Structure of Trapped Degenerate Fermi Gases

Robert Roth

18 January 2002





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

Boulder / Colorado — September 1999

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^{540} K 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 ⁴⁰K atoms kept in a magnetic trap tive cooling and as a modification of the total spin: fermion

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

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

 $\approx 0.5 \varepsilon_F$

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

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

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

two-component mixture

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

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

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

Houston / Texas — March 2001

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 \rightarrow $F = 2 \rightarrow$ **boson** ⁶Li \rightarrow $F = \frac{3}{2} \rightarrow$ **fermion**

 $\begin{array}{l} \text{evaporative cooling of the} \\ \text{bosons} \ \rightarrow \ \text{sympathetic} \\ \text{cooling of the fermions} \end{array}$

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

Fermion Experiments — Today

Two-Component Fermi Gases

09/1999	⁴⁰ K	$T = 0.5\varepsilon_F$	$N_F \sim 10^6$	JILA, Boulder/Colorado, B. DeMarco, D.S. Jin
11/2001	⁶ Li	$T = 0.5\varepsilon_F$	$N_F \sim 10^5$	Duke Univ., Durham/North Carolina, S.R. Granade,, J.E. Thomas

Binary Boson-Fermion Mixtures

03/2001	⁷ Li/ ⁶ Li	$T = 0.25\varepsilon_F$	$N_F \sim 10^5$	Rice Univ., Houston/Texas, A.G. Truscott,, R.G. Hulet
07/2001	⁷ Li/ ⁶ Li	$T = 0.2\varepsilon_F$	$N_F \sim 10^4$	ENS, Paris F. Schreck,, C. Salomon
08/2001	87 Rb $/^{40}$ K		$N_F \sim 10^7$	JILA, Boulder/Colorado J. Goldwin,, D.S. Jin
12/2001	23 Na $/^{6}$ Li	$T = 0.5 \varepsilon_F$	$N_F \sim 10^6$	MIT, Cambridge/Massachusetts Z. Hadzibabic,, W. Ketterle

Theoretical Description of Trapped Degenerate (Fermi) Gases

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

Route Through the Many-Body Problem

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



Model Space

mean-field states: antisym. 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

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,...)







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

Correlated States

include correlations in many-body model-space

Effective Contact Interaction

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

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



Construction of an

Effective Contact Interaction

Energy Shift

• relative two-body wave function w/o and with interaction (outside the 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 *l*th partial wave

$$\mathbf{v}_{l}^{\text{ECI}} = (\vec{\mathbf{q}} \cdot \frac{\vec{\mathbf{r}}}{\mathbf{r}})^{l} g_{l} \delta^{(3)}(\vec{\mathbf{r}}) (\frac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}})^{l}$$
$$= \int d^{3}r \left| \vec{r} \right\rangle \frac{\overleftarrow{\partial}^{l}}{\partial r^{l}} g_{l} \delta^{(3)}(\vec{r}) \frac{\overleftarrow{\partial}^{l}}{\partial r^{l}} \langle \vec{r} |$$

 expectation value in non-interacting twobody states

$$\left\langle \phi_{nlm} \right| \mathbf{v}_{l}^{\mathrm{ECI}} \left| \phi_{nlm} \right\rangle \stackrel{!}{=} \Delta E_{nl}$$

• interaction strengths g_l determined by $\hat{\eta}_l(q)$ $4\pi [(2l+1)!!]^2 \hat{\eta}_l(q)$

$$g_l = -\frac{4\pi}{2m_{\rm red}} \left[\frac{(2l+1)!!}{l!} \right] \frac{\eta_l(q)}{q^{2l+1}}$$

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

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

A Model for a Trapped Degenerate Fermi Gas

- trapped gas of Ξ distinguishable fermionic species (ξ = 1,...,Ξ) interacting via the sand p-wave contact interaction
- for simplicity: equal trapping potentials and s- and p-wave scattering lengths, a₀ and a₁, for all components

Hamiltonian

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

Mean-Field States (homogeneous)

