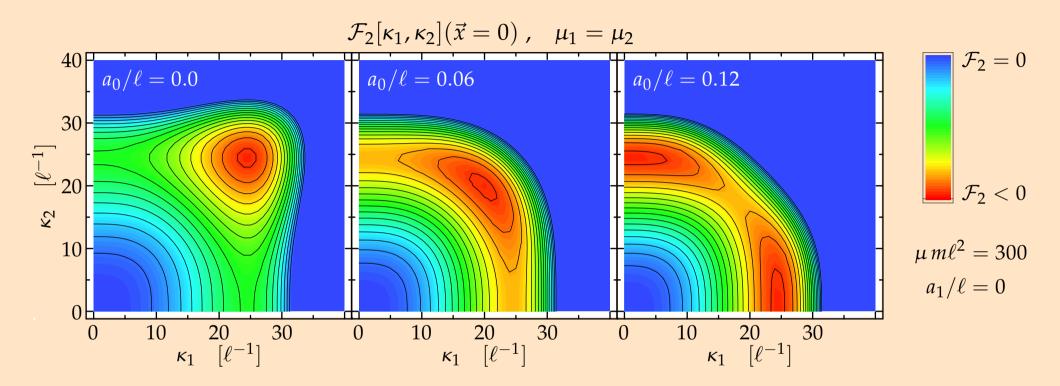
abs. stabilization due to p-wave repulsion $a_1/|a_0| > 2/(3\pi^{2/3})$

p-wave attraction lowers critical particle number substantially

p-wave induced collapse and interference with separation



Energy-Density Landscape: $a_0 > 0$



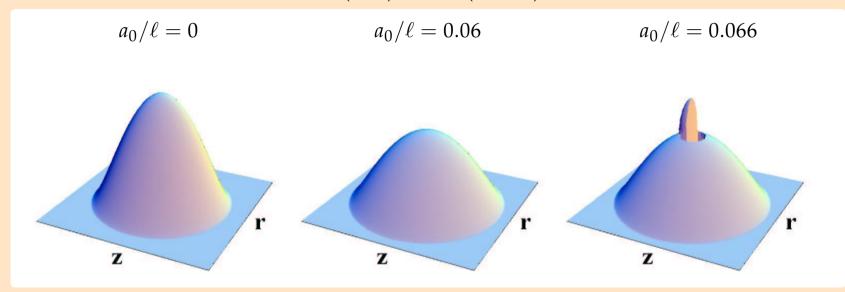
- overlapping configuration: for moderate repulsive s-wave interactions a unique minimum exists at $\kappa_1 = \kappa_2$
- **separation**: beyond a critical interaction strength two separate minima emerge at

$$\kappa_1 = 0, \ \kappa_2 > 0$$
 and $\kappa_1 > 0, \ \kappa_2 = 0$

repulsive interactions can induce a spatial **separation** of the two components

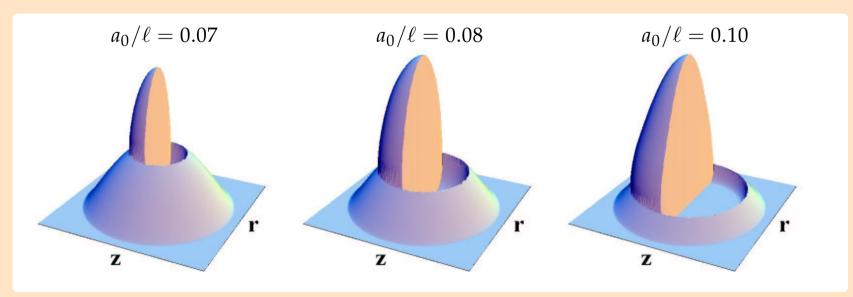
Separation — Density Distributions

$$\rho_1(r,z) = \rho_2(r,-z)$$



$$N_1 = N_2 = 10^7$$

$$a_1/\ell = 0$$



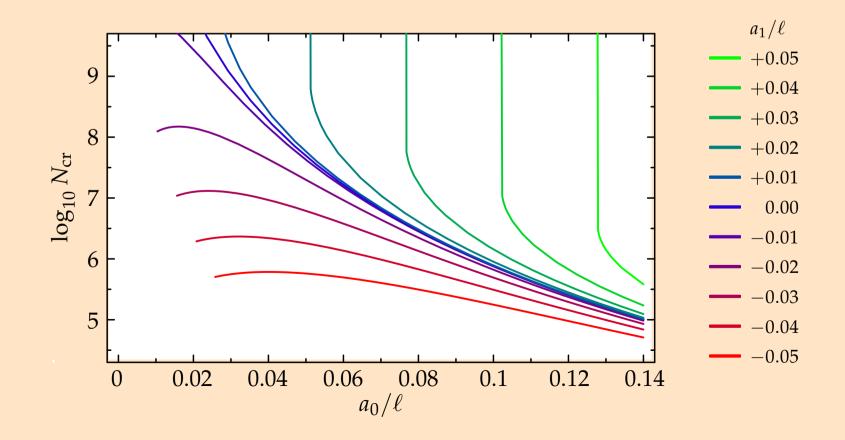
Separation — Critical Particle Number

- ullet assume parabolic trapping potential with mean oscillator length ℓ
- obtain the density profile for the critical chemical potential $\mu_{\rm cr}$ and calculate $N_{\rm cr}$

