Specific heat of a fermionic atomic cloud in the bulk and in traps

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Outline

- Some general remarks
- Path integral Monte Carlo for many fermions on the lattice at finite temperatures and bulk finite T properties
- Specific heat of fermionic clouds in traps
- Conclusions
Superconductivity and superfluidity in Fermi systems

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

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*units (1 eV $\approx 10^4$ K)*
A little bit of history
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.

• Thomas’ Duke group (2002) demonstrated experimentally that such systems are (meta)stable.
Bertsch’s regime is nowadays called the unitary regime

The system is very dilute, but strongly interacting!

\[
\begin{align*}
n r_0^3 & \ll 1 \\
n |a|^3 & \gg 1 \\
r_0 & \ll n^{-1/3} \approx \frac{\lambda_F}{2} \ll |a|
\end{align*}
\]

- \( n \) - number density
- \( r_0 \) - range of interaction
- \( a \) - scattering length
Expected phases of a two species dilute Fermi system

**BCS-BEC crossover**

- High T, normal atomic (plus a few molecules) phase
- **Strong interaction**
  - weak interaction
  - BCS Superfluid
    - \(a<0\)
      - no 2-body bound state
  - strong interaction
  - Molecular BEC and Atomic+Molecular Superfluids
    - \(a>0\)
      - shallow 2-body bound state
      - halo dimers
Early theoretical approach to BCS-BEC crossover
Dyson (?), Eagles (1969), Leggett (1980) …

\(| gs \rangle = \prod_k \left( u_k + v_k a_k^\uparrow a_k^\downarrow \right) | \text{vacuum} \rangle \quad \text{BCS wave function}

\[ \frac{m}{4\pi \hbar^2 a} = \sum_k \left( \frac{1}{2\varepsilon_k} - \frac{1}{2E_k} \right) \quad \text{gap equation} \]

\[ n = 2 \sum_k \left( 1 - \frac{\varepsilon_k - \mu}{E_k} \right) \quad \text{number density equation} \]

\[ \Delta \approx \frac{8}{\varepsilon_F} \exp \left( \frac{\pi}{2k_F a} \right) \quad \text{pairing gap} \]

\[ \varepsilon_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2} \quad \text{quasi-particle energy} \]

\[ E_k = \frac{\hbar^2 k^2}{2m}, \quad u_k^2 + v_k^2 = 1, \quad v_k^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_k - \mu}{E_k} \right) \]

\[ E_{\text{total}} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} + \frac{\pi \hbar^2 a}{m} n + \ldots - \frac{3\Delta^2}{8\mu}, \quad n = \frac{k_F^3}{3\pi^2} \quad \text{Neglected/overlooked} \]
Consequences:

• Usual BCS solution for small and negative scattering lengths, with exponentially small pairing gap

• For small and positive scattering lengths this equations describe a gas a weakly repelling (weakly bound/shallow) molecules, essentially all at rest (almost pure BEC state)

\[ \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \ldots) \approx A[\varphi(\vec{r}_{12})\varphi(\vec{r}_{34})\ldots] \]

In BCS limit the particle projected many-body wave function has the same structure (BEC of spatially overlapping Cooper pairs)

• For both large positive and negative values of the scattering length these equations predict a smooth crossover from BCS to BEC, from a gas of spatially large Cooper pairs to a gas of small molecules
What is wrong with this approach:

- The BCS gap (a<0 and small) is overestimated, thus the critical temperature and the condensation energy are overestimated as well.

- In BEC limit (a>0 and small) the molecule repulsion is overestimated.

- The approach neglects of the role of the “meanfield (HF) interaction,” which is the bulk of the interaction energy in both BCS and unitary regime.

- All pairs have zero center of mass momentum, which is reasonable in BCS and BEC limits, but incorrect in the unitary regime, where the interaction between pairs is strong!!! (this situation is similar to superfluid $^4$He)

$$\Psi\left(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4, \ldots\right) \approx \mathcal{A}\left[\varphi(\vec{r}_{12})\varphi(\vec{r}_{34})\ldots\right]$$

Fraction of non-condensed pairs (perturbative result)!!?

