Between Bose-Einstein condensate and fermionic superfluid



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- **BCS-BEC crossover.** Universality of the unitary regime.
- Physical realization of the unitary regime: ultra cold atomic gases.
- Equation of state for the uniform Fermi gas in the unitary regime. <u>Critical temperature</u>.
- Measurements of the entropy and the critical temperature in a harmonic trap: <u>experiment vs. theory.</u>

Scattering at low energies (s-wave scattering)







 $f = \frac{1}{-ik - \frac{1}{a} + \frac{1}{2}r_0k^2}, \ a \text{ - scattering length, } r_0 \text{ - effective range}$

If $k \rightarrow 0$ then the interaction is determined by the scattering length alone.

two-particle wave function for small $r \ge R$ (range of the potential): $r\psi(r) \sim (r-a)$



Fermi gas: *n* - number density, *a* - scattering length

What is the energy of the dilute Fermi gas? $E(k_F a) = ?$ $\begin{pmatrix} \uparrow \\ (k_F r_0 << 1) \end{pmatrix}$ $\varepsilon_F = \frac{\hbar^2 k_F^2}{2m}; n = \frac{k_F^3}{3\pi^2}$ - particle density

$$E_{FG} = 1 + \frac{10}{9\pi} (k_F a) \left[1 + \frac{0}{35\pi} (k_F a) (11 - 2ln2) + \dots \right] + \text{pairing}$$

 $E_{FG} = \frac{3}{5} \varepsilon_F N$ - Energy of the noninteracting Fermi gas

Perturbation series (works if: $|k_Fa| < 1$)

A gas of interacting fermions is in the unitary regime if the average separation between particles is large compared to their size (range of interaction), but small compared to their scattering length.

$$\begin{array}{c} n \ r_0^{\ 3} \ll 1 \\ \hline n \ |a|^3 \gg 1 \\ \hline n \ |a|^3 \rightarrow 1 \\ \hline n$$



Superconductivity and superfluidity in Fermi systems

20 orders of magnitude over a century of (low temperature) physics

 $T_c \approx 10^{-12} - 10^{-9} eV$ ✓ Dilute atomic Fermi gases $T_c \approx 10^{-7} eV$ ✓ Liquid ³He $T_{c} \approx 10^{-3} - 10^{-2} eV$ ✓ Metals, composite materials $T_{c} \approx 10^{5} - 10^{6} \, eV$ ✓ Nuclei, neutron stars QCD color superconductivity $T_{c} \approx 10^{7} - 10^{8} \, eV$

units (1 eV \approx 10⁴ K)



A little bit of history

Bertsch Many-Body X challenge, Seattle, 1999

What are the ground state properties of the many-body system composed of spin ½ fermions interacting via a zero-range, infinite scattering-length contact interaction.

Why? Besides pure theoretical curiosity, this problem is relevant to neutron stars!

In 1999 it was not yet clear, either theoretically or experimentally, whether such fermion matter is stable or not! A number of people argued that under such conditions fermionic matter is unstable.

- systems of bosons are unstable (Efimov effect)
- systems of three or more fermion species are unstable (Efimov effect)

Baker (winner of the MBX challenge) concluded that the system is stable.
 See also Heiselberg (entry to the same competition)

• Carlson et al (2003) Fixed-Node Green Function Monte Carlo and Astrakharchik et al. (2004) FN-DMC provided the best theoretical estimates for the ground state energy of such systems: $\mathcal{E}(T-0) \approx 0.44$

 Thomas' Duke group (2002) demonstrated experimentally that such systems are (meta)stable.

In dilute atomic systems experimenters can control nowadays almost anything:

• The number of atoms in the trap: typically about 10⁵⁻10⁶ atoms divided 50-50 among the lowest two hyperfine states.

Who does experiments?

• Jin's group at Boulder

- The density of atoms
- Mixtures of various atoms
- The temperature of the atomic cloud
- The strength of this interaction is fully tunable!



One fermionic atom in magnetic field



Collision of two atoms: At low energies (low density of atoms) only L=0 (s-wave) scattering is effective.

- Due to the high diluteness atoms in the same hyperfine state do not interact with one another.
- Atoms in different hyperfine states experience interactions only in s-wave.



Regal and Jin, PRL 90, 230404 (2003)

Interatomic distance



Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) or 500 ms (b–h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the

magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (**a**), 766 G (**b**), 792 G (**c**), 812 G (**d**), 833 G (**e**), 843 G (**f**), 853 G (**g**) and 863 G (**h**). The field of view of each image is 880 μ m × 880 μ m.

Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \int d^3r \sum_{s=\uparrow\downarrow} \hat{\psi}_s^{\dagger}(\vec{r}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \hat{\psi}_s(\vec{r}) - g \int d^3r \, \hat{n}_{\uparrow}(\vec{r}) \hat{n}_{\downarrow}(\vec{r})$$

$$\hat{N} = \int d^3r \left(\hat{n}_{\uparrow}(\vec{r}) + \hat{n}_{\downarrow}(\vec{r}) \right); \, \hat{n}_s(\vec{r}) = \hat{\psi}_s^{\dagger}(\vec{r}) \hat{\psi}_s(\vec{r})$$
Theoretical approach: Fermions on 3D lattice
$$\begin{array}{c} \text{Volume} = L^3 \\ lattice \ spacing = \Delta x \\ 0 \ -\text{Spin up fermion:} \end{array}$$

$$k_{cut} = \frac{\pi}{\Delta x}; \, \Delta x \downarrow$$

$$k_{cut} = \frac{\pi}{\Delta x}; \, \Delta x \downarrow$$

Periodic boundary conditions imposed

Theoretical approach: Fermions on 3D lattice



MOMENTUM SPACE



Hamiltonian

$$\hat{H} = \hat{T} + \hat{V} = \int d^3 r \sum_{s=\uparrow\downarrow} \hat{\psi}_s^{\dagger}(\vec{r}) \left(-\frac{\hbar^2 \Delta}{2m} \right) \hat{\psi}_s(\vec{r}) - g \int d^3 r \, \hat{n}_{\uparrow}(\vec{r}) \hat{n}_{\downarrow}(\vec{r})$$
$$\hat{N} = \int d^3 r \, \left(\hat{n}_{\uparrow}(\vec{r}) + \hat{n}_{\downarrow}(\vec{r}) \right); \quad \hat{n}_s(\vec{r}) = \hat{\psi}_s^{\dagger}(\vec{r}) \hat{\psi}_s(\vec{r})$$

$$\frac{1}{g} = -\frac{m}{4\pi\hbar^2 a} + \frac{mk_{cut}}{2\pi^2\hbar^2}$$

Running coupling constant g defined by lattice

$$\frac{1}{g} = \frac{m}{2\pi\hbar^2\Delta x} - \text{UNITARY LIMIT}$$

Grand-canonical ensemble:

$$E(T) = \left\langle \hat{H} \right\rangle = \frac{1}{Z(T)} Tr \left\{ \hat{H} \rho(\hat{H}, \hat{N}, T) \right\} = \frac{1}{Z} \sum_{n} E_{n} e^{-\frac{1}{kT}(E_{n} - \mu N_{n})}$$
$$Z(T) = Tr \left\{ \rho(\hat{H}, \hat{N}, T) \right\} = \sum_{n} e^{-\frac{1}{kT}(E_{n} - \mu N_{n})}; \ \rho(\hat{H}, \hat{N}, T) = e^{-\frac{1}{kT}(\hat{H} - \mu \hat{N})}$$

Eigenenergies of the Hamiltonian are unknown!

Path integral approach:

Single-particle quantum mechanics:

$$\left\langle \vec{r}_{1} \left| e^{-i\hat{H}(t-t_{0})} \right| \vec{r}_{1} \right\rangle = \int D[r(t)] e^{i\int_{t_{0}}^{t} L(\vec{r}(t), \dot{\vec{r}}(t)) dt} L(r(t), \dot{r}(t)) = \frac{m\dot{\vec{r}}(t)}{2} - V(\vec{r}); \quad e^{i\int_{t_{0}}^{t} L(\vec{r}(t), \dot{\vec{r}}(t)) dt} = e^{iS[\vec{r}(t)]}$$

Quantum statistical mechanics:

$$Z(\beta) = Tr\left\{\exp(-\beta(\hat{H} - \mu\hat{N}))\right\} = \sum_{n-many} \langle n | \exp(-\beta(\hat{H} - \mu\hat{N}) | n \rangle$$

 \bar{v}

 e^{iS}

 e^{iS_2}

$$3 = \frac{1}{kT}$$
; imaginary time: $\tau = it$

$$Z(\boldsymbol{\beta}) = \left[D[\boldsymbol{\sigma}(\vec{r},\tau)] e^{\ln\{\det[1+U(\{\boldsymbol{\sigma}\})]\}} \right]$$

