The Unitary Fermi Gas: so simple yet so complex!

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Why would one want to study this system?

One reason:

(for the nerds, I mean the hard-core theorists, not for the phenomenologists)

Bertsch's 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.

What are the scattering length and the effective range?

$$k \cot a \delta_0 = -\frac{1}{a} + \frac{1}{2}r_0k^2 + \cdots$$
$$\sigma = \frac{4\pi}{k^2}\sin^2\delta_0 + \cdots = 4\pi a^2 + \cdots$$

If the energy is small only the s-wave is relevant.

Let me consider as an example the hydrogen atom.

The ground state energy could only be a function of:

✓ Electron charge
 ✓ Electron mass
 ✓ Planck's constant

and then trivial dimensional arguments lead to

$$E_{gs} = \frac{e^4 m}{\hbar^2} \times \frac{1}{2}$$

Only the factor ½ requires some hard work.

Let me now turn to dilute fermion matter

The ground state energy is given by such a function:

$$E_{gs} = f(N, V, \hbar, m, a, r_0)$$

Taking the scattering length to infinity and the range of the interaction to zero, we are left with:

$$E_{gs} = F(N, V, \hbar, m) = \frac{3}{5} \varepsilon_F N \times \xi_F$$
$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

number

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 (LANL, 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.

Carlson et al (2003) have also shown that the system has a huge pairing gap !

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

What George Bertsch essentially asked in 1999 is: What is the value of ξ !

But he wished to know the properties of the system as well: *The* system turned out to be superfluid !

$$E_{gs} = \frac{3}{5} \varepsilon_F N \times \xi \qquad \Delta = \varepsilon_F \times \zeta$$
$$\xi = 0.40(1), \qquad \zeta = 0.50(1)$$

Now these results are a bit unexpected.

The energy looks almost like that of <u>a non-interacting system</u>! (there are no other dimensional parameters in the problem)
The system has <u>a huge pairing gap</u>!
This system is a very strongly interacting one, since the <u>elementary cross section is infinite</u>! The initial Bertsch's Many Body challenge has evolved over time and became the problem of *Fermions in the Unitary Regime*

And this is part of the BCS-BEC crossover problem

The system is very dilute, but strongly interacting!



Why Study Fermi Gases ?



- Fermions are the building blocks of matter
- Strongly-interacting Fermi gases are stable
- Link to other interacting Fermi systems:
 - High-T_C superconductors Neutron stars
 - Lattice field theory
 - Quark-gluon plasma of Big Bang
 - String theory!

O'Hara et al., Science 2002

Superconductivity and Superfluidity in Fermi Systems

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

- ✓ Dilute atomic Fermi gases $T_c \approx 10^{-12} 1$
- ✓ Liquid ³He $T_c \approx 10^{-7} \text{ eV}$
- ✓ Metals, composite materials
- ✓ Nuclei, neutron stars
- QCD color superconductivity

 $T_c \approx 10^{-12} - 10^{-9} \, eV$

- $T_c \approx 10^{-3} 10^{-2} \text{ eV}$
- $T_c \approx 10^5 10^6 \text{ eV}$
- $T_c \approx 10^7 10^8 \,\mathrm{eV}$

units (1 eV \approx 10⁴ K)

Optical Trap Loading





Forced Evaporation



High-Field Imaging









FIG. 4: Scattering lengths versus magnetic field from multichannel quantum scattering calculations for the (1, 2), (1, 3), and (2, 3) scattering channels. The arrows indicate the resonance positions.

Bartenstein et al. Phys. Rev. Lett. 94, 103201 (2005)

Feshbach resonance

$$H = \frac{\vec{p}^2}{2\mu_r} + \sum_{i=1}^2 (V_i^{hf} + V_i^Z) + V_0(\vec{r})P_0 + V_1(\vec{r})P_1 + \mathcal{M}^d$$
$$V^{hf} = \frac{a_{hf}}{\hbar^2} \vec{S}^e \cdot \vec{S}^n, \quad V^Z = (\gamma_e S_z^e - \gamma_n S_z^n)B$$

Channel coupling

Tiesinga, Verhaar, and Stoof Phys. Rev. A<u>47</u>, 4114 (1993)



Regal and Jin Phys. Rev. Lett. <u>90</u>, 230404 (2003)







Fig. 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) to 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 (a) 740 G, (b) 766 G, (c) 792 G, (d) 812 G, (e) 833 G, (f) 843 G, (g) 853 G and (h) 863 G. The field of view of each image is $880 \ \mu m \times 880 \ \mu m$.