$$\frac{n_{ex}}{n_0} = \frac{8}{3\sqrt{\pi}} \sqrt{n_m a_{mm}^3}, \quad n_m = \frac{n}{2}, \quad a_{mm} \approx 0.6a$$
Two-body density matrix and condensate fraction

\[ \langle \psi_{\uparrow}^+(\vec{r}_1 + \vec{r})\psi_{\downarrow}^+(\vec{r}_2 + \vec{r})\psi_{\uparrow}(\vec{r}_1)\psi_{\downarrow}(\vec{r}_2) \rangle \xrightarrow{r \to \infty} F^2(\mid \vec{r}_1 - \vec{r}_2 \mid) \]

where

\[ F(\mid \vec{r}_1 - \vec{r}_2 \mid) = \langle \psi_{\uparrow}(\vec{r}_1)\psi_{\downarrow}(\vec{r}_2) \rangle \quad \text{order parameter} \]

\[ g_2(r) = \frac{2}{N} \int d^3 r_1 d^3 r_2 \langle \psi_{\uparrow}^+(\vec{r}_1 + \vec{r})\psi_{\downarrow}^+(\vec{r}_2 + \vec{r})\psi_{\uparrow}(\vec{r}_1)\psi_{\downarrow}(\vec{r}_2) \rangle \]

From a talk of Stefano Giorgini (Trento)
What is the best theory for the $T=0$ case?
Fixed-Node Green Function Monte Carlo approach at $T=0$

$$\Delta_{\text{BCS}} \approx \frac{8}{e^2} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

$$\Delta_{\text{Gorkov}} \approx \left(\frac{2}{e}\right)^{7/3} \varepsilon_F \exp\left(\frac{\pi}{2k_F a}\right)$$

Carlson et al. PRL 91, 050401 (2003)
Chang et al. PRA 70, 043602 (2004)
Astrakharchik et al. PRL 93, 200404(2004)
Even though two atoms can bind, there is no binding among dimers!

Fixed node GFMC results, J. Carlson et al. (2003)
Theory for fermions at $T > 0$
in the unitary regime

Put the system on a spatio-temporal lattice and use
a path integral formulation of the problem
A short detour

Let us consider the following one-dimensional Hilbert subspace (the generalization to more dimensions is straightforward)

\[ P^2 = P \] projector in this Hilbert subspace

\[ \langle x \mid P \mid y \rangle = \int_{-\frac{\pi}{l}}^{\frac{\pi}{l}} \frac{dk}{2\pi} \exp[ik(x - y)] = \frac{\sin\left(\frac{\pi}{l}(x - y)\right)}{\pi(x - y)} \]

\[ \Delta_\alpha(x) = P \left[ \delta(x - x_\alpha) \right] , \quad \langle \Delta_\alpha \mid \Delta_\beta \rangle = \Delta_\alpha(x_\beta) = \Delta_\beta(x_\alpha) = K_\alpha \delta_{\alpha\beta} \]

\[ \psi(x) = \sum_{\alpha=1}^{N} c_\alpha \Delta_\alpha(x) + O(\exp(-cN)) \approx \sum_{n} \psi(nl) \frac{\sin\left(\frac{\pi}{l}(x - nl)\right)}{\frac{\pi}{l}(x - nl)} \]

\[ c_\alpha = \int dx \frac{1}{K_\alpha} \Delta_\alpha(x)\psi(x) = \frac{1}{K_\alpha} \psi(x_\alpha), \quad x_\alpha = nl \]

Schroedinger equation

\[ \psi(x) = \sum_{\alpha=1}^{N} d_{\alpha} F_{\alpha}(x) + O(\exp(-cN)) \]

\[ F_{\alpha}(x) = \frac{1}{\sqrt{K_{\alpha}}} \Delta_{\alpha}(x), \quad x_{\alpha} = nl, \quad \langle F_{\alpha} \mid F_{\beta} \rangle = \delta_{\alpha\beta} \]

\[ \sum_{\beta} \left[ \langle F_{\alpha} \mid T \mid F_{\beta} \rangle + V(x_{\alpha})\delta_{\alpha\beta} \right] d_{\beta} = Ed_{\alpha} \]
\[ \Delta, \epsilon_F, T \ll \frac{\hbar^2 \pi^2}{2m l^2} \]
\[ \delta \epsilon > \frac{2\hbar^2 \pi^2}{m L^2} \]
\[ \epsilon_F, \Delta \gg \frac{2\hbar^2 \pi^2}{m L^2} \]
\[ \xi \ll L = N_s l \]
\[ \delta p > \frac{2\pi \hbar}{L} \]
Grand Canonical Path-Integral Monte Carlo

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

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

**Trotter expansion (trotterization of the propagator)**

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

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

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

No approximations so far, except for the fact that the interaction is not well defined!
Recast the propagator at each time slice and put the system on a 3d-spatial lattice, in a cubic box of side $L=\text{N}_s l$, with periodic boundary conditions.

$$\exp\left[-\tau\left(\hat{H} - \mu\hat{N}\right)\right] \approx \exp\left[-\tau\left(\hat{T} - \mu\hat{N}\right)/2\right]\exp(-\tau\hat{V})\exp\left[-\tau\left(\hat{T} - \mu\hat{N}\right)/2\right] + O(\tau^3)$$

