Short-range correlations and entropy in ultracold atomic Fermi gases


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BEC-BCS crossover


In a two component fermion gas with attractive interactions

Pair size ~ mean distance
Feshbach resonances

The interaction couples scattering in multiple channels.

\[ V(r) = f(r) + g(r)S_1 \cdot S_2 \]

Zeeman energy difference
\[ \sim B_z \Delta S_z \]

Spin singlet
Spin triplet

BEC limit
BCS limit

e.g., I. Bloch, J. Dalibard, and W. Zwerger
Rev. Mod. Phys. 80, 885 (2008)
Feshbach resonances

The s-wave scattering length tells the effective scattering in one channel.

Strongly interacting regime

\[ |n^{1/3}a| \gg 1 \]

Challenging for microscopic theories

Correlations at short distances

In a gas consisting of particles of species \( |i> \) and \( |j> \) interacting with a potential with range \( r_0 \), in the dilute limit \( r_0 \ll d \) (mean distance between particles), the correlation functions have the asymptotic form

\[
\langle \psi_i^+ (\vec{r}) \psi_j^+ (0) \psi_j (0) \psi_i (\vec{r}) \rangle \sim C_{ij} \left( \frac{1}{r} - \frac{1}{a_{ij}} \right)^2
\]

Jastrow factor

in the regime \( r_0 \ll r \ll d \)

Where \( a_{ij} \) is the s-wave scattering length characterizing the low energy scattering between \( |i> \) and \( |j> \).

The Jastrow factor comes from solving the zero-energy Schrodinger equation of the relative coordinates at short distances

\[
\langle \psi_i^+ (\vec{r}) \psi_i^+ (0) \psi_i (0) \psi_i (\vec{r}) \rangle \sim \chi_{ij}^2 (r) / r^2
\]

\[
\left( -\frac{1}{m} \frac{d^2}{dr^2} + V_{ij} (r) \right) \chi_{ij} (r) = 0
\]

for \( r_0 \ll r \ll d \)

\[
\chi_{ij} (r) \sim 1 - r / a_{ij}
\]

Determined by two-body physics
The correlation strength (contact) is determined by non-trivial many-body physics

\[ C_{ij}(a_{ij}, n_i, n_j, T) \]

The contact encapsulates essential thermodynamic information

\[ C = -\frac{m}{4\pi} \frac{\partial (F/V)}{\partial a^{-1}} \]


The hamiltonian

\[ H = \sum_{\sigma=1}^{2} \int d\vec{r} \psi_{\sigma}^+(\vec{r}) \left( -\frac{\nabla^2}{2m} \right) \psi_{\sigma}(\vec{r}) + \int d\vec{r} \int d\vec{r}' V(|\vec{r} - \vec{r}'|) \psi_1^+(\vec{r}) \psi_2^+(\vec{r}') \psi_2(\vec{r}') \psi_1(\vec{r}) \]

Let us \( V(r) \to \lambda V(r) \) \( a \to a_\lambda \) \hspace{1cm} We will take \( \lambda=1 \) at the end.

\[ \frac{\partial (F_\lambda/V)}{\partial a_\lambda^{-1}} = \frac{\partial (F_\lambda/V)}{\partial \lambda} \frac{\partial \lambda}{\partial a_\lambda^{-1}} \]

\[ = \int d\vec{r} V(r) \langle \psi_1^+(\vec{r}) \psi_2^+(0) \psi_2(0) \psi_1(\vec{r}) \rangle \frac{\partial \lambda}{\partial a_\lambda^{-1}} = C_\lambda \int_0^\infty dr V(r) \chi_\lambda^2(r) \frac{\partial \lambda}{\partial a_\lambda^{-1}} \]

\[ \int_0^{r_c} dr X_\lambda'(r) \left( -\frac{1}{m} \frac{d^2}{dr^2} + \lambda V(r) \right) X_\lambda(r) = 0 \quad r_0 \ll r_c \ll n^{-1/3} \]