Zweirlein et al. Nature <u>435</u>, 1047 (2005)

Theoretical tools and features:

- Canonical and Grand Canonical Ensembles
- Hubbard-Stratonovich transformation
- Auxiliary Field Quantum Monte-Carlo
- Absence of Fermion sign problem
- Markov process, Metropolis importance sampling, decorrelation, ...
- Renormalization of the two-body interaction
- Spatio- (imaginary) temporal lattice formulation of the problem
- One-particle temperature (Matsubara) propagator
- Extension of Density Functional Theory to superfluid systems and timedependent phenomena
- Superfluid to Normal phase transition (second order)
- Off-diagonal long range order, condensate fraction, finite size scaling and extraction of critical temperature
- S- and P-wave superfluidity, induced interactions
 - (NB bare interaction in s-wave only)
- Larkin-Ovchinnikov-Fulde-Ferrell superfluidity (LOFF/FFLO)
- Quantum phase transitions (T=0, first and second order)
- Phase separation
- Pairing gap and pseudo-gap
- Supersolid





$$E_{\text{phonons}}(T) = \frac{3}{5} \varepsilon_F N \frac{\sqrt{3}\pi^4}{16\xi_s^{3/2}} \left(\frac{T}{\varepsilon_F}\right)^4, \qquad \xi_s \approx 0.44$$

$$E_{\text{quasi-particles}}(T) = \frac{3}{5} \varepsilon_F N \frac{5}{2} \sqrt{\frac{2\pi\Delta^3 T}{\varepsilon_F^4}} \exp\left(-\frac{\Delta}{T}\right)$$

$$\Delta = \left(\frac{2}{e}\right)^{1/3} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

7 10

Bulgac, Drut, and Magierski Phys. Rev. Lett. <u>96</u>, 090404 (2006)

Normal Fermi Gas (with vertical offset, solid line)

Bogoliubov-Anderson phonons and quasiparticle contribution (dot-dashed line)

Bogoliubov-Anderson phonons contribution only

Quasi-particles contribution only (dashed line)

νμ - chemical potential (circles)

Experiment (about 100,000 atoms in a trap):

Measurement of the Entropy and Critical Temperature of a Strongly Interacting Fermi Gas, Luo, Clancy, Joseph, Kinast, and Thomas, Phys. Rev. Lett. <u>98</u>, 080402 (2007)



Ab initio theory (no free parameters)

Bulgac, Drut, and Magierski, Phys. Rev. Lett. 99, 120401 (2007)

Long range order and condensate fraction



$$g_{2}(\vec{r}) = \left(\frac{2}{N}\right)^{2} \int d^{3}\vec{r_{1}} \int d^{3}\vec{r_{2}} \left\langle \psi_{\uparrow}^{\dagger}(\vec{r_{1}}+\vec{r})\psi_{\downarrow}^{\dagger}(\vec{r_{2}}+\vec{r})\psi_{\downarrow}(\vec{r_{2}})\psi_{\uparrow}(\vec{r_{2}})\right\rangle$$
$$\alpha = \lim_{r \to \infty} \frac{N}{2} g_{2}(\vec{r}) - n(\vec{r})^{2}, \qquad n(\vec{r}) = \frac{2}{N} \int d^{3}\vec{r_{1}} \left\langle \psi_{\uparrow}^{\dagger}(\vec{r_{1}}+\vec{r})\psi_{\uparrow}(\vec{r_{1}})\right\rangle$$

Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

Critical temperature for superfluid to normal transition



Bulgac, Drut, and Magierski, Phys. Rev. A 78, 023625 (2008)

 Amherst-ETH:
 Burovski et al. Phys. Rev. Lett. <u>101</u>, 090402 (2008)

 Hard and soft bosons: Pilati et al. PRL <u>100</u>, 140405 (2008)