 $S[\boldsymbol{\sigma}(\vec{r},\tau)] = -\ln\{\det[1+\hat{U}(\{\boldsymbol{\sigma}\})]\} - \operatorname{action}$

 $\hat{U}(\{\sigma\}) = T_{\tau} \exp\{-\int_{\sigma}^{\rho} d\tau [\hat{h}(\{\sigma\}) - \mu]\}; \ \hat{h}(\{\sigma\}) - \text{one-body operator}$ $U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle; \quad | \psi_l \rangle$ - single-particle wave function $E(T) = \left\langle \hat{H} \right\rangle = \int \frac{D[\sigma(\vec{r}, \tau)]e^{-S[\sigma]}}{Z(T)} E[U(\{\sigma\})]$ $E[U(\{\sigma\})]$ - energy associated with a given sigma field Quantum Monte-Carlo: Sigma space sampling $\overline{E}(T) = \frac{1}{N_{\sigma}} \sum_{k=1}^{N_{\sigma}} E(U(\{\sigma_k\}))$ - stochastic variable $\left\langle \overline{E}(T) \right\rangle = \overline{E}(T)$ $\sqrt{\left\langle \overline{E}(T)^2 \right\rangle - \left\langle \overline{E}(T) \right\rangle^2} \propto \frac{1}{\sqrt{N_{\pi}}}$ N_{σ} - number of uncorrelated samples $P(\sigma) \propto e^{-S[\sigma]}$

Quantum Monte-Carlo: parallel computing

$$\begin{split} \hat{U}(\{\sigma\}) &= T_{\tau} \exp\{-\int_{0}^{\beta} d\tau [\hat{h}(\{\sigma\}) - \mu]\}; \ \hat{h}(\{\sigma\}) - \text{one-body operator} \\ U(\{\sigma\})_{kl} &= \left\langle \psi_{k} \middle| \hat{U}(\{\sigma\}) \middle| \psi_{l} \right\rangle; \ \left| \psi_{l} \right\rangle - \text{single-particle wave function} \end{split}$$

For each sigma *n* single particle states have to be evolved.



More details of the calculations:

- Lattice sizes used from <u>8³ x 257</u> (high Ts) to <u>8³ x 1732</u> (low Ts), <N>=50, and <u>6³ x 257</u> (high Ts) to <u>6³ x 1361</u> (low Ts), <N>=30.
- Effective use of FFT(W) makes all imaginary time propagators diagonal (either in real space or momentum space) and there is no need to store large matrices.
- Update field configurations using the Metropolis importance sampling algorithm.
- Change randomly at a fraction of all space and time sites the signs the auxiliary fields $\sigma(r,\tau)$ so as to maintain a running average of the acceptance rate between 0.4 and 0.6.
- Thermalize for 50,000 100,000 MC steps or/and use as a start-up field configuration a $\sigma(x,\tau)$ -field configuration from a different T
- At low temperatures use Singular Value Decomposition of the evolution operator $U(\{\sigma\})$ to stabilize the numerics.
- Use 200,000-2,000,000 $\sigma(x,\tau)$ field configurations for calculations
- MC correlation "time" $\approx 150 200$ time steps at T $\approx T_{e}$

 $\mathfrak{S} = \pm \infty$

Superfluid to Normal Fermi Liquid Transition





<u>Thermodynamics of the unitary Fermi gas</u>

ENERGY:
$$E(x) = \frac{3}{5}\xi(x)\varepsilon_F N; \quad x = \frac{T}{\varepsilon_F}$$

$$C_{V} = T \frac{\partial S}{\partial T} = \frac{\partial E}{\partial T} = \frac{3}{5} N \xi'(x) \Longrightarrow S(x) = \frac{3}{5} N \int_{0}^{x} \frac{\xi'(y)}{y} dy$$

ENTROPY/PARTICLE: $\sigma(x) = \frac{S(x)}{N} = \frac{3}{5} \int_{0}^{x} \frac{\xi'(y)}{y} dy$

