Thermodynamics of Interacting Fermions in Atomic Traps

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We calculate the entropy in a trapped, resonantly interacting Fermi gas as a function of temperature for a wide range of magnetic fields between the BCS and Bose-Einstein condensation endpoints. This provides a basis for the important technique of adiabatic sweep thermometry, and serves to characterize quantitatively the evolution and nature of the excitations of the gas. The results are then used to calibrate the temperature in several ground breaking experiments on $^6\text{Li}$ and $^{40}\text{K}$.

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The claims [1, 2, 3, 4, 5] that superfluidity has been observed in fermionic atomic gases have generated great excitement. Varying a magnetic field, one effect is a smooth evolution from BCS superfluidity to Bose-Einstein condensation (BEC) [6, 7]. In this Letter we use a BCS-BEC crossover theory to study the entropy $S$ over the entire experimentally accessible crossover regime. Our goal is to help establish a methodology for obtaining the temperature $T$ of a strongly interacting Fermi gas via adiabatic sweeps. This addresses an essential need of the experimental cold atom community by providing a temperature calibration for their ground breaking experiments [2, 3, 4]. In the process, we characterize quantitatively the evolution of the excitations and show how their character evolves smoothly from fermionic to bosonic, and conversely.

In adiabatic sweeps, the starting $T$ at either a BEC or BCS endpoint is estimated from the “known” shape of the profile in the trapped cloud. Then, the temperature (near unitarity, say) is obtained by equating the entropy before the sweep to that in the strongly interacting regime after the sweep. Conventionally, the temperature scale which appears in the superfluid phase diagram [2, 3] involves an isentropic sweep between the unitary and the non-interacting Fermi gas regimes. The direction of the sweep is irrelevant in these reversible processes. The important experimental phase diagrams plot the condensate fraction, $N_c/N$ near unitarity vs this Fermi gas-projected temperature, $T_{\text{eff}}$.

In this paper, our thermodynamical calculations are used to relate the actual physical temperatures $T$ to $T_{\text{eff}}$, where, in general, $T$ is significantly greater than $T_{\text{eff}}$. A calculation of $N_c(T)$ is simultaneously undertaken [10, 11] which provides an important self-consistency condition on the thermodynamics, since the same excitations appear in both. Moreover, a calculation of $N_c$ has to be done with proper attention paid to collective modes and gauge invariance [12]. Here we address the various condensate fractions found experimentally [1, 2], (with emphasis on $^6\text{Li}$), as a function of $T_{\text{eff}}$, in the experimental range of magnetic fields.

Our work is based on the BCS-Leggett ground state [6, 7] and its finite $T$ extension [11]. Four different classes of experiments have been successfully addressed in this framework. These include (i) $T \approx 0$ breathing modes experiments [2, 4] and theory [12, 14], (ii) radio frequency (RF) pairing gap experiments [5] and theory [15, 16], and (iii) $T$-dependent density profiles [17]. Finally, (iv) plots of the energy $E$ vs $T$ at unitarity [18] yield very good agreement with experiment and serve to characterize quantitatively the evolution and nature of the excitations of the gas. The results are then used to calibrate the temperature in several ground breaking experiments [6] and theory [15, 16].

Because previous thermodynamic theories did not address unitarity, it has not been possible until now to arrive at a temperature scale in the experimentally interesting resonant superfluid regime. Carr et al. [20, 21] calculated $S$ at the BCS and weakly interacting, deep-BEC endpoints. The latter true Bose limit which they considered does not appear to be appropriate to current collective mode experiments. [3, 4], which show [13, 14] that for physically accessible (i.e., near-BEC) fields, fermions are playing an important role. Thus, the BCS-Leggett ground state appears to be more appropriate than one deriving from Bose-liquid-based theory. Williams et al. [22] calculated $S$ for a BCS-BEC crossover theory using a mixture of noninteracting fermions and bosons. This work, omits the important and self consistently determined fermionic excitation gap $\Delta$ which is an essential component for describing the thermodynamics of fermionic superfluids.