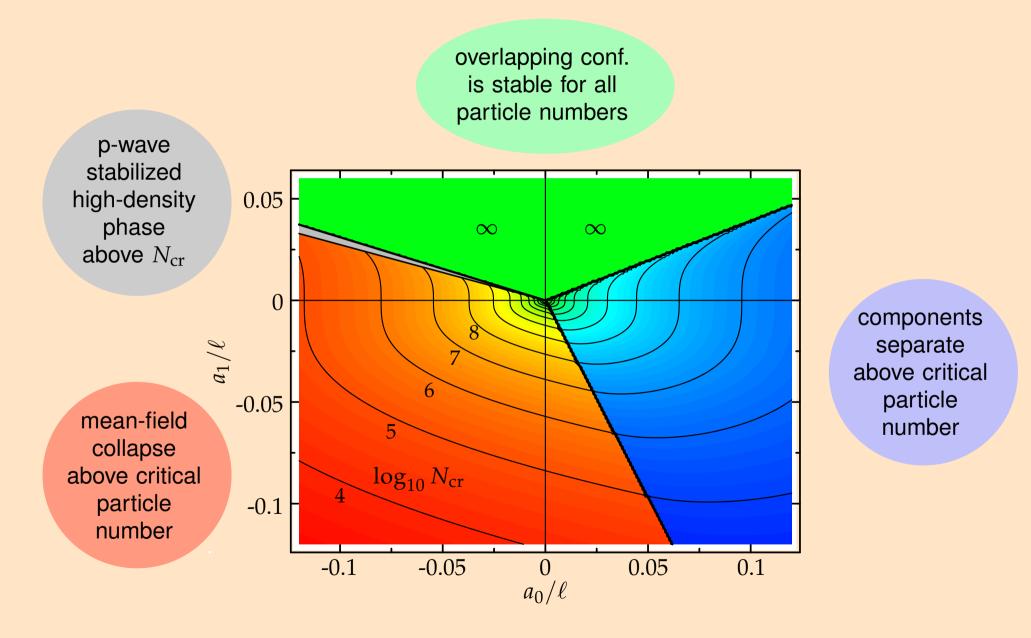
interference with collapse induced by p-wave attraction

p-wave attraction lowers critical particle number substantially

abs. stabilization due to p-wave repulsion $a_1/a_0 > 2^{4/3}/(3\pi^{2/3})$



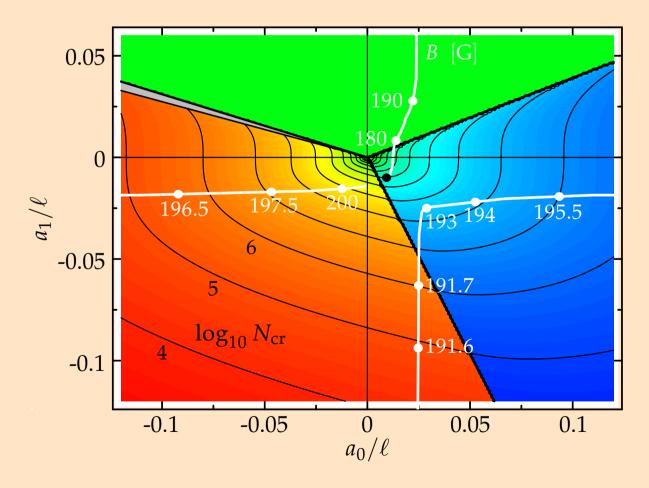
Stability Map



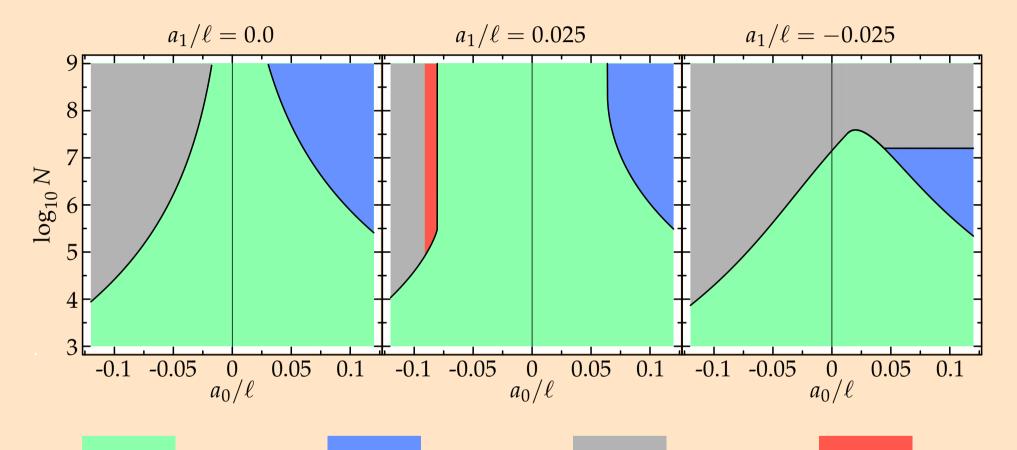
Stability Map & Feshbach Resonances

- Feshbach resonances allow to tune the strength of the atom-atom interaction (scattering lengths) via an external magnetic field
- simultaneous s- and p-wave Feshbach resonance predicted for a two-component $^{40}{\rm K}$ system with $F=\frac{9}{2},\ m_F=-\frac{9}{2},-\frac{7}{2}$

J. Bohn, Phys. Rev. A61 (2000) 053409



Phase Diagram



identical overlapping density distributions spatial separation of the components

unstable against collapse towards high densities

p-wave stabilized high-density phase

Summary

Strategy

- developed a simple framework to describe interacting degenerate quantum gases
- effective contact interaction + mean-field states + Thomas-Fermi approximation → energy functional
- investigated the influence of s- and p-wave interactions on structure and stability of degenerate Fermi gases

Results

- s- and p-wave interactions have strong influence on the density profiles and the stability of the gas
- collapse: attractive interactions can induce a collapse of the dilute gas towards high densities
- separation: repulsive interactions can cause a spatial separation of the different components
- in all cases a complex interplay between s- and p-wave interactions is observed