\[-\frac{1}{m} \left( X_\lambda', X_\lambda' - X_\lambda, X_\lambda \right)_{r_c} + \int_0^{r_c} dr \left( -\frac{1}{m} \frac{d^2}{dr^2} + \lambda V(r) \right) X_\lambda'(r) \right] X_\lambda(r) = 0 \]

\[\left( -\frac{1}{m} \frac{d^2}{dr^2} + \lambda' V(r) \right) X_\lambda'(r) = 0 \quad X_\lambda(0) = 0 \quad X_\lambda(r) = 1 - r/a_\lambda, \quad @ r \sim r_c \]

\[
\frac{1}{a_\lambda} - \frac{1}{a_\lambda'} = -m(\lambda' - \lambda) \int_0^\infty dr V(r) X_\lambda(r) X_\lambda'(r)
\]

In the limit \( \lambda \to \lambda' \)

\[
\int_0^\infty dr V(r) X_\lambda^2(r) \frac{\partial \lambda}{\partial a_\lambda^{-1}} = -\frac{1}{m}
\]

Taking \( \lambda = 1 \)

\[ C = -\frac{m}{4\pi} \frac{\partial (F/V)}{\partial a^{-1}} \]
Correlation strength at zero temperature

The ground state energy per particle

\[ \frac{E_{\text{gnd}}}{2N} = \frac{3}{5} \left(1 + \beta(\xi)\right) E_F \quad E_F = k_F^2/2m, \ n = k_F^3/6\pi^2, \ \xi = -1/k_F a \]

The contact

\[ C(T=0) = \frac{k_F^4}{40\pi^3} \frac{\partial \beta}{\partial \xi} \]

In the BEC limit, \( a \to 0^+ \), fermions form bosonic molecules with bound energy \( E_b = -1/ma^2 \)

\[ \frac{E}{2N} = \frac{E_b}{2} + \frac{\pi}{6} E_F k_F a m \left(1 + \frac{128}{15\sqrt{6\pi^3}} (k_F a_m)^{3/2} + \ldots \right) \quad C = \frac{n}{2\pi a} \]

the scattering length between molecules

In the BCS limit, \( a \to 0^- \), BCS pairing is exponentially small

\[ \frac{E}{2N} = E_F \left[ \frac{3}{5} + \frac{2}{3\pi} k_F a + \frac{4(11-2\log 2)}{35\pi^2} (k_F a)^2 + \ldots \right] \quad C = a^2 n^2 \]
Correlation strength @ T=0

Generally, $\beta$ can be calculated by quantum Monte Carlo simulation.


In the BEC limit, $a \rightarrow 0^+$, fermions form bosonic molecules with bound energy $E_b = -1/ma^2$.

In the BCS limit, $a \rightarrow 0^-$, BCS pairing is exponentially small; the leading interaction energy is the Hartree mean field energy.
How does $C(T)$ vary with $T$?

By thermodynamic identity

$$\frac{\partial C}{\partial T} = - \frac{m}{4\pi} \frac{\partial}{\partial a^{-1}} \left( \frac{F}{V} \right) = \frac{m}{4\pi} \frac{\partial (S/V)}{\partial a^{-1}}$$

$C$ is related to the isentropes in the $T$-$a$ plane.

In the limit $T \to 0$, in the superfluid phase, phonons are the only gapless excitations

$$S \approx S_{\text{phonon}} = \frac{2\pi^2}{45} V \left( \frac{T}{v_s} \right)^3$$