Response of the two-component Fermi gas in the unitary regime

Bulgac, Drut, and Magierski, arXiv:0801:1504

$$\chi(\vec{p}) = -T \frac{d}{dg} \frac{\text{Tr}\{\exp[-\beta(\text{H}-\mu\text{N}+g\psi(\vec{p}))]\psi^{\dagger}(\vec{p})\}}{\text{Tr}\{\exp[-\beta(\text{H}-\mu\text{N}+g\psi(\vec{p}))]\}} \bigg|_{g=0} = -\int_{0}^{\beta} d\tau G(\vec{p},\tau)$$

One-body temperature (Matsubara) Green's function







The pseudo-gap vanishes at T₀

Magierski, Wlazlowski, Bulgac, and Drut arXiv:0801.1504v3





Using photoemission spectroscopy to probe a strongly interacting Fermi gas Stewart, Gaebler, and Jin, Nature, <u>454</u>, 744 (2008) Until now we kept the numbers of spin-up and spin-down equal.

What happens when there are not enough partners for everyone to pair with?

(In particular this is what one expects to happen in color superconductivity, due to a heavier strange quark)

What theory tells us?

Green – Fermi sphere of spin-up fermions Yellow – Fermi sphere of spin-down fermions

If
$$|\mu_{\uparrow} - \mu_{\downarrow}| < \frac{\Delta}{\sqrt{2}}$$
 the same solution as for $\mu_{\uparrow} = \mu_{\downarrow}$



LOFF/FFLO solution (1964) Pairing gap becomes a spatially varying function Translational invariance broken



Muether and Sedrakian (2002) Translational invariant solution Rotational invariance broken

What we think is happening in spin imbalanced systems?

Induced P-wave superfluidity

Two new superfluid phases where before they were not expected



Going beyond the naïve BCS approximation



Eliashberg approx. (red)

BCS approx. (black)

Full momentum and frequency dependence of the selfconsistent equations (red)

Bulgac and Yoon, Phys. Rev. A 79, 053625 (2009)

What happens at unitarity?

Bulgac and Forbes, PRA 75, 031605(R) (2007)



Predicted quantum first phase order transition, subsequently observed in MIT experiment , Shin *et al*. Nature, <u>451</u>, 689 (2008)

Red points with error bars – subsequent DMC calculations for normal state due to Lobo et al, PRL <u>97</u>, 200403 (2006)

$$E(n_a, n_b) = \frac{3}{5} \frac{(6\pi^2)^{2/3} \hbar^2}{2m} \left[n_a g\left(\frac{n_b}{n_a}\right) \right]^{5/3}, \quad n_a \ge n_b$$

How to construct and validate an *ab initio* Energy Density Functional (EDF)?

Given a many body Hamiltonian determine the properties of the infinite homogeneous system as a function of density

Extract the EDF

Add gradient corrections, if needed or known how (?)

Determine in an *ab initio* calculation the properties of a select number of wisely selected finite systems

Apply the energy density functional to inhomogeneous systems and compare with the *ab initio* calculation, and if lucky declare Victory!

The SLDA energy density functional at unitarity for equal numbers of spin-up and spin-down fermions

Only this combination is cutoff independent

$$\varepsilon(\vec{r}) = \left[\alpha \frac{\tau_c(\vec{r})}{2} - \Delta(\vec{r})\nu_c(\vec{r})\right] + \beta \frac{3(3\pi^2)^{2/3}n^{5/3}(\vec{r})}{5}$$

$$\begin{split} n(\vec{r}) &= 2 \sum_{0 < E_k < E_c} \left| \mathbf{v}_{\mathbf{k}}(\vec{r}) \right|^2, \quad \tau_c(\vec{r}) = 2 \sum_{0 < E_k < E_c} \left| \vec{\nabla} \mathbf{v}_{\mathbf{k}}(\vec{r}) \right|^2, \\ \nu_c(\vec{r}) &= \sum_{0 < E < E_c} \mathbf{u}_{\mathbf{k}}(\vec{r}) \mathbf{v}_{\mathbf{k}}^*(\vec{r}) \end{split}$$

$$\begin{split} U(\vec{r}) &= \beta \frac{(3\pi^2)^{2/3} n^{2/3}(\vec{r})}{2} - \frac{\left| \Delta(\vec{r}) \right|^2}{3\gamma n^{2/3}(\vec{r})} + V_{ext}(\vec{r}) + \text{small correction} \\ \Delta(\vec{r}) &= -g_{eff}(\vec{r}) v_c(\vec{r}) \end{split}$$