FREE ENERGY:
$$F = E - TS = \frac{3}{5}\varphi(x)\varepsilon_F N$$

 $\varphi(x) = \xi(x) - x\sigma(x)$

Low temperature behaviour of a Fermi gas in the unitary regime

$$F(T) = \frac{3}{5} \varepsilon_F N \varphi \left(\frac{T}{\varepsilon_F}\right) = E - TS \text{ and } \frac{\mu(T)}{\varepsilon_F} \approx \xi_s \approx 0.41(2) \text{ for } T < T_C$$

$$\mu(T) = \frac{dF(T)}{dN} = \varepsilon_F \left[\varphi\left(\frac{T}{\varepsilon_F}\right) - \frac{2}{5} \frac{T}{\varepsilon_F} \varphi'\left(\frac{T}{\varepsilon_F}\right) \right] \approx \varepsilon_F \xi_s$$

$$\varphi\left(\frac{T}{\varepsilon_F}\right) = \varphi_0 + \varphi_1\left(\frac{T}{\varepsilon_F}\right)^{5/2}$$

$$E(T) = \frac{3}{5} \varepsilon_F N \left[\xi_s + \zeta_s \left(\frac{T}{\varepsilon_F} \right)^n \right]$$

Lattice results disfavor either n≥3 or n≤2 and suggest n=2.5(0.25)

This is the same behavior as for a gas of <u>noninteracting</u> (!) bosons below the condensation temperature.

$$\begin{split} \rho_{2}(\vec{r}_{1},\vec{r}_{2},\vec{r}_{3},\vec{r}_{4}) &= \left\langle \hat{\psi}^{\dagger}_{\uparrow}(\vec{r}_{1})\hat{\psi}^{\dagger}_{\downarrow}(\vec{r}_{2})\hat{\psi}_{\downarrow}(\vec{r}_{4})\hat{\psi}_{\uparrow}(\vec{r}_{3})\right\rangle \\ \rho_{2}^{P}(\vec{r}) &= \frac{2}{N} \int d^{3}r_{1}d^{3}r_{2}\rho_{2}(\vec{r}_{1}+\vec{r},\vec{r}_{2}+\vec{r},\vec{r}_{1},\vec{r}_{2}) \\ \lim_{r \to \infty} \rho_{2}^{P}(\vec{r}) &= \alpha - \text{condensate fraction} \end{split}$$

More Results...

Condensate fraction **α**: Order parameter for Off Diagonal Long Range Order (C.N. Yang)

Free Bose gas-like: $\alpha(T) = \alpha(0) \left[1 - \left(\frac{T}{T_c}\right)^{3/2} \right]$

> Free : $\alpha(0) = 1$ Unitary: $\alpha(0) \approx 0.6$

> > $T_c = 0.23(2)$



From a talk of J.E. Drut

$$E(T) \approx \frac{3}{5} \varepsilon_F N \xi_s + \frac{m_B^{3/2} \Gamma\left(\frac{3}{2}\right) \varsigma\left(\frac{3}{2}\right)}{2^{1/2} \pi^2 \hbar^3} T^{5/2} V, \quad \text{if} \quad T \gg m_B c^2$$

and fitting to lattice results $\Rightarrow m_B \approx 3m$

- Why this value for the bosonic mass?
- Why these bosons behave like noninteracting particles?

Experiment

John Thomas' group at Duke University, L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007)

Dilute system of fermionic ${}^{6}Li$ atoms in a harmonic trap

- The number of atoms in the trap: N=1.3(0.2) x 10⁵ atoms divided 50-50 among the lowest two hyperfine states.
- Fermi energy: $\varepsilon_F^{ho} = \hbar \Omega (3N)^{1/3}; \ \Omega = \left(\omega_x \omega_y \omega_z\right)^{1/3}$

 $\varepsilon_F^{ho} / k_B \approx 1 \mu K$

- Depth of the potential: $U_0 \approx 10 \varepsilon_F^{ho}$
- How they measure: energy, entropy and temperature?

$$PV = \frac{2}{3}E$$

$$\Rightarrow N\langle U \rangle = \frac{E}{2} - \text{virial theorem}$$

$$\vec{\nabla}P = -n(\vec{r})\vec{\nabla}U$$

$$\text{Holds at unitarity and for noninteracting Fermi gas}$$

•For the weakly interacting gas $(B=1200G \Rightarrow 1/k_Fa \approx -0.75)$ the energy and entropy is calculated. In this limit one can use Thomas-Fermi approach to relate the energy to the given density distribution. The entropy can be estimated as for the noninteracting system with 1% accuracy. In practice: $\langle z^2 \rangle_{B=1200} \Rightarrow E, S$