The sound velocity $v_s$ can be calculated by the formula

$$m v_s^2 = n \frac{\partial \mu}{\partial n}$$

@ $T=0$

$$\mu = \frac{\partial E}{\partial N} = E_F \left( 1 + \beta - \frac{1}{5} \beta' \xi \right) \left( \frac{v_s}{k_F \sqrt{3m}} \right)^2 = 1 + \beta - \frac{3}{5} \beta' \xi + \frac{1}{10} \beta'' \xi^2$$
Correlation strength in the low $T$ limit

\[ \frac{\partial v_s}{\partial a^{-1}} < 0 \quad \frac{\partial S_{\text{phonon}}}{\partial a^{-1}} = -\frac{3 S_{\text{phonon}}}{v_s} \frac{\partial v_s}{\partial a^{-1}} > 0 \]

\[ \delta C = C(T) - C(0) = -\frac{\pi m}{120} \left( \frac{T}{v_s} \right)^4 \frac{\partial v_s}{\partial a^{-1}} > 0 \]

Phonon enhanced correlations
Correlation strength in the low $T$ limit

At higher temperatures, pairs are dissociated by thermal energy; fermionic excitations reduce $C$.

\[
\frac{\partial C}{\partial T} = \frac{m}{4\pi} \frac{\partial (S/V)}{\partial a^{-1}}
\]

Within the BCS mean field approach,

\[
\frac{\delta (S_f/V)}{\delta a^{-1}} = \frac{1}{V} \sum_k \frac{\delta S_f}{\delta f_k} \frac{\delta f_k}{\delta \Delta} \frac{\delta \Delta}{\delta a^{-1}}
\]

Since

\[
\frac{\delta F}{\delta f_k} = 0, \quad \frac{\delta S_f}{\delta f_k} = \frac{E_k}{T}
\]

\[
\frac{\delta f_k}{\delta \Delta} < 0, \quad \frac{\delta \Delta}{\delta a^{-1}} > 0
\]

Thus

\[
\frac{\delta (S_f/V)}{\delta a^{-1}} < 0
\]
\[
\lim_{r \to 0} \langle \psi_1^+ (\vec{r}) \psi_2^+ (0) \psi_2 (0) \psi_1 (\vec{r}) \rangle
\]

measures the probability of fermions staying close to each other.

The pair structure of the molecules is rigid since \( |E_b| \gg T \)
The same low temperature physics is described by the boson model

\[
H_m = \int d \vec{r} \phi^+ (\vec{r}) \left( -\frac{\nabla^2}{2M} \right) \phi (\vec{r}) + \frac{1}{2} \int d \vec{r} \int d \vec{r}' V_m (|\vec{r} - \vec{r}'|) \phi^+ (\vec{r}) \phi^+ (\vec{r}') \phi (\vec{r}') \phi (\vec{r})
\]

Characterized by \(a_m\)

The boson correlation function has the similar asymptotic form

\[
\lim_{r \to 0} \langle \phi^+ (\vec{r}) \phi^+ (0) \phi (0) \phi (\vec{r}) \rangle \sim C_m (1/r - 1/a_m)^2
\]

\[
C_m = -\frac{M}{2\pi} \frac{\partial (F_m / V)}{\partial a_m^{-1}} \quad M = 2m
\]

Since the thermal induced variation \(\delta F = \delta F_m\)

\[
\delta C = -\frac{m}{4\pi} \frac{\partial (\delta F / V)}{\partial a^{-1}} = -\frac{m}{4\pi} \frac{\partial (\delta F_m / V)}{\partial a_m^{-1}} \frac{\partial a_m^{-1}}{\partial a^{-1}} = \frac{m}{2M} \frac{\partial a_m^{-1}}{\partial a^{-1}} \delta C_m
\]
Bogoliubov approximation in the BEC limit

Let us assume the contact pseudopotential

\[ V_m(r) = U_0 \delta(\vec{r}), \quad U_0 = 4\pi a_m / M \]

Divide the field operator into the condensate and fluctuation parts

\[ \Phi(\vec{r}) = \Phi_0 + \delta \Phi(\vec{r}) \]