 α can take any positive value, but the best results are obtained when α is fixed by the qp-spectrum

Fermions at unitarity in a harmonic trap Total energies E(N)



GFMC - Chang and Bertsch, Phys. Rev. A 76, 021603(R) (2007) FN-DMC - von Stecher, Greene and Blume, PRL <u>99</u>, 233201 (2007) PRA <u>76</u>, 053613 (2007)

Bulgac, PRA 76, 040502(R) (2007)

Fermions at unitarity in a harmonic trap Pairing gaps



Bulgac, PRA 76, 040502(R) (2007)

Quasiparticle spectrum in homogeneous matter



solid/dotted blue line red circles dashed blue line

- SLDA, homogeneous GFMC due to Carlson et al
- GFMC due to Carlson and Reddy
- SLDA, homogeneous MC due to Juillet

black dashed-dotted line – meanfield at unitarity

Two more universal parameter characterizing the unitaryFermi gas and its excitation spectrum:effective mass, meanfield potentialBulgac, PRA 76, 040502(R) (2007)

Asymmetric SLDA (ASLDA)

$$n_{a}(\vec{r}) = \sum_{E_{n}<0} |\mathbf{u}_{n}(\vec{r})|^{2}, \qquad n_{b}(\vec{r}) = \sum_{E_{n}>0} |\mathbf{v}_{n}(\vec{r})|^{2},$$
$$\tau_{a}(\vec{r}) = \sum_{E_{n}<0} |\vec{\nabla}\mathbf{u}_{n}(\vec{r})|^{2}, \qquad \tau_{b}(\vec{r}) = \sum_{E_{n}>0} |\vec{\nabla}\mathbf{v}_{n}(\vec{r})|^{2},$$
$$\nu(\vec{r}) = \frac{1}{2} \sum_{E_{n}} \operatorname{sign}(E_{n}) \mathbf{u}_{n}(\vec{r}) \mathbf{v}_{n}^{*}(\vec{r}),$$

$$E(\vec{r}) = \frac{\hbar^2}{2m} \Big[\alpha_a(\vec{r}) \tau_a(\vec{r}) + \alpha_b(\vec{r}) \tau_b(\vec{r}) \Big] - \Delta(\vec{r}) \nu(\vec{r}) + \frac{3 \Big(3\pi^2 \Big)^{2/3} \hbar^2}{10m} \Big[n_a(\vec{r}) + n_b(\vec{r}) \Big]^{5/3} \beta[x(\vec{r})],$$

$$\alpha_a(\vec{r}) = \alpha [x(\vec{r})], \quad \alpha_b(\vec{r}) = \alpha [1/x(\vec{r})], \quad x(\vec{r}) = n_b(\vec{r})/n_a(\vec{r}),$$

$$\Omega = -\int d^{3}\vec{r} \ \mathrm{P}(\vec{r}) = \int d^{3}\vec{r} \ \left[\mathrm{E}(\vec{r}) - \mu_{a}n_{a}(\vec{r}) - \mu_{b}n_{b}(\vec{r})\right]$$

A refined EOS for spin unbalanced systems



Red line: Larkin-Ovchinnikov phase

Black line:normal part of the energy densityPhys. Rev. Lett. <u>101</u>, 215301 (2008)Blue points:DMC calculations for normal state, Lobo et al, PRL <u>97</u>, 200403 (2006)Gray crosses:experimental EOS due to Shin, Phys. Rev. A 77, 041603(R) (2008)

Bulgac and Forbes,

$$E(n_a, n_b) = \frac{3}{5} \frac{(6\pi^2)^{2/3} \hbar^2}{2m} \left[n_a g\left(\frac{n_b}{n_a}\right) \right]^{5/3}$$

