Short-range correlations and entropy in ultracold atomic Fermi gases

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We relate short-range correlations in ultracold atomic Fermi gases to the entropy of the system over the entire temperature, T, vs. coupling strength, −1/kF a, plane. In the low temperature limit the entropy is dominated by phonon excitations and the correlations increase as T4. In the BEC limit, we calculate a boson model within the Bogoliubov approximation to show explicitly how phonons enhance the fermion correlations. In the high temperature limit, we show from the virial expansion that the correlations decrease as 1/T. The correlations therefore reach a maximum at a finite temperature. We infer the general structure of the isentropes of the Fermi gas in the T, −1/kF a plane, and the temperature dependence of the correlations in the unitary, BEC, and BCS limits. Our results compare well with measurements of the correlations via photoassociation experiments at higher temperatures.

I. INTRODUCTION

The thermodynamics of an ultracold atomic gas interacting via short range interactions is encoded in the short range two-body correlations of the particles. Such connections between short range correlations and physical properties of systems with short range interactions have been long recognized, e.g., Ref. [1], and have been employed recently to study the rf spectra of paired Fermi gases [2, 3, 4]. Tan has derived a number of remarkable relations between the properties of ultracold atomic gases, e.g., the ground state energy and their short range correlations [5] (see also [6]). These links open new perspectives to examine the many particle physics of systems with short range interactions.

By using Feshbach resonances to tune the scattering length a, one can study atomic Fermi gases through the crossover from a weakly coupled BCS superfluid to a weakly coupled Bose-Einstein condensate (BEC) of molecules. In the strongly correlated unitarity regime, |a| → ∞, the many-body correlations are highly non-trivial and one has to resort to Monte-Carlo calculations to obtain controlled results [2, 3, 4]. At non-zero temperatures T, information on the correlations is even more limited. We study here how knowledge of the free energy and entropy can illuminate the nature of the finite temperature short range two particle correlations. The two-body correlation function in a two component Fermi gas has the general structure

\[ \langle \psi_1^\dagger(r') \psi_2^\dagger(0) \psi_2(0) \psi_1(r) \rangle = \sum_i \gamma_i \phi_i(r) \phi_i^*(r') , \]

as one sees by regarding the correlation function as a Hermitian operator in r, r'. For r ≪ d, the interparticle spacing, the functions \( \phi_i \), essentially s-wave Jastrow factors in the many-body wavefunction at short interparticle distance, are determined by two-body physics, and outside the range of the potential, r0, at temperatures of interest, are \( \sim \sin(kr + \delta)/r = \sin\delta \chi(r)/r \), where \( \chi(r) = 1 - r/a, \) \( \delta \) is the s-wave phase shift, and \( \cot \delta = -1/ka \), where a is the s-wave scattering length. Thus

\[ \langle \psi_1^\dagger(r) \psi_2^\dagger(0) \psi_2(0) \psi_1(r) \rangle = C \left( \frac{\chi(r)}{r} \right)^2 = C \left( \frac{1 - 1/a}{r} \right)^2 . \]

The correlation (or contact) strength C, which is determined by many-body physics, can be measured directly in photoassociation experiments [3, 10].

Here we examine the temperature dependence of the correlations by calculating C(T) from the finite temperature thermodynamics. Quite generally, the short range correlations are related to the free energy density f = Tr e−H/T/Ω (where Ω is the volume of the system) by [4]:

\[ C = -\frac{m}{4\pi} \frac{\partial f}{\partial a} . \]

Differentiating with respect to the temperature, T, we find

\[ \frac{\partial C}{\partial T} = -\frac{m}{4\pi} \frac{\partial f}{\partial T} \frac{\partial a}{\partial a} = -\frac{m}{4\pi} \frac{\partial s}{\partial a} , \]

thus linking the variation of C with temperature to the coupling constant dependence of the entropy density s.

The connection is illustrated below in Fig. which shows the temperature dependence of C, and the related Fig. 2 which shows the isentropes in the T, −1/kF a plane.

We focus on the unitarity, BEC, and BCS limits and provide controlled results for C for both high and low T. Using the virial expansion, we show that the correlations decrease with C ∝ n2/T in the high temperature limit, where n is the density. From the relation between the T dependence of C and the entropy density, we show that C(T) increases with temperature as T4 for low T, owing...
II. CORRELATION FUNCTION AND FREE ENERGY

We consider a homogenous two-component Fermi gas described by the Hamiltonian ($\hbar = 1$ throughout)

$$H = \int d^3r \sum_{i=1,2} \frac{1}{2m} \nabla \psi_i^\dagger(r) \cdot \nabla \psi_i(r) + \int d^3r \int d^3r' V(|r - r'|) \psi_i^\dagger(r) \psi_2^\dagger(r') \psi_2(r') \psi_1(r),$$

(5)

where the $\psi_i$ are the field operators for fermions in internal state $|i\rangle$. We take the range $r_0$ of the interaction $V(r)$ to be short compared to the interparticle spacing $d$.