Discrete Hubbard-Stratonovich transformation

$$\exp(-\tau\hat{V}) = \prod_{\vec{x}} \sum_{\sigma_{\pm}(\vec{x})=\pm 1} \frac{1}{2} \left[ 1 + \sigma_{\pm}(\vec{x})\hat{A}\hat{n}_{\uparrow}(\vec{x}) \right] \left[ 1 + \sigma_{\pm}(\vec{x})\hat{A}\hat{n}_{\downarrow}(\vec{x}) \right], \quad A = \sqrt{\exp(\tau g) - 1}$$

$\sigma$-fields fluctuate both in space and imaginary time

$$\frac{m}{4\pi\hbar^2 a} = -\frac{1}{g} + \frac{mk_c}{2\pi^2\hbar^2}, \quad k_c < \frac{\pi}{l}$$

Running coupling constant $g$ defined by lattice
How to choose the lattice spacing and the box size

\[ n(k) \]

\[ 2\pi/L \]

\[ L \text{ – box size} \]

\[ l \text{ - lattice spacing} \]

\[ k_{\text{max}} = \pi/l \]
\[ Z(T) = \int \prod_{\vec{x}, \tau} D\sigma(\vec{x}, \tau) \, \text{Tr} \, \hat{U}(\{\sigma\}) \]

\[ \hat{U}(\{\sigma\}) = T_{\tau} \prod_{\tau} \exp\{-\tau[\hat{h}(\{\sigma\}) - \mu]\} \]

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

\[ \text{Tr} \, \hat{U}(\{\sigma\}) = \{\det[1 + \hat{U}(\{\sigma\})]\}^2 = \exp[-S(\{\sigma\})] > 0 \]

\[ n_{\uparrow}(\vec{x}, \vec{y}) = n_{\downarrow}(\vec{x}, \vec{y}) = \sum_{k,l<k_c} \varphi_{\vec{k}}^\dagger(\vec{x}) \left[ \frac{\hat{U}(\{\sigma\})}{1 + \hat{U}(\{\sigma\})} \right]_{\vec{k}} \varphi_{\vec{l}}^* (\vec{y}), \quad \varphi_{\vec{k}}(\vec{x}) = \frac{\exp(i\vec{k} \cdot \vec{x})}{\sqrt{V}} \]

No sign problem! One-body evolution operator in imaginary time

All traces can be expressed through these single-particle density matrices
More details of the calculations:

- Lattice sizes used from $6^3 \times 300$ (high Ts) to $6^3 \times 1361$ (low Ts) $8^3$ running (incomplete, but so far no surprises) and larger sizes to come.

- 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 $\sigma(x,\tau)$ 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 $100,000 - 2,000,000$ $\sigma(x,\tau)$- field configurations for calculations.

- MC correlation “time” $\approx 250 - 300$ time steps at $T \approx T_c$. 
\[ a = \pm \infty \]

Superfluid to Normal Fermi Liquid Transition

Normal Fermi Gas
(with vertical offset, solid line)

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

Bogoliubov-Anderson phonons
contribution only (little crosses)
People never consider this ???

Quasi-particles contribution only
(dashed line)

\[ \mu - \text{chemical potential} \]

(circles)

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

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

\[
\Delta = \left( \frac{2}{e} \right)^{7/3} \varepsilon_F \exp\left( \frac{\pi}{2k_F a} \right)
\]
\[ E = \mu N - PV + TS = \frac{3}{5} \varepsilon_F(n)N \exp \left( \frac{T}{\varepsilon_F(n)} \right) = \varepsilon(n)nV \]

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

\[ S = \frac{5}{3} \frac{e(n) - \mu}{T} N = N\sigma \left( \frac{T}{\varepsilon_F(n)} \right), \quad P = \frac{2}{3} e(n)n \]

\[ E(T), F(T), [0.6\varepsilon_F(N), \mu, \varepsilon_F(N), S[N]] \]
Specific heat of a fermionic cloud in a trap

At $T << T_c$ only the Bogoliubov-Anderson modes in a trap are excited

In a spherical trap

$$\Omega_{nl} = \omega \sqrt{\frac{4}{3} n(n + l + 2) + l} \approx \frac{\omega}{\sqrt{3}} (2n + l)$$