A Unitary Fermi Supersolid: the Larkin-Ovchinnikov phase



 Δ/Δ_0 0 10 L/l_0 5 y_{LO} y_1 -0.20.0 $y = \mu_b/\mu_a$

 y_{LO-N}

 y_{LO-SF}

Bulgac and Forbes, arXiv:0804:3364 PRL accepted

$$P[\mu_a,\mu_b] = \frac{2}{30\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \left[\mu_a h\left(\frac{\mu_b}{\mu_a}\right)\right]^{5/2}$$

Some of the lessons learned so far:

We have (finally) control over the calculation of the pairing gap in dilute fermion/neutron matter (second order phase transition superfluid to normal)

There are strong indications that the pseudo-gap (spectral gap above the critical temperature) is present in these systems

At moderate spin imbalance the system turns into a supersolid with pairing of the LOFF type (first and second order quantum phase transitions)

At large spin imbalance two <u>simbiotic</u> superfluids appear (most likely p-wave superfluidity)

There is a controlled way to construct an energy density functional for superfluid systems, relevant for UNEDF

Time Dependent Phenomena and Formalism

The time-dependent density functional theory is viewed in general as a reformulation of the exact quantum mechanical time evolution of a many-body system when only single-particle properties are considered.

A.K. Rajagopal and J. Callaway, Phys. Rev. B <u>7</u>, 1912 (1973)
V. Peuckert, J. Phys. C <u>11</u>, 4945 (1978)
E. Runge and E.K.U. Gross, Phys. Rev. Lett. <u>52</u>, 997 (1984)

http://www.tddft.org

$$[h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathbf{u}_{i}(\vec{r},t) + [\Delta(\vec{r},t) + \Delta_{ext}(\vec{r},t)] \mathbf{v}_{i}(\vec{r},t) = i\hbar \frac{\partial \mathbf{u}_{i}(\vec{r},t)}{\partial t}$$
$$[\Delta^{*}(\vec{r},t) + \Delta^{*}_{ext}(\vec{r},t)] \mathbf{u}_{i}(\vec{r},t) - [h(\vec{r},t) + V_{ext}(\vec{r},t) - \mu] \mathbf{v}_{i}(\vec{r},t) = i\hbar \frac{\partial \mathbf{v}_{i}(\vec{r},t)}{\partial t}$$

Full 3D implementation of TD-SLDA is a petaflop problem and is almost complete.

Bulgac and Roche, J. Phys. Conf. Series <u>125</u>, 012064 (2008)

Lots of contributions due to Y. Yu, S. Yoon, Y.-L. Luo, P. Magierski, and I. Stetcu

New issues arising in formulating and implementing a TD-DFT:

In ground states currents vanish, but they are present in excited states.

The dependence of the EDF on some currents can be established from general principles, e.g. Galilean invariance:

$$\tau(\vec{r}) \Rightarrow \tau(\vec{r}) - \frac{\vec{j}^2(\vec{r})}{n(\vec{r})}$$

Not all currents and densities can be introduced into the formalism in a such a manner however.

Energy of a (unitary) Fermi system as a function of the pairing gap



Response of a unitary Fermi system to changing the scattering length with time

Tool: TD DFT extension to superfluid systems (TD-SLDA)



• All these modes have a very low frequency below the pairing gap and a very large amplitude and excitation energy as well

 None of these modes can be described either within Quantum Hydrodynamics or Landau-Ginzburg like approaches

Bulgac and Yoon, Phys. Rev. Lett. 102, 085302 (2009)

3D unitary Fermi gas confined to a 1D ho potential well (pancake) New qualitative excitation mode of a superfluid Fermi system (non-spherical Fermi momentum distribution)



Black solid line – Time dependence of the cloud radius Black dashed line – Time dependence of the quadrupole moment of momentum distribution

Bulgac and Yoon, Phys. Rev. Lett. <u>102</u>, 085302 (2009)







4vortices_1.avi







7vortices_1.avi

In case you've got lost: What did I talk about so far?

What is a unitary Fermi gas?

Thermodynamic properties

Pairing gap and pseudo-gap

EOS for spin imbalanced systems

P-wave pairing

Small systems in traps and (A)SLDA

Unitary Fermi supersolid: the Larkin-Ovchinnikov phase

Time-dependent phenomena, vortex generation, pairing Higgs mode