We first present an elementary derivation of the relation (8) between the two-body correlation function and the free energy density, using the device of scaling the interaction (3) between the two-body correlation function and $\chi$, where we use vanishing of the s-wave function $\chi$ at the origin, and extend the upper bound of the integral from $r_c$ to infinity since $V(r)$ is nonzero only for $r < r_0$. On the other hand, from the Feynman-Hellmann theorem, the variation of the free energy density with coupling strength is

$$\frac{\partial f}{\partial a_\lambda} = \frac{\partial f}{\partial \lambda} \frac{\partial \lambda}{\partial a_\lambda} = \frac{1}{\Omega} \left( \int \frac{\partial H}{\partial \lambda} \frac{\partial \lambda}{\partial a_\lambda} \right),$$

(8)

Combining (8) and (8), and setting $\lambda = 1$, we arrive at the desired relation (3).

We review the application of (8) to a homogeneous equally populated two-component Fermi gas of volume $\Omega$, at $T = 0$. The ground state energy per particle $E/2N$ can be written as $(3/5)(1 + \beta)E_F$, where $\beta$ is a function of the dimensionless quantity $\xi = -1/k_Fa$. The Fermi momentum $k_F$ is defined in terms of the single component density $n = N/\Omega$ by $n = k_F^2/6\pi^2$, and the Fermi energy by $E_F = k_F^2/2m$. Equation (7) implies that $C(T = 0) = (k_F^2/4\pi^2)\partial/\partial \xi$. The function $\beta$ has been calculated by quantum Monte Carlo simulations near unitarity ($1/a \rightarrow 0$); at unitarity $\partial/\partial \xi \approx 0.9$ [1], a result which agrees well with the value $C = 2.7(k_F^4/36\pi^4)$ extracted directly from the correlation function calculated by quantum Monte Carlo methods [8]. In the BCS limit, $-1/k_Fa \gg 1$, a perturbative expansion in $k_Fa$ gives $\frac{E}{2N} = \frac{3}{5}E_F \left[1 + \frac{10}{9\pi}k_Fa + \ldots\right].$ (9)

Corrections to $E$ due to pairing are exponentially small in this limit. Keeping the leading term yields $C = a^{-1}$. In the BEC limit, $1/k_Fa \gg 1$, fermions form molecules and $E/2N = \frac{E_b}{2} + \frac{E_Fk_Fa_m}{6\pi} \left[1 + \frac{128}{15\sqrt{6}\pi^3} (k_Fa_m)^{3/2} + \ldots\right].$ (10)

with $E_b = -1/ma^2$ the molecular binding energy, and $a_m$ the scattering length between molecules. The second term is the Hartree-Fock mean field energy and the third the nonperturbative Lee-Yang correction [11]. Few body calculations give $a_m = 0.6a$ [12]. In the BEC limit, $C = n/2\pi a$ to leading order. The divergent behavior, as $a \rightarrow 0$, arises from the normalization of the molecular wave function, $\chi/r \sim e^{-r^2/a}/ra^{1/2}$.

III. LOW TEMPERATURE

We now consider the temperature dependence of $C$ for $T$ well below the superfluid transition temperature $T_c$, in which regime phonon excitations dominate. The contribution of the phonons to the entropy density is

$$s_{\text{phonon}} = \frac{2\pi^2}{45} \left( \frac{T}{T_c} \right)^3,$$

(11)
where the zero temperature sound velocity \( c_s \) is given by \( mc_s^2 = n\partial\mu/\partial n \), with \( \mu \) is the chemical potential. The change of \( C \) to leading order for \( T \ll T_F = E_F \) \((k_B = 1)\) is thus

\[
\delta C = C(T) - C(0) = -\frac{\pi m}{120} \left( \frac{T}{c_s} \right)^4 \frac{\partial c_s}{\partial \alpha^4}.
\]

The zero temperature sound velocity appears to increase monotonically from the BEC side to the BCS side \([14,15]\), so that the short range pair correlations as parametrized via \( C \) increase from zero temperature as \( T^4 \). At \( T = 0, \mu = E_F \) \((1 + \beta - \beta/\xi/5)\), so that

\[
\left( \frac{c_s}{v_F/\sqrt{3}} \right)^2 = 1 + \frac{3}{5} \beta' \xi + \frac{1}{10} \beta'' \xi^2,
\]

with \( \beta' = \partial\beta/\partial\xi \), etc. Recent measurements of \( c_s \) are in good agreement with \([12]\) combined with Monte Carlo results for \( \beta \) around unitarity \([21]\).