The magnetic field is changed adiabatically (S=const.) to the value corresponding to the unitary limit: B = 840G ⇒ 1/k_Fa ≈ 0
Relative energy in the unitary limit is calculated from virial theorem:

 $\frac{E(T_1)}{E(T_2)} = \frac{\left\langle z^2 \right\rangle_{T_1}}{\left\langle z^2 \right\rangle_{-}}$

•Temperature is calculated from the identity: $\frac{1}{2} = \frac{2\pi}{2}$

•The plot S(E) contains a cusp related to the phase transition:



$$\begin{split} E(T_c) - E(0) &\approx 0.41(5) N \varepsilon_F^{ho}, \\ S_c / N &\approx 2.7(2) k_B, \\ T_c &\approx 0.29(3) \varepsilon_F^{ho} \end{split}$$

 ∂S

 ∂E

Theory: local density approximation (LDA)

Uniform system

$$\Omega = F - \lambda N = \frac{3}{5}\varphi(x)\varepsilon_F N - \lambda N$$

$$\Omega = \int d^3r \left[\frac{3}{5} \varepsilon_F(\vec{r}) \varphi(x(\vec{r})) + U(\vec{r}) - \lambda \right] n(\vec{r})$$

$$T \qquad \hbar^2 \Gamma = 2^{2/3}$$

 $x(\vec{r}) = \frac{1}{\varepsilon_F(\vec{r})}; \quad \varepsilon_F(r) = \frac{1}{2m} \int \frac{3\pi}{2m} \int \frac{3$

The overall chemical potential λ and the temperature *T* are constant throughout the system. The density profile will depend on the shape of the trap as dictated by:

$$\frac{\delta\Omega}{\delta n(\vec{r})} = \frac{\delta(F - \lambda N)}{\delta n(\vec{r})} = \mu(x(\vec{r})) + U(r) - \lambda = 0$$

Using as an input the Monte Carlo results for the uniform system and experimental data (trapping potential, number of particles), we determine the density profiles.

<u>Comparison with experiment</u> John Thomas' group at Duke University, L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007)



Entropy as a function of energy (relative to the ground state) for the unitary Fermi gas in the harmonic trap. Inset: log-log plot of energy as a function of temperature.



The radial (along shortest axis) density profiles of the atomic cloud in the Duke group experiment at various temperatures.



Ratio of the mean square cloud size at B=1200G to its value at unitarity (B=840G) as a function of the energy. Experimental data are denoted by point with error bars.

 $B = 1200G \Longrightarrow 1/k_F a \approx -0.75 \qquad B = 840G \Longrightarrow 1/k_F a \approx 0$

Summary

We presented the first model-independent comparison of recent measurements of the entropy and the critical temperature, performed by the Duke group: L.Luo, et al. Phys. Rev. Lett. 98, 080402, (2007), with our recent finite temperature Monte Carlo calculations.

EXP.

$$\begin{split} E(T_c) - E(0) &\approx 0.41(5) N \varepsilon_F^{ho}, \\ S_c \,/\, N &\approx 2.7(2) k_B, \\ T_c &\approx 0.29(3) \varepsilon_F^{ho} \end{split}$$

<u>THEORY</u>

$$\begin{split} E(T_c) - E(0) &\approx 0.34(2) N \varepsilon_F^{ho}, \\ S_c / N &\approx 2.4(3) k_B, \\ T_c &\approx 0.27(3) \varepsilon_F^{ho} \end{split}$$

A.Bulgac, J.E. Drut, P. Magierski, Phys. Rev. Lett 99, 120401 (2007)

The results are consistent with the predicted value of the critical temperature for the uniform unitary Fermi gas: $0.23(2)\mathcal{E}_F$

Conclusions

✓ Fully non-perturbative calculations for a spin ½ many fermion system in the unitary regime at finite temperatures are feasible and apparently the system undergoes a phase transition in the bulk at $T_{\rm c} = 0.23$ (2) $\varepsilon_{\rm F}$

- Chemical potential is constant up to the critical temperature note similarity with Bose systems!
- Below the transition temperature, both phonons and fermionic quasiparticles contribute almost equaly to the specific heat. In more than one way the system is at crossover between a Bose and Fermi systems.

There are reasons to believe that below the critical temperature this system is a new type of fermionic superfluid, with unusual properties.

Quest for unitary point critical temperature



Boris Svistunov's talk (updated), Seattle 2005