In an anisotropic trap

$$\Omega(n_x, n_y, n_z) \approx \frac{1}{\sqrt{3}} \left[ (n_x + n_y) \omega_\perp + n_z \omega_\parallel \right]$$
Now we can estimate $E(T)$

$$E_s(T) \approx E_{gs} + \sum_{n_x, n_y, n_z} \frac{\hbar \Omega(n_x, n_y, n_z)}{\exp[\beta \hbar \Omega(n_x, n_y, n_z)] - 1}, \quad \beta = \frac{1}{T}$$

$$\Omega(n_x, n_y, n_z) \approx \frac{1}{\sqrt{3}} \left[ (n_x + n_y) \omega_\perp + n_z \omega_\parallel \right]$$

$$E_s(T) \approx E_{gs} + \begin{cases} 
\hbar \omega_\parallel \exp(-\beta \hbar \omega_\parallel), & T \ll \hbar \omega_\parallel \\
\frac{\sqrt{3} \pi^2}{6} \frac{T^2}{\hbar \omega_\parallel}, & \hbar \omega_\parallel \ll T \ll \hbar \omega_\perp \\
3^{3/2} \pi^4 \frac{T^4}{30 \hbar^3 \omega_\parallel \omega_\perp^2}, & \hbar \omega_\perp \ll T \ll T_c 
\end{cases}$$
The previous estimate used an approximate collective spectrum. Let us use the exact one for spherical traps:

\[
\Omega_{nl} = \omega \sqrt{\frac{4}{3} n(n + l + 2) + l} \quad \Rightarrow \quad \Omega_{\text{surf}} = \omega \sqrt{1 + \frac{4n}{3}} l
\]

\[
E_s(T) \approx E_{gs} + \sum_{n,l}^1 \frac{(2l + 1) \hbar \Omega_{nl}}{\exp[\beta \hbar \Omega_{nl}] - 1} \approx \sqrt{\xi_s \hbar \omega} (3N)^{4/3} + 142 \frac{T^5}{\hbar^4 \omega^4}
\]

\[
E_s(T) \approx E_{gs} + 2\hbar \omega \sum_{n=0}^{\infty} \sqrt{1 + \frac{4n}{3}} \int dl \ l^{3/2} \exp\left(-\frac{\hbar \omega l^{1/2}}{T} \sqrt{1 + \frac{4n}{3}}\right)
\]

\[
\approx \frac{\sqrt{\xi_s \hbar \omega} (3N)^{4/3}}{4} + 140 \frac{T^5}{\hbar^4 \omega^4}
\]

The last estimate includes only the surface modes.
Let us try to estimate the contribution from surface modes in a deformed trap (only n=0 modes):

\[ \Omega_{\text{surf}}^2(S) = k \frac{F(S)}{m}, \quad F(S) = |\nabla U(\vec{r})|_S \]

\[ U(\vec{r}) = \frac{m\omega^2}{2} \left( x^2 + y^2 + \lambda^2 z^2 \right) \]

\[ E_s(T) \approx E_{gs} + \int \frac{dS d^2k}{(2\pi)^2} \frac{\hbar \Omega_{\text{surf}}(S)}{\exp\left[ \beta \hbar \Omega_{\text{surf}}(S) \right] - 1} \]

\[ \approx \sqrt{\xi} \hbar \omega \left( 3N \right)^{4/3} + \frac{96T^5}{\hbar^4 \omega^4} \arctan \sqrt{\lambda^2 - 1} \]

\[ \frac{4}{\lambda \sqrt{\lambda^2 - 1}} \]
Let us estimate the maximum temperature for which this formula is reasonable:

\[ l^2 \approx \frac{T}{\hbar \omega} < l_{\text{max}}^2 \approx \xi_s (24N)^{2/3} \]

\[ E_s(T) < \frac{\sqrt{\xi_s} \hbar \omega (3N)^{4/3}}{4} + 140\hbar \omega \xi_s^{5/2} (24N)^{5/3} \]

\[ F_s(T) \approx \frac{\sqrt{\xi_s} \hbar \omega (3N)^{4/3}}{4} - 35 \frac{T^5}{\hbar^4 \omega^4} > \frac{\sqrt{\xi_s} \hbar \omega (3N)^{4/3}}{4} - 35\hbar \omega \xi_s^{5/2} (24N)^{5/3} \]

\[ F_n(T) \approx \frac{\sqrt{\xi_n} \hbar \omega (3N)^{4/3}}{4} - \frac{\pi^2 (3N)^{2/3} T^2}{6 \xi_n^{1/2} \hbar \omega} \]
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 $T_c = 0.22 (3) \varepsilon_F$

(One variant of the fortran 90 program, version in matlab, has about 500 lines, and it can be shortened also. This is about as long as a PRL!)

✓ 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

✓ In a trap the surface modes seem to affect significantly the thermodynamic properties of a fermionic atomic cloud