Equation \((9)\) implies that in the BCS limit, \( c_s^2 = (v_F^2/3)(1 + 2k_Fa/\pi) \), and thus at low \( T \),

\[
C(T) = n^2 a^2 \left[ 1 + \frac{9\sqrt{3}\pi^4}{160} \left( \frac{T}{T_F} \right)^4 \right].
\]

For \( T_c < T \ll T_F \), the weakly attractive Fermi gas can be described by Landaum Fermi liquid theory. The entropy density is given by \([25]\) \( s_f = \frac{3}{2}m^*k_F^2T \) with \( m^* = m[1 + 8(7\log T - 1)(k_Fa)^2/15\pi] \) the effective mass of the quasiparticles \([20]\). From \([1]\), we then have the temperature dependence

\[
\delta C(T)/n^2a^2 = \frac{\pi}{8}(7\log T - 1)k_Fa \left( \frac{T}{T_F} \right)^2 > 0.
\]

In the BEC limit, the Bogoliubov sound speed is \( c_s = \sqrt{sg_m/M} \) with \( g_m = 4\pi a_m/M \) and \( M = 2m \) \([22]\). Thus

\[
C(T) = \frac{n}{2\pi a} \left[ 1 + \frac{(\partial a_m/a)}{12\pi} \left( \frac{k_Fa}{3(1 + 2k_Fa^3/12\pi)(k_Fa^3)^{3/2}} \right) + \left( \frac{48\pi^3}{15k^5} \right) \left( \frac{T}{T_F} \right)^4 \right].
\]

At unitarity,

\[
C(T) = \frac{k_F^4\beta^4}{40\pi^4} \left[ 1 + \frac{\sqrt{3}\pi^4}{80(1 + \beta^3)^2} \left( \frac{T}{T_F} \right)^4 \right].
\]

**IV. CORRELATIONS IN THE BEC LIMIT**

The universal behavior \( \delta C \sim T^4 \) as \( T \to 0 \) shows that thermally excited phonons enhance the fermion pair correlations. In the BEC limit, the enhancement of the correlations can be understood directly in terms of a gas of molecules interacting with a short range potential with a scattering length \( a_m > 0 \). The boson correlation function is similar in structure to that for fermions:

\[
\lim_{r \to 0} \langle \phi^\dagger(\mathbf{r})\phi(0)\phi(0)\phi(\mathbf{r}) \rangle = C_m \left( \frac{1}{r} - \frac{1}{a_m} \right)^2,
\]

where the \( \phi(\mathbf{r}) \) are the bosonic field operators. As for fermions,

\[
C_m = -\frac{M}{2\pi} \frac{\partial f_m}{\partial a_m^{-1}},
\]

with \( f_m \) the free energy density for the bosonic molecules. The factor of 2 difference from \([38]\) is due to the factor \( 1/2 \) in the interaction energy for identical bosons written in terms of the \( \phi \).

Since the low temperature physics described in terms of the fundamental fermions or bosonic molecules must be the same, the leading temperature variation \( \delta f = f(T) - f(0) \) is equal to \( \delta f_m = f_m(T) - f_m(0) \). Therefore

\[
\delta C = -\frac{m}{4\pi} \frac{\partial \delta f}{\partial a_m^{-1}} = -\frac{m}{4\pi} \frac{\partial \delta f_m}{\partial a_m^{-1}} = \frac{m}{2M} \frac{\partial a_m^{-1}}{\partial a_m^{-1}} \delta C_m,
\]

with \( \delta C_m = C_m(T) - C_m(0) \). We calculate the boson correlation function within the Bogoliubov approximation using a pseudopotential \( V_m(r) = g_m\delta(r) \). We divide the field operator \( \phi(\mathbf{r}) = \phi_0 + \delta\phi(\mathbf{r}) \) into a condensate part \( \phi_0 \) and a fluctuation \( \delta\phi \), assumed to be small. To second order in the fluctuations, at small \( r \),

\[
\langle \phi^\dagger(\mathbf{r})\phi^\dagger(0)\phi(0)\phi(\mathbf{r}) \rangle = n^2 + 2n_0 \langle \delta\phi^\dagger(0)\delta\phi(0) \rangle + \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle,
\]

