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Strong Coupling Effects on the Specific Heat of an Ultracold Fermi Gas in the Unitarity Limit

P. van Wyk[1] · **H. Tajima**[1] · **R. Hanai**[1] · **Y. Ohashi**[1]

Abstract We investigate strong-coupling corrections to the specific heat C_V in the normal state of an ultracold Fermi gas in the BCS–BEC crossover region. A recent experiment on a ^{6}Li unitary Fermi gas (Ku et. al. in Science 335:563 2012) shows that C_V is remarkably amplified near the superfluid phase transition temperature T_c, being similar to the well-known λ-structure observed in liquid ^{4}He. Including pairing fluctuations within the framework of the strong-coupling theory developed by Nozières and Schmitt-Rink, we show that strong pairing fluctuations are sufficient to explain the anomalous behavior of C_V observed in a ^{6}Li unitary Fermi gas near T_c. We also show that there is no contribution from *stable* preformed Cooper pairs to C_V at the unitarity. This indicates that the origin of the observed anomaly is fundamentally different from the case of liquid ^{4}He, where *stable* ^{4}He Bose atoms induce the λ-structure in C_V near the superfluid instability. Instead, the origin is the suppression of the entropy S, near T_c, due to the increase of *metastable* preformed Cooper pairs. Our results indicate that the specific heat is a useful quantity to study the effects of pairing fluctuations on the thermodynamic properties of an ultracold Fermi gas in the BCS–BEC crossover region.

Keywords Ultracold Fermi gas · Many-body physics · Quantum gas · BCS–BEC crossover

1 Introduction

Ultracold Fermi gases have recently gathered much theoretical and experimental attention as highly controllable many-body systems [1–8]. A tunable pairing interaction

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associated with a Feshbach resonance [6] has realized the so-called BCS (Bardeen–Cooper–Schrieffer)-BEC (Bose Einstein condensation) crossover phenomenon, where we can study a Fermi superfluid and a Bose superfluid in a unified manner. In the BCS–BEC crossover region, the system is dominated by strong pairing fluctuations, so that the formation of preformed Cooper pairs, as well as their effects on physical properties, have extensively been discussed [9–11]. Recently various thermodynamic quantities have become accessible in the field of cold Fermi gas physics [12–15], allowing us to directly compare theoretical studies of the strong-coupling properties of an ultracold Fermi gas [10,11,16,17] with experimental results.

Since the formation of preformed Cooper pairs due to a strong pairing interaction is expected to affect the entropy S of the system, the specific heat (which is directly related to the change in entropy) is a useful thermodynamic quantity to study this key many-body phenomenon in the BCS–BEC crossover region. Indeed, a recent experiment on a ^{6}Li unitary Fermi gas [17] observed that the specific heat at constant volume C_V deviates from the linear temperature dependence known in a normal Fermi liquid [18]. In the normal state near T_c, the observed C_V exhibits an anomalous enhancement with decreasing temperature, which resembles the so-called λ-structure observed in liquid ^{4}He [19]. Although this resemblance infers that some form of Bose excitations are responsible for the anomalous behavior of C_V in a ^{6}Li unitary Fermi gas near T_c, it is unclear to what extent a unitary Fermi gas with strong pairing fluctuations can be regarded as an interacting Bose system, like liquid ^{4}He.

In this paper, we investigate the specific heat at constant volume C_V, and effects of pairing fluctuations in the BCS–BEC crossover regime of an ultracold Fermi gas, above the superfluid phase transition temperature T_c. Including pairing fluctuations within the framework developed by Nozières and Schmitt-Rink (NSR) [20], we show that strong-coupling corrections to C_V, near T_c, in the unitarity limit are sufficient to explain the anomalous enhancement of C_V that has recently been observed in a ^{6}Li Fermi gas. We also clarify that this phenomenon originates from pairing fluctuations leading to the formation of *metastable* preformed pairs, which is quite different from the case of liquid ^{4}He, where *stable* ^{4}He Bose atoms induce the λ-structure in the temperature dependence of C_V near the superfluid instability [19]. Throughout this paper, we take $\hbar = k_B = 1$, and the system volume V is taken to be unity, for simplicity.
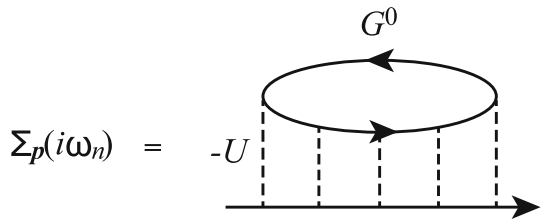
2 Formulation