To the second order of the fluctuations,

\[ \lim_{r \to 0} \langle \delta \Phi^+(\vec{r}) \delta \Phi^+(0) \Phi(0) \Phi(\vec{r}) \rangle = n_0^2 + 2n_0 (2 \langle \delta \Phi^+ \delta \Phi \rangle + \langle \delta \Phi^+(\vec{r}) \delta \Phi^+(0) \rangle) \quad + \ldots \]

\[ \langle \delta \Phi^+ \delta \Phi \rangle = \frac{1}{V} \sum_k \left[ v_k^2 + (u_k^2 + v_k^2) \langle \alpha_k^+ \alpha_k \rangle \right] \]

\[ \lim_{r \to 0} \langle \delta \Phi^+(\vec{r}) \delta \Phi^+(0) \rangle = -\frac{n_0 a_m}{r} - \frac{1}{V} \sum_k \left( u_k v_k - \frac{U_0 n_0}{k^2} \right) - \frac{2}{V} \sum_k u_k v_k \langle \alpha_k^+ \alpha_k \rangle \]

\[ v_k^2 = (\xi_k / E_k - 1)/2, \quad u_k^2 = (\xi_k / E_k + 1)/2, \quad \xi_k = k^2 / 2 M + U_0 n_0 \]
Bogoliubov approximation in the BEC limit

To calculate $\delta C_m$, we only need to focus on the temperature variance of r-independent part of

$$\lim_{r \to 0} \langle \phi^+(\vec{r}) \phi^+(0) \phi(0) \phi(\vec{r}) \rangle \sim C_m (1/r - 1/a_m)^2$$

which is

$$\frac{\delta C_m}{a_m^2} = \frac{2n}{V} \sum_k (u_k^2 + v_k^2 - 2u_k v_k) \langle \alpha_k^+ \alpha_k \rangle = \frac{\pi}{30} n T^4 v_{\sigma}^{-4}$$

$\nu_s^2 = U_0 n_0 / M^2$

$$\delta C = -\frac{\pi m}{120} \left( \frac{T}{\nu_s} \right)^4 \frac{\partial \nu_s}{\partial a^{-1}}$$

agrees with the general phonon argument
In the number conversed state,

\[ \int d \vec{r} \langle \phi^+(\vec{r}) \phi^+(0) \phi(0) \phi(\vec{r}) \rangle = (N - 1)n \quad \text{normalized} \]

For repulsive bosons \( a_m \sim r_0 \)  \( a_m \ll d \ll \xi \)

\[ \langle \phi^+(\vec{r}) \phi^+(0) \phi(0) \phi(\vec{r}) \rangle \]

\[ C_m \left( 1/r - 1/a_m \right)^2 \quad \text{Thermal energy overcomes the repulsive interactions.} \]
Correlation strength in high T limit

Calculate the partition function

\[ Z = \text{Tr} \ e^{-\beta (H - \mu_1 N_1 - \mu_2 N_2)} \]


To the second order in the fugacity \( z_i = e^{\beta \mu} \)

\[ \ln (Z / Z_0) = 2^{3/2} V \ z_1 \ z_2 \ b_2 / \lambda^3 \]

\[ b_2 = \sum_i e^{\beta |E_i|} + \int_0^\infty \frac{dk}{\pi} \frac{d \delta(k)}{dk} e^{-\beta k^2 / m} \]

Bound states due to \( V(r) \)

the thermal wavelength \( \lambda = \sqrt{2 \pi \beta / m} \)

the s-wave phase shift for the scattering states

E. Beth and G. E. Uhlenbeck, Physica (Amsterdam) 4, 915 (1937)
In the BEC-BCS crossover regime, we consider the only relevant bound state with

\[ E_b = -1/ma^2 \]

For the scattering continuum

\[ k \cot \delta(k) = -\frac{1}{a} \]

\[ b_2(\lambda/a) = \left( \frac{1}{2} - \frac{1}{\sqrt{\pi}} \int_{0}^{\lambda/a} e^{-t^2} dt \right) e^{\lambda^2/2\pi a^2} \]


\[ C = \frac{m}{4\pi \beta V} \frac{\partial \log Z}{\partial a^{-1}} = \sqrt{2} n_1 n_2 \lambda^2 \frac{\partial b_2(\lambda/a)}{\partial (\lambda/a)} \rightarrow \frac{2n^2}{mT} \]

for \( \lambda/a \to 0 \), \( \frac{\partial b_2(\lambda/a)}{\partial (\lambda/a)} = \frac{1}{\sqrt{2\pi}} \)
Correlation strength at finite $T$

