Equation of state for dilute and strongly interacting Fermi gas

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Outline

- General remarks

- Path integral Monte Carlo description of strongly interacting Fermi gases.


- Conclusions.
Superconductivity and superfluidity in Fermi systems

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

<table>
<thead>
<tr>
<th>System</th>
<th>$T_c \approx$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dilute atomic Fermi gases</td>
<td>$10^{-12} - 10^{-9}$ eV</td>
</tr>
<tr>
<td>Liquid $^3$He</td>
<td>$10^{-7}$ eV</td>
</tr>
<tr>
<td>Metals, composite materials</td>
<td>$10^{-3} - 10^{-2}$ eV</td>
</tr>
<tr>
<td>Nuclei, neutron stars</td>
<td>$10^5 - 10^6$ eV</td>
</tr>
<tr>
<td>QCD color superconductivity</td>
<td>$10^7 - 10^8$ eV</td>
</tr>
</tbody>
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units (1 eV $\approx 10^4$ K)
Fermi gas: \( n \) - number density, \( a \) - scattering length

What is the energy of the dilute Fermi gas? \( E(k_Fa) = ? \)

\[
E_{\text{FG}} = \frac{3}{5} \epsilon_F N \quad \text{- Energy of the noninteracting Fermi gas}
\]

BCS pairing gap

\[
\Delta_{\text{BCS}} = \frac{8 \hbar^2 k_F^2}{\epsilon^2} \exp \left( \frac{\pi}{2k_F a} \right) , \quad \text{iff} \quad k_F a \ll 1 \quad \text{and} \quad \frac{1}{k_F} \ll \eta = \frac{1}{k_F} \frac{\epsilon_F}{\Delta} \quad \text{- size of the Cooper pair}
\]

\[
\frac{E_{\text{HF+BCS}}}{E_{\text{FG}}} = 1 + \frac{10}{9\pi} (k_F a) + \ldots - \frac{5}{8} \left( \frac{\Delta_{\text{BCS}}}{\epsilon_F} \right)^2 = 1 + \frac{10}{9\pi} (k_F a) + \ldots - \frac{40}{\epsilon^3} \exp \left( \frac{\pi}{k_F a} \right)
\]

Mean-field term

BCS term
What is the unitary regime?

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.

\[ n r_0^3 \ll 1 \quad \text{and} \quad n |a|^3 \gg 1 \]

\[ i.e. \quad r_0 \to 0, \quad a \to \pm \infty \]

The only scale:

\[ \frac{E_{FG}}{N} = \frac{3}{5} \varepsilon_F \]

UNIVERSALITY:

\[ E(T) = \xi \left( \frac{T}{\varepsilon_F} \right) E_{FG} \]

QUESTIONS:

What is the shape of \( \xi \left( \frac{T}{\varepsilon_F} \right) \)?

What is the critical temperature for the superfluid-to-normal transition?

...
Expected phases of a two species dilute Fermi system
BCS-BEC crossover

T

Strong interaction
UNITARY REGIME

EASY!
weak interaction
BCS Superfluid

?  
Molecular BEC and
Atomic+Molecular
Superfluids

EASY!
weak interactions

1/a

a<0
no 2-body bound state

a>0
shallow 2-body bound state

Boise molecule

EASY!
**A little bit of history**

Bertsch Many-Body X challenge, Seattle, 1999

<table>
<thead>
<tr>
<th>What are the ground state properties of the many-body system composed of spin $\frac{1}{2}$ fermions interacting via a zero-range, infinite scattering-length contact interaction.</th>
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<td>Why? Besides pure theoretical curiosity, this problem is relevant to neutron stars!</td>
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</tbody>
</table>

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: $\zeta(T=0) \approx 0.44$

- Thomas’ Duke group (2002) demonstrated experimentally that such systems are (meta)stable.
Neutron matter:

Effective range: \( r_0 \approx 2.8 \text{ fm} \)
Scattering length: \( a \approx -18.5 \text{ fm} \)

Density range
\[
\begin{align*}
r_0 & \ll n^{-1/3} \approx \frac{\lambda_F}{2} \ll |a|
\end{align*}
\]
corresponds to
\[
\begin{align*}
n & \approx 0.001 - 0.01 \text{ fm}^{-3} \\
k_F & \approx 0.3 - 0.7 \text{ fm}^{-1}
\end{align*}
\]
**Neutron matter**