Our thermodynamical calculations focus on this self-consistently determined $\Delta$; they are based, for completeness, on a two-channel Hamiltonian [11, 23, 24]. Here $\Delta$ appears in the fermionic dispersion $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$. (We define $\epsilon_k = h^2k^2/2m$ as the kinetic energy of free atoms, and $\mu$ the fermionic chemical potential.) Importantly, this $\Delta$ provides a measure of bosonic degrees of freedom. In the fermionic regime ($\mu > 0$), $\Delta$ is just the energy required to dissociate the pairs and thereby excite fermions. At finite $T$, the closed-channel molecular bosons and the open-channel finite momentum Cooper pairs are strongly hybridized with each other, making up the “bosonic” excitations which contribute to thermodynamics.
Our many-body formalism has been described below the superfluid transition temperature \( T_c \)). The parameter \( \Delta \), (when squared), is the analogue of the total number of particles, in the simplest theory of BEC. Just as in BEC, there are two self-consistency conditions: (i) the effective chemical potential of the pairs, \( \mu_{\text{pair}} \), is zero, for \( T \leq T_c \) (as is that of the closed-channel molecular bosons \( \mu_{\text{mb}} \)), and, (ii) the number of pairs, reflected in \( \Delta^2(T) \) contains two additive contributions representing condensed \( (\Delta^2_c) \) and non-condensed \( (\Delta^2_{pg}) \) pairs. This first condition implies that \( \Delta(T) \) satisfies a BCS-like gap equation. Then, the condensate is deduced, just as in BEC, by determining the difference between \( \Delta^2 \) and \( \Delta^2_{pg} \). In this approach the hybridized pairs have dispersion \( \Omega_q = \hbar^2 q^2/2M^* \), with effective pair mass \( M^* \).

We now extend this approach above \( T_c \). Our first equation represents the important defining condition on \( \mu_{\text{pair}} \): that the inverse pair propagator (or \( T \)-matrix) \( t^{-1}(Q)|_{Q=0} = Z \mu_{\text{pair}} \), with (inverse) “residue” \( Z \). While in the superfluid regions \( \mu_{\text{pair}} \) and \( \mu_{\text{mb}} \) vanish, in general, we have

\[
U^{-1}_{\text{eff}}(0) + \sum_k \frac{1 - 2f(E_k)}{2E_k} = Z \mu_{\text{pair}},
\]

where \( U_{\text{eff}}(0) = U + g^2/(2\mu - \nu) \) involves the sum of the direct attraction \( U \) between open-channel fermions, as well as the virtual processes associated with the Feshbach resonance. Here \( f(x) \) is the Fermi distribution function. The determination of the inter-channel coupling constant, \( g \), and the magnetic field detuning, \( \nu \), is described elsewhere \[25\], as are the residues \( Z \) and \( Z_b \)). The contribution from hybridized bosons will lead to a normal state excitation gap or pseudogap (pg). This can be written in terms of the Bose distribution function \( b(x) \) as

\[
\Delta^2_{pg} = Z^{-1} \sum_q b(\Omega_q - \mu_{\text{pair}}).
\]

We use the local density approximation (LDA) throughout with a harmonic trap potential \( V(r) \). For notational simplicity, we omit writing \( V(r) \) in favor of \( \mu(r) \) according to the LDA prescription: \( \mu \rightarrow \mu(r) \equiv \mu - V(r) \), where \( \mu \equiv \mu(0) \). The total atomic number \( N \equiv \int d^3r \, n(r) \), where

\[
n = 2n_{b0} + 2Z^{-1} \sum_q b(\Omega_q - \mu_{\text{mb}})
+ 2 \sum_k [v_k^2(1 - f(E_k)) + u_k^2 f(E_k)].
\]

Here \( n_{b0} = g^2 \Delta^2_c /[(\nu - 2\mu(r))U]^2 \) is the density of condensed closed-channel molecules, and \( u_k^2, v_k^2 = [1 \pm (\epsilon_k - \mu(r))/E_k]/2 \). The total order parameter \( \Delta_{sc} = \Delta_{c} + |g|\sqrt{n_{mb}} \).

To make progress, we numerically solve Eqs. (1)-(2) at each \( r \) for given \( \mu \) and then self-consistently adjust \( \mu \) via the total number constraint. Next we obtain the entropy \( S \) directly from the thermodynamical potential \[23\]. This potential contains fermionic contributions from bare fermions, \( \Omega_f \), and bosonic contributions \( \Omega_b \). The latter is given by the sum of all possible ring diagrams shown in Fig. 1. It can be easily shown that this \( \Omega_b \) is consistent with the self energy diagrams for the fermions and the molecular bosons. After regrouping, we see that \( S \) has two contributions, from fully dressed fermions \( (S_f) \) and from their bosonic counterpart \( (S_b) \). The total entropy involves an integral over the trap, given by \( S = \int d^3r \, s(r) \) (and similarly for \( S_f \) and \( S_b \)), where

\[
s = s_f + s_b,
\]