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

 $\left|\Psi\right\rangle = \mathcal{A}\left(\left|\vec{k}_{1},\xi_{1}
ight
angle\otimes\cdots\otimes\left|\vec{k}_{N},\xi_{N}
ight
angle
ight)$

• 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

Two-Component System

• energy expectation value $E_{\Xi}[\kappa_1, ..., \kappa_{\Xi}] = \int d^3x \ \mathcal{E}_{\Xi}[\kappa_1, ..., \kappa_{\Xi}](\vec{x}) \qquad \bullet \text{ density} \qquad \bullet \text{ particle number}$ $\rho_{\xi}(\vec{x}) = \frac{1}{6\pi^2} \kappa_{\xi}^3(\vec{x}) \qquad N[\kappa_{\xi}] = \frac{1}{6\pi^2} \int d^3x \ \kappa_{\xi}^3(\vec{x})$

Ground State — Variationally

Functional Variation

minimization of the energy $E_{\Xi}[\kappa_1, ..., \kappa_{\Xi}]$ 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

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

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

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

• 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 $\mathcal{F}_{\Xi}[\kappa_1, ... \kappa_{\Xi}](\vec{x})$ 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



for a typical trap w	with $\ell = 1 \mu \mathrm{m}$	
$a_0 = 200 a_{Bohr}$	$\rightarrow a_0/\ell =$	0.01

 $a_0 = 2000 \, a_{\mathsf{Bohr}} \quad o \quad a_0/\ell = 0.1$

• Two-Component Fermi Gas

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 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

Two-Component Fermi Gas

Collapse — Stability Condition

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



- 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

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

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

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

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

Two-Component Fermi Gas

Collapse — Critical Particle Number

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



• Two-Component Fermi Gas

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

Two-Component Fermi Gas
Separation — Density Distributions •

$$\rho_{1}(r, z) = \rho_{2}(r, -z)$$

$$a_{0}/\ell = 0 \qquad a_{0}/\ell = 0.06 \qquad a_{0}/\ell = 0.066$$

$$N_{1} = N_{2} = 10^{7}$$

$$a_{1}/\ell = 0$$

$$a_{0}/\ell = 0.07 \qquad a_{0}/\ell = 0.08 \qquad a_{0}/\ell = 0.10$$

$$a_{0}/\ell = 0.07 \qquad a_{0}/\ell = 0.08 \qquad a_{0}/\ell = 0.10$$



• Two-Component Fermi Gas

Stability Map



Two-Component Fermi Gas 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 ${}^{40}\text{K}$ system with $F = \frac{9}{2}$, $m_F = -\frac{9}{2}, -\frac{7}{2}$ [J. Bohn, Phys. Rev. A61 (2000) 053409]



• Two-Component Fermi Gas

Phase Diagram



What's about the Single-Component Fermi Gas?

- Density Profiles
- p-Wave Induced Collapse

Single-Component Fermi Gas

Density Profiles & Collapse

$$\mathcal{F}_1[\kappa](\vec{x}) = \frac{1}{6\pi^2} \left[U(\vec{x}) - \mu \right] \kappa^3(\vec{x}) + \frac{1}{20\pi^2 m} \kappa^5(\vec{x}) + \frac{a_1^3}{30\pi^3 m} \kappa^8(\vec{x}) + \frac{a_1^3}{$$

- the p-wave interaction can have a strong effect on the density profile
- attractive p-wave interactions can cause a collapse of the single component gas
- **stability conditions** for the existence of a metastable state

$$\kappa_{\rm cr} = \frac{\sqrt[3]{3\pi}}{2|a_1|} \qquad \mu_{\rm cr} = \frac{3(3\pi)^{2/3}}{40m|a_1|^2}$$
$$N_{\rm cr} = \left(0.445\frac{\ell}{|a_1|}\right)^6$$

• p-wave attraction can cause a severe limitation of the fermion number

$$a_1/\ell = -0.01 \rightarrow N_{\rm cr} = 7.8 \times 10^9$$

 $a_1/\ell = -0.1 \rightarrow N_{\rm cr} = 7800$





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