Neutron-neutron scattering

Scattering length: \( a \approx -18.5 \, \text{fm} \)

Effective range: \( r_0 \approx 2.8 \, \text{fm} \)

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**s-wave pairing gap in infinite neutron matter with realistic NN-interactions**

\[ \Delta_r [\text{MeV}] \]

- Chen et al., NPA 451, 509 (1986)
- Ainsworth et al., PLB 222, 173 (1989)
- Chen et al., NPA 555, 59 (1993)
- Wambach et al., NPA 555, 128 (1993)
- Schulze et al., PLB 375, 1 (1996)

**BCS**

---

Dilute matter: only neutron matter

- Nuclear density

- \( n \approx 0.001 - 0.01 \, \text{fm}^3 \)

- \( k_F \approx 0.3 - 0.7 \, \text{fm}^{-1} \)

---

Close to the unitary limit
Theoretical approach: Fermions on 3D lattice

Coordinate space

Hamiltonian

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

\[ \hat{N} = \int d^3r \ (\hat{n}_\uparrow (\vec{r}) + \hat{n}_\downarrow (\vec{r})) \]

\[ \hat{n}_s (\vec{r}) = \hat{\psi}_s^\dagger (\vec{r}) \hat{\psi}_s (\vec{r}) \]

Volume = \( L^3 \)

Lattice spacing = \( \Delta x \)

- Spin up fermion: \( \uparrow \)
- Spin down fermion: \( \downarrow \)

External conditions:
- \( T \) - temperature
- \( \mu \) - chemical potential

Periodic boundary conditions imposed
Theoretical approach: Fermions on 3D lattice

\[ \Lambda = \Delta \ll \Lambda_{UV} \ll \frac{2\pi}{L} \]

**Momentum space**

UV momentum cutoff \( \Lambda_{UV} = \frac{\pi}{\Delta x} \)

IR momentum cutoff \( \Lambda_{IR} = \frac{2\pi}{L} \)

\[ \frac{\hbar^2 \Lambda_{IR}^2}{2m} \ll \varepsilon_F, \Delta \ll \frac{\hbar^2 \Lambda_{UV}^2}{2m} \]

**REAL SPACE** ↔ **MOMENTUM SPACE**
Grand Canonical Path-Integral Monte Carlo

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

\[ \hat{N} = \int d^3x \left[ \hat{n}_\uparrow(\vec{x}) + \hat{n}_\downarrow(\vec{x}) \right], \quad \hat{n}_s(\vec{x}) = \psi^+_s(\vec{x}) \psi_s(\vec{x}), \quad s = \uparrow, \downarrow \]

**Trotter expansion**

\[ Z(\beta) = \text{Tr} \exp \left[ -\beta \left( \hat{H} - \mu \hat{N} \right) \right] = \text{Tr} \left\{ \exp \left[ -\tau \left( \hat{H} - \mu \hat{N} \right) \right] \right\}^{N_\tau}, \quad \beta = \frac{1}{T} = N_\tau \tau \]

\[ E(T) = \frac{1}{Z(T)} \text{Tr} \hat{H} \exp \left[ -\beta \left( \hat{H} - \mu \hat{N} \right) \right] \]

\[ N(T) = \frac{1}{Z(T)} \text{Tr} \hat{N} \exp \left[ -\beta \left( \hat{H} - \mu \hat{N} \right) \right] \]
\[
\exp\left[-\tau\left(\hat{H} - \mu\hat{N}\right)\right] \approx \exp\left[-\tau\left(\hat{T} - \mu\hat{N}\right)/2\right] \exp(-\tau\hat{V}) \exp\left[-\tau\left(\hat{T} - \mu\hat{N}\right)/2\right] + O(\tau^3)
\]

Discrete Hubbard-Stratonovich transformation

\[
\exp(-\tau\hat{V}) = \prod \sum_{\vec{r}} \frac{1}{2} \left[1 + \sigma(\vec{r}) \hat{\sigma}^\uparrow(\vec{r}) \right] \left[1 + \sigma(\vec{r}) \hat{\sigma}^\downarrow(\vec{r}) \right], \quad A = \sqrt{\exp(\tau g) - 1}
\]

\[\sigma\text{-fields fluctuate both in space and imaginary time}\]