\[
s_f = -2 \sum_k \left| f_k \ln f_k + (1 - f_k) \ln(1 - f_k) \right|,
\]

\[
s_b = - \sum_{q \neq 0} \left[ b_q \ln b_q - (1 + b_q) \ln(1 + b_q) \right],
\]

where \( f_k \equiv f(E_k) \), and \( b_q \equiv b(\Omega_q - \mu_{\text{mb}}) \); a relatively small contribution associated with the \( T \) dependence of \( \Omega_q \) has been dropped. The fermion contribution coincides formally with the standard BCS result for non-interacting quasiparticles [although here \( \Delta(T_c) \neq 0 \)]. And the bosonic contribution is given by the expression for non-directly-interacting bosons with dispersion \( \Omega_q \). These bosons are not free, however; because of interactions with the fermions, their propagator contains important self-energy and mass renormalization effects.

Figure 2 illustrates the behavior of \( S \) as a function of \( T \) obtained from our self-consistent equations, over the entire experimentally relevant crossover regime. The magnetic field is contained in the parameter \( 1/k_Fa \), which increases with decreasing field. Here \( a \) is the s-wave fermionic scattering length, \( k_F \) is the Fermi wavevector at the trap center, and \( k_B T_F = \hbar^2 k_F^2 / 2m \) is the noninteracting Fermi temperature. Two important aspects of the fermionic contribution \( S_f \) should be noted. Generally, the fermions have a gap \( \Delta \) in their excitation spectrum (which increases with decreasing field) and moreover this \( T \) dependent gap is inhomogeneous so that the fermions near the trap edge often behave as free particles at \( T > \Delta \). These quasi-“free” fermions change the \( T \) dependence of \( S_f \) from exponential to power law. They have also been seen in RF experiments \[8,15\], as a free fermion peak in the spectra.

We refer to Fig. 2 starting from the high field or BCS regime where \( S \) is linear in \( T \). As the field is lowered to-

![FIG. 1: Bosonic contribution to the thermodynamical potential. Here \( G_0(G) \) and \( D_0(Q) \) are the “bare” (“full”) propagators associated with the fermions and closed-channel molecular bosons, respectively, and \( K \) and \( Q \) are four-momenta, and \( U_{k,k'} \) is the open-channel pairing interaction.](Image)
FIG. 2: (color online) Entropy per atom as a function of $d$. Dotted lines show an isentropic sweep between $s_f$ and $s_b$ component contributions at unitarity for $T = T_c/4$. Here $R_{TF}$ is the Thomas-Fermi radius, and $T_c = 0.27T_F$.

Towards unitarity, $s_f$ will vary as a low-$T$ power law which is higher than linear. Simultaneously, the bosonic degrees of freedom emerge. Here one sees a $T^{3/2}$ power law from these excited bosons. At unitarity, bosonic effects dominate for $T/T_F \lesssim 0.05$ or $T/T_c \lesssim 0.2$. For an extended range of $T < T_c$, the fermions and bosons combine to yield, $S \propto T^3$, which can be compared with the experimental power law \cite{18}. Finally, in the near-BEC regime one sees an essentially pure bosonic $T^{3/2}$ power law in $S$ at low $T$ in the superfluid phase. The relative contribution of the bosonic excitations, $S_b/S$, evolves continuously from 0 to 1 as $1/k_F a$ increases from $-\infty$ to $+\infty$. $S$ becomes dominantly bosonic once $\mu$ becomes negative.

The bosonic $T^{3/2}$ power law found in the trap is the same as found for the homogeneous situation. Inhomogeneity effectively disappears here because the fermion-boson interactions lead to the self-consistent constraint that $\mu_{pair} = 0$ for the entire superfluid region. This same disappearance of inhomogeneity is found in Ref. \cite{20}. This is different from a strictly non-interacting Bose system (dashed line in Fig. 2) where one does not have a vanishing boson chemical potential below $T_c$ except at the trap center. The previous work of Ref. \cite{20} is based on interacting but true bosons. The present situation is more complex since Cooper pair operators do not obey Bose commutation relations, (nor does the linear combination of Cooper pair and closed-channel boson operators). This suggests that a theory based on a true Bose liquid may not be appropriate for the fields that have been accessed experimentally. Moreover, if one were to contemplate contributions from the linearly dispersing Goldstone bosons, albeit within a more general ground state, their contribution, at unitarity, will not be as important as that from the edge fermions.