where

\[
\langle \delta\phi(0)\delta\phi(0) \rangle = \int \frac{d^3k}{(2\pi)^3} [u_k^2 + (u_k^2 + v_k^2)\langle \alpha_k^\dagger\alpha_k \rangle],
\]

\[
\lim_{r \to 0} \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle = -\int \frac{d^3k}{(2\pi)^3} u_k v_k [e^{ik\cdot\mathbf{r}} + 2\langle \alpha_k^\dagger\alpha_k \rangle]
\]

\[
= -\frac{n_0 a_m}{r} - \int \frac{d^3k}{(2\pi)^3} \left( u_k v_k - \frac{M g_m a_0}{k^2} + 2u_k v_k \langle \alpha_k^\dagger\alpha_k \rangle \right),
\]

here \( v_k^2 = (\xi_k/E_k - 1)/2 \), \( u_k^2 = (\xi_k/E_k + 1)/2 \), \( \xi_k = k^2/2M + g_m a_0 \), and the \( \alpha_k \) annihilate phonons with energy dispersion \( E_k = \sqrt{\xi_k^2 - (g_m a_0)^2} \). The 1/r divergence in \( \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle \) corresponds to the cross term in \([18]\). The \( \sim 1/r^2 \) term in \([18]\) appears from the higher order term \( \lim_{r \to 0} \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle = \lim_{r \to 0} \langle \delta\phi^\dagger(\mathbf{r})\delta\phi^\dagger(0) \rangle^2 \) and \( \leq 2 \). The lowest order Bogoliubov approximation produces the correlation function \([18]\) to leading order in \( (n a_m^3)^{1/2} \).

In \([21]\), the \( r \) independent term is reliable to order \( (n a_m^3)^{1/2} \), the term proportional to \( 1/n^{1/3}r \) to order.
is the s-wave scattering phase shift, and the term proportional to $1/(n^{1/3}\rho) = (na^3_m)^{1/3}$, and the term proportional to $1/(n^{1/3}\rho)$ to order $(na^3_m)^{2/3}$. To derive the full $C_m(1-a_m/r)^2$ structure to higher order in $(na^3_m)^{1/2}$ requires calculating terms beyond the simple ones in (21), a task we defer. To extract $C_m$ from the $r$ independent term in (21) we write $n_0 = n - (\delta\phi(0)^2/\delta\phi(0))$. At $T = 0$, $C_m/(na^3_m)^{1/2} = 1 + (64/3)(na^3_m)^{1/2}$, which agrees with the calculation of $C_m$ from (19) using the ground state energy of weakly interacting bosons [cf. (10)]. The thermally induced change $\delta C_m$ is

$$\frac{\delta C_m}{2na^3_m} = \int \frac{d^3k}{(2\pi)^3} \left( \frac{k^2}{2E_k} e^{E_k/T} - 1 \right) = \frac{\pi^2 T^4}{60} c^2_r,$$

where we consider only the phonon contribution ($E_k = c_k k$). Substituting (24) into (20), we obtain the same result as in (16).

The $T^4$ dependence can be understood in terms of the effect of thermal sound waves on the eigenstates, $\phi_i(r)$, of the two particle density matrix $\rho$. At distances beyond the interparticle spacing, Eq. (13) for the $\phi$ (with $\lambda = 1$) contains potential terms from the mean field $\rho_m n$ and its fluctuations. At fixed normalization, the latter change the magnitude of $\phi_i(r)$ at short distances by terms $\sim \langle (\delta n)^2 \rangle \sim T^4$, which translates into the $T^4$ dependence of $C$ at low temperature.

V. HIGH TEMPERATURE

In the high temperature limit, $T \gg T_F$, where the fugacity $z = e^{\mu/T}$ is small, the free energy can be calculated via a virial expansion. To second order in $z$, the partition function for a two-component Fermi gas is given by (23, 24)

$$\log(Z/Z_0) = \frac{2^{3/2}\Omega}{\lambda^3} z^2 b_2,$$

where

$$b_2 = \sum_i e^{E_i^0/T} + \int_0^\infty \frac{dk \delta(k)}{\pi} e^{-k^2/mT}$$

is the second virial coefficient. Here the $E_i^0$ are the bound energies of the two-body attractive interaction $V(r)$, $\delta(k)$ is the s-wave scattering phase shift, and $\lambda = (2\pi/mT)^{1/2}$ is the thermal wavelength. In the BEC regime, we consider only the relevant bound state with $E_b = -1/ma^2$. In the regime $T \ll 1/ma^2$, the values of $k$ entering (24) are $\ll 1/r_0$, so that $\cot \delta(k) = -1/ka$; hence $d\delta(k)/dk = -a/((ka)^2 + 1)$, and