Running coupling constant \( g \) defined by lattice

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

\[
\frac{1}{g} = \frac{m}{2\pi\hbar^2 \Delta x} \quad - \text{UNITARY LIMIT}
\]
\[ Z(T) = \int D\sigma(\bar{x}, \tau) \, \text{Tr} \, \hat{U}(\{\sigma\}); \]
\[ \int D\sigma(\bar{r}, \tau) \equiv \sum_{\{\sigma(\bar{r},1)=\pm1\}} \sum_{\{\sigma(\bar{r},2)=\pm1\}} \cdots \sum_{\{\sigma(\bar{r},N_r)=\pm1\}} ; \quad N_r \tau = \frac{1}{T} \]
\[ \hat{U}(\{\sigma\}) = T_\tau \exp\left\{ -\int_0^\beta d\tau [\hat{h}(\{\sigma\}) - \mu] \right\} \]

One-body evolution operator in imaginary time

\[ E(T) = \int \frac{D\sigma(\bar{x}, \tau)\text{Tr} \hat{U}(\{\sigma\})}{Z(T)} \, \frac{\text{Tr} \left[ \hat{H} \hat{U}(\{\sigma\}) \right]}{\text{Tr} \hat{U}(\{\sigma\})} \]

\[ \text{Tr} \hat{U}(\{\sigma\}) = \{\text{det}[1 + \hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0 \quad \text{No sign problem!} \]

\[ n^\uparrow(\bar{x}, \bar{y}) = n^\downarrow(\bar{x}, \bar{y}) = \sum_{k,l<k_c} \psi^*_k(\bar{x}) \left[ \frac{U(\{\sigma\})}{1 + U(\{\sigma\})} \right] \psi^*_l(\bar{y}), \quad \psi^*_k(\bar{x}) = \frac{\exp(ik\cdot\bar{x})}{\sqrt{L^3}} \]

All traces can be expressed through these single-particle density matrices
\[ \hat{U}(\{\sigma\}) = T_\tau \exp\left\{ -\int_0^\beta d\tau [\hat{h}(\{\sigma\}) - \mu] \right\}; \quad \hat{h}(\{\sigma\}) - \text{one-body operator} \]

\[ U(\{\sigma\})_{kl} = \left\langle \psi_k \left| \hat{U}(\{\sigma\}) \right| \psi_l \right\rangle; \quad |\psi_i\rangle - \text{single-particle wave function} \]

\[ E(T) = \left\langle \hat{H} \right\rangle = \int \frac{D[\sigma(\vec{r}, \tau)]e^{-S[\sigma]}}{Z(T)} E[U(\{\sigma\})] \]

\[ E[U(\{\sigma\})] - \text{energy associated with a given sigma field} \]

**Quantum Monte-Carlo:**

**Sigma space sampling**

- Energy associated with a given sigma field

\[ \bar{E}(T) = \frac{1}{N_\sigma} \sum_{k=1}^{N_\sigma} E(U(\{\sigma_k\})) \]

\[ \bar{E}(T) - \text{stochastic variable} \]
\[ \left\langle \bar{E}(T) \right\rangle = E(T) \]
\[ \sqrt{\left\langle (\bar{E}(T))^2 \right\rangle - \left\langle \bar{E}(T) \right\rangle^2} \propto \frac{1}{\sqrt{N_\sigma}} \]

\[ N_\sigma - \text{number of uncorrelated samples} \]

\[ P(\sigma) \propto e^{-S[\sigma]} \]
Quantum Monte-Carlo: parallel computing

\[ \hat{U}({\{\sigma}\}}) = T_\tau \exp\{-\int_0^\beta d\tau [\hat{h}(\{\sigma\}) - \mu]\}; \quad \hat{h}(\{\sigma\}) \quad \text{one-body operator} \]

\[ U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle; \quad |\psi_l\rangle \quad \text{- single-particle wave function} \]

For each sigma \( \sigma \) single particle states have to be evolved.

\[ |\psi_n \rangle \cdots |\psi_3 \rangle |\psi_2 \rangle |\psi_1 \rangle \]

\[ \hat{U}(\{\sigma\}) \quad \hat{U}(\{\sigma\}) \quad \hat{U}(\{\sigma\}) \quad \cdots \quad \hat{U}(\{\sigma\}) \]

\[ U(\{\sigma\})_{kl} = \langle \psi_k | \hat{U}(\{\sigma\}) | \psi_l \rangle \]
More details of the calculations:

- Lattice sizes used from $8^3 \times 257$ (high Ts) to $8^3 \times 1732$ (low Ts), $<N>=50$, and $6^3 \times 257$ (high Ts) to $6^3 \times 1361$ (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 $T \approx T_c$. 
Superfluid to Normal Fermi Liquid Transition

\[ a = \pm \infty \]

\[ \xi(T=0) \approx 0.41(2) \]

\[ E_{\text{quasi-particles}}(T) = \frac{3}{5} \varepsilon_F N \left( \frac{2}{e} \right)^{7/3} \varepsilon_F \exp \left( \frac{\pi}{2k_F a} \right) \]

\[ \Delta = \left( \frac{2}{e} \right)^{7/3} \varepsilon_F \exp \left( \frac{\pi}{2k_F a} \right) \exp \left( \frac{-\Delta}{T} \right) \]

\[ E_{\text{phonons}}(T) = \frac{3}{5} \varepsilon_F N \left( \frac{3\pi^4}{16\xi^3} \right)^{\frac{1}{2}} \left( \frac{T}{\varepsilon_F} \right)^{\frac{1}{4}}, \quad \xi_s \approx 0.44 \]

\[ E = \frac{3}{5} \varepsilon_F(n) N \left( \frac{T}{\varepsilon_F(n)} \right) \]

\[ n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}, \quad \varepsilon_F(n) = \frac{\hbar^2 k_F^2}{2m} \]

\[ S(T) = S(0) + \int_0^T \frac{\partial E}{\partial T} \frac{dT}{T} \]

\[ S(T) = \frac{3}{5} N \int_0^{e_F} dy \frac{\xi'(y)}{y} \]
\[ \rho_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = \langle \hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_4)\hat{\psi}^\dagger(\mathbf{r}_3) \rangle \]

\[ \rho_2^p(\mathbf{r}) = \frac{2}{N} \int d^3 r_1 d^3 r_2 \rho_2(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2 + \mathbf{r}, \mathbf{r}_1, \mathbf{r}_2) \]

\[ \lim_{r \to \infty} \rho_2^p(\mathbf{r}) = \alpha - \text{condensate fraction} \]

More Results...

Condensate fraction \( \alpha \):
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
Low temperature behaviour of a Fermi gas in the unitary regime

\[
E(T) = \frac{3}{5} \varepsilon_F N \xi \left( \frac{T}{\varepsilon_F} \right) \quad \text{and} \quad \frac{\mu(T)}{\varepsilon_F} \approx \xi_s \approx 0.41(2) \quad \text{for} \quad T < T_C
\]

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

\[
\xi \left( \frac{T}{\varepsilon_F} \right) = \xi_s + \zeta_s \left( \frac{T}{\varepsilon_F} \right)^{5/2} , \quad \zeta_s \approx 11(1)
\]

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

Lattice results disfavor either \( n \geq 3 \) or \( n \leq 2 \) and suggest \( n = 2.5(0.25) \)

This is the same behavior as for a gas of noninteracting (!) bosons below the condensation temperature.
\[ E(T) \approx \frac{3}{5} \varepsilon_F N \xi_s + \frac{m_B^{3/2} \Gamma \left( \frac{3}{2} \right) \zeta \left( \frac{3}{2} \right)}{2^{1/2} \pi^2 \hbar^3} T^{5/2} V, \quad \text{if} \quad T \gg m_B c^2 \]

and fitting to lattice results \( \Rightarrow \quad m_B \approx 3m \)

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

✓ Fully non-perturbative calculations for a spin $\frac{1}{2}$ many fermion system in the unitary regime at finite temperatures are feasible and apparently the system undergoes a phase transition in the bulk at $T_c = 0.23 (2) \varepsilon_F$

(Exp: $T_c = 0.27(2) \varepsilon_F$, J. Kinast et al. Science, 307, 1296 (2005): Based on theoretical assumptions).

✓ 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 equally 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


T. Lee, D. Schafer, nucl-th/0509018

X.-J. Liu, H. Hu, cond-mat/0505572

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Quest for unitary point critical temperature

Boris Svistunov’s talk (updated), Seattle 2005