Virial expansion of fermions

$C \downarrow$

$C \sim 1/T$

$E_b / \log(1/k_F a)$

$T < T_c$, $\delta C \sim T^4$

$\lambda \ll a$

Virial expansion of bosons

$C \downarrow$

$T \gg T_F$, Virial expansion

$C \downarrow$

$T < T_F$, Fermi liquid

$S \sim m^* k_F T$, $\delta C \sim T^2$

$T \gg T_F$, Virial expansion

$C \downarrow$

BEC Limit

BCS Limit

$-1/k_F a$
Maximum of the correlation strength at finite $T$

$T_{max} \sim T_F @ 1/a = 0$

$T \sim 1/T$

$\sim T^4$
Correlation strength and isentropes

**FIG. 1.** (Color online) The correlation strength $C(T)$ in the (a) BCS, (b) unitary, and (c) BEC limits. The dashed lines at high $T$ are the virial results, and the dashed line at low $T$ in (b) is from Eq. (17). The solid lines are qualitative interpolations between the increasing low $T$ results and the decreasing high $T$ results. The maximum in $C(T)$ for $T=T_{\text{max}}$ is prominent in the strong-coupling limit, but in the BCS and BEC limits are too small to be visible here.

$T_{\text{max}}\sim T_F$ prominent around unitarity
Correlation strength and isentropes

\[
\frac{\partial C}{\partial T} = \frac{m}{4\pi} \frac{\partial (S/V)}{\partial a^{-1}}
\]


\[ S(T=0.2T_F, a \to 0^-) = S(T=0.2T_F, 1/a = 0) \]

At unitarity, \( T_{\text{max}} > 0.2 \ T_F \)

FIG. 2. (Color online) Sketches of isentropes of a balanced two-component Fermi gas, from which one can infer the temperature dependence of \( C(T) \).
FIG. 3: (Color online) Summary of results for $C/(Nk_F)$ as a function of $T/\varepsilon_F$. The solid datapoints are determined from the large $k/k_F$ behavior of $n(k)$, and the errorbars are dominated by systematics related to the residual fluctuations in the plateaux, as shown in Fig. 2. Also shown are the results of the virial expansion of Ref. [29], as well as the $t$-matrix calculations of Refs. [27, 28].
A resonant electrical field $E$, coupled to the electronic dipole moment, converts fermions into a molecular state which loses from the trap.

The loss rate of the atoms from the trap

$$\Gamma \propto \langle \psi_1^+(\vec{r}) \psi_2^+(0) \psi_2(0) \psi_1(\vec{r}) \rangle$$


coupled to the closed channel

$$\frac{dN(t)}{dt} = -\frac{\Omega^2}{\gamma} \frac{4 \pi a_{bg}}{m \mu_B \Delta B} \left( \frac{1}{a_{bg}} - \frac{1}{a} \right)^2 C$$

$$\Omega = \langle f | d | i \rangle$$


Photoassociation of $^6$Li

BEC side, $k_F a = 0.15$

$T = 0.75T_F$

$T \sim 0$

BSC side, $k_F a = -1$

$T = 0.75T_F$

$T \sim 0$

Virial expansion theoretical result with no fitting parameters

FIG. 2. (Color online) Sketches of isentropes of a balanced two-component Fermi gas, from which one can infer the temperature dependence of $C(T)$. 

\[ T_{\text{max}} \]

\[ T_{\text{c}} \]

\[ \sim T^4 \]

\[ \sim 1/T \]

\[ T_{\text{min}} \]
Thank You

谢谢