To shed additional light on the component fermionic and bosonic contributions, in the inset to Fig. 2, we decompose the various terms in the entropy to reveal their spatial distributions, for the unitary case at $T = T_c/4$. It can be seen that the fermionic contribution $s_f$ (red curve) is limited to the trap edge, where $\Delta$ is small. By contrast, the bosonic contribution $s_b$ (blue curve) is evenly distributed over the superfluid region and rapidly decays at larger radii.

Figure 2 provides a basis for thermometry in adiabatic sweep experiments. The vertical lines illustrate how to choose an initial temperature ($T_i = 0.5T_F$ at point “A”) with an initial value of $1/k_F a = 1$ and use an isentropic sweep (represented by the horizontal line through “A” and “B”) to obtain the final temperature ($T_f = 0.28T_F$ at point “B”) with the final value of $1/k_F a = 0$. It is most convenient to begin with either the BCS regime or BEC regimes, since here $T_c$ can, in principle, be determined by fitting the density profiles.

Figure 3 provides a plot of the superfluid fraction $N_s/N$ in the intermediate regime as a function of an effective temperature $T_{eff}/T_F$ for different values of initial fields or $1/k_F a$. Here $T_{eff}$ is the temperature reached after an adiabatic sweep to a BCS-like state. Based on experiment, we take the final state as $1/k_F a = -0.59$ at 1025 G for $^6$Li \cite{2} and a noninteracting Fermi gas for $^{40}$K \cite{8}.

The same vertical axis appears in the inset but with the physical temperature scale $T_s$ so that this figure provides a means of directly calibrating the temperature scale $T_{eff}$ which has been used in the important phase diagrams of $^6$Li and $^{40}$K. Figure 3 also provides a means of comparing the condensate fractions with those in the phase diagrams. For $^6$Li at 900 G, with $T_{eff}/T_F = 0.2, 0.1$ and 0.05, the experimental condensate fractions are 0.0, 0.1 and 0.6. This should be compared with our calculated values, 0.006 0.36, and 0.73, respectively. For $^6$Li at 770 G, the condensate first appears at $T_{eff}/T_F = 0.18$, consistent with theory. From the values of $k_F a$ and $T_c$ at both ends (importantly, the latter can be read from the inset), one can easily see that the sweep from 770 G to 1025 G is still very far from a full BEC-BCS sweep.

There are two reasons for the larger condensate fractions found theoretically for $^6$Li. A calculation of the BEC-like density profiles shows that the noncondensed pairs inside the superfluid region have a flat density distribution, which reflects the vanishing of $\mu_{pair}$. The superfluid fraction extracted experimentally (assuming a Gaussian form for the noncondensed particles inside the condensate core) is, thus, underestimated, most notably around $T_c/2$. In addition, earlier work \cite{13} shows that when the system is treated as a non-interacting Fermi gas, $T_{eff}$ will be underestimated whenever a condensate is present (at $T < T_c \approx 0.17T_F$ at 1025 G). This suggests that theory and experiment can be brought into rather good agreement for the case of $^6$Li. For $^{40}$K, one has to appeal to non-adiabaticity and other complications of the sweep process to understand the small measured fractions.

For this case, we emphasize temperature scales. For a full
resonance in these states. Also plotted in the inset is a critical temperature at each field value. The system is not far from the magnetic field. The inset plots the same

\[ T \]

chosen based on Refs. \[2\] and \[8\]. For experiment \[8\] and in theory are assumed a

\[ T \]

measured in a near-BCS (at 1025G for \(^6\)Li) or noninteracting Fermi gas (FG, \(^{40}\)K) state accessed via reversible adiabatic sweeps of magnetic field. The inset plots the same
density profile. Similarly calculated

\[ T \]

should serve as upper bounds. Our calculations and DOE, No. W-31-109-ENG-38 (QC).

Without knowing the temperature, measurements in this

field cannot be directly compared to any theory. The present work presents a theory for the entropy \( S \) of a Fermi gas, at general accessible magnetic fields, which thereby calibrates \( T \) in various existing

and future experiments.

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![Diagram of density profile](image)

**FIG. 3:** (color online) Superfluid density \( N_s/N \) at different magnetic fields for \(^6\)Li and \(^{40}\)K as a function of the effective temperature, \( T_{\text{eff}} \), measured in a near-BCS (at 1025G for \(^6\)Li) or noninteracting Fermi gas (FG, \(^{40}\)K) state accessed via reversible adiabatic sweeps of magnetic field. The inset plots the same density profile. Similarly calculated uncertainties and DOE, No. W-31-109-ENG-38 (QC).