$$b_2 = \left( \frac{1}{2} + 1 \sqrt{\frac{a}{\pi}} \int_0^{\lambda/\sqrt{\pi a}} e^{-t^2} dt \right) e^{\lambda^2/2\pi a^2}.$$
It follows from \( f \cdot \) and the virial expansion result \( g \), that the isentropes have a negative slope in the \( T_c - 1/k_Fa \) plane for high \( T \). Likewise, the increase in \( C(T) \) given by \( h \) has a positive slope for low \( T \). The correlation strength \( C(T) \) has an extremum where the slope of the isentropes as a function of \(-1/k_Fa\) vanishes. Additional information is obtained from a recent experiment, where a Fermi gas was prepared in the BCS limit with initial energy \( E_i \) and entropy \( S_i \) and then adiabatically tuned to the unitary point where the final energy \( E_f \) was measured \( j \). The temperature was deduced from \( T = \partial E/\partial S \). Within the experimental regime the final temperatures \( T_f \) at unitarity were generally higher than the initial temperatures \( T_i \) in the BCS limit \( k \). However, for the isentrope ending at \( T_f \approx 0.2T_c \), \( T_i \approx T_f \), which indicates that this isentrope (as well as neighboring ones) first bends upwards and then downwards from the unitarity region to the BCS limit. Well below the BCS transition, where phonons dominate the entropy, the isentropes have positive slope, not visible on the scale of Fig. 2.

**VI. PHOTOASSOCIATION EXPERIMENT**

Photoassociation experiments provide a direct measure of the correlation strength \( l \). In a recent experiment, \(^6\)Li atoms were trapped in the lowest two hyperfine states \( m \) and \( n \). Then the bare closed channel spin-singlet molecular state \(|\psi_{v'=0}\rangle \) associated with the 834G Feshbach resonance in the 1-2 channel was excited by a laser field \( E_L \) to a spin-singlet molecular state \(|\psi_{v'=68}\rangle \), with linewidth \( \gamma = (2\pi)1.7 \) MHz. The excited molecules were lost from the trap and the remaining atoms counted for various durations of the laser pulse \( o \). By Fermi’s golden rule, the local loss rate of the number of atoms, \( 2n_i \), in the trap is \( p \)

\[
\Gamma = -2\frac{dn(t)}{dt} = 2\frac{\Omega_R^2}{\gamma}n_b, \tag{31}
\]

where \( \Omega_R = \langle \psi_{v'=68}|E_L \cdot \mathbf{d}|\psi_{v'=38}\rangle \) is the Rabi frequency, \( \mathbf{d} \) is the atomic dipole operator, and \( n_b \) the local density of molecules in the closed channel. The density of closed channel molecules \( n_b \) is related to the correlation function between the states \( m \) and \( n \) in the open channel by \( q \)

\[
n_b = \frac{4\pi a_{bg}C}{m_B \Delta B} \left( \frac{1}{a_n} - \frac{1}{a} \right)^2, \tag{32}
\]

where \( a_{bg} \) is the background scattering length, the molecular magnetic moment \( \mu_B \) is twice the Bohr magneton \( \mu_B \), and \( \Delta B \) is the width of the Feshbach resonance.

In a homogeneous gas in the high temperature limit, we find from \( r \), \( s \), and \( t \) that \( \Gamma \sim n^2/T \). In a trap, the local density approximation gives \( u/V(r) = N(\omega/XT)^3 \exp[-\beta V(r)] \) with \( V(r) = (m/2)(\omega^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2 \) and \( \omega = (\omega_x \omega_y \omega_z)^{1/3} \). The average of \( C \) over the trap, and thus the average rate \( \bar{\Gamma} \), is \( \propto \gamma^3 N^2/\gamma^3/2 \), and Eq. \( u \) has the solution

\[
N(t)/N(0) = \left( 1 + \frac{\Omega_R^2 n_b}{\gamma N t} \right)^{-1}. \tag{33}
\]

Analogous expressions for the \( T = 0 \) trap-averaged loss rate were given in \( v \).

In Fig. 3 we compare the high \( T \) result \( w \) with the experimental data obtained on the BCS side of the resonance \( x \). Initially the temperature is below \( T_f \), where
FIG. 3: (color online) Loss of $^6$Li atoms in the trap through photoassociation vs. the probe duration at $B = 865$ G. The solid curve is the numerical evaluation of (33). The circles are the $T_F = 0.75T$ experimental data from Ref. [9]. (31) underestimates the loss; however, owing to depletion the Fermi temperature falls below $T$, and (33) provides reasonable agreement with the data – with no fitting parameters.

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