We consider a two-component Fermi gas, described by the BCS Hamiltonian,

$$H = \sum_{\boldsymbol{p},\sigma} \xi_{\boldsymbol{p}} c_{\boldsymbol{p},\sigma}^{\dagger} c_{\boldsymbol{p},\sigma} - U \sum_{\boldsymbol{p},\boldsymbol{p}',\boldsymbol{q}} c_{\boldsymbol{p}+\boldsymbol{q}/2,\uparrow}^{\dagger} c_{-\boldsymbol{p}+\boldsymbol{q}/2,\downarrow}^{\dagger} c_{-\boldsymbol{p}'+\boldsymbol{q}/2,\downarrow} c_{\boldsymbol{p}'+\boldsymbol{q}/2,\uparrow}, \quad (1)$$

where $c_{\boldsymbol{p},\sigma}$ is the annihilation operator of a Fermi atom with pseudospin $\sigma = \uparrow, \downarrow$, describing two atomic hyperfine states. $\xi_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} - \mu = p^2/(2m) - \mu$ is the kinetic energy, measured from the Fermi chemical potential μ, where m is an atomic mass. The pairing interaction $-U$ (< 0) is assumed to be tunable by adjusting the threshold

$$\Sigma_p(i\omega_n) \quad = \quad -U$$

energy of a Feshbach resonance [6]. As usual, we measure the interaction strength in terms of the inverse s-wave scattering length a_s^{-1}, which is related to $-U$ through

$$\frac{4\pi a_s}{m} = \frac{-U}{1 - U \sum_p \frac{1}{2\varepsilon_p}}. \tag{2}$$

We include fluctuations in the Cooper channel within the framework of the strong-coupling theory developed by Nozières and Schmitt-Rink (NSR) [20]. In the Green's function formalism, the NSR theory is described by the single-particle thermal Green's function,

$$G_p(i\omega_n) = G_p^0(i\omega_n) + G_p^0(i\omega_n)\Sigma_p(i\omega_n)G_p^0(i\omega_n), \tag{3}$$

where ω_n is the fermion Matsubara frequency, and $G_p^0(i\omega_n)^{-1} = i\omega_n - \xi_p$ is the Green's function for a free Fermi particle. The NSR self-energy $\Sigma_p(i\omega_n)$, which describes strong-coupling corrections to single-particle excitations, is diagrammatically drawn as Fig. 1, which gives,

$$\Sigma_p(i\omega_n) = T \sum_{q,i\nu_n} \Gamma_q(i\nu_n)G_{p-q}^0(i\omega_n - i\nu_n). \tag{4}$$

Here, ν_n is the boson Matsubara frequency. The NSR particle-particle scattering matrix,

$$\Gamma_q(i\nu_n) = \frac{1}{\frac{m}{4\pi a_s} + \left[\Pi_q(i\nu_n) - \sum_p \frac{1}{2\varepsilon_p}\right]}, \tag{5}$$

describes fluctuations in the Cooper channel, where

$$\Pi_q(i\nu_n) = -\sum_p \frac{1 - f(\xi_{p+q/2}) - f(\xi_{p-q/2})}{i\nu_n - \xi_{p+q/2} - \xi_{p-q/2}} \tag{6}$$

is the lowest order pair correlation function (where $f(x)$ is the Fermi distribution function). We briefly note that, although the pair correlation function $\Pi_q(i\nu_n)$ has an ultraviolet divergence, this singularity is renormalized into the s-wave scattering length in Eq. (2).

The specific heat at constant volume C_V is calculated from the formula,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{V,N}. \tag{7}$$

Here, the NSR internal energy E is given by

$$E = 2T \sum_{\boldsymbol{p}, i\omega_n} \left[\varepsilon_{\boldsymbol{p}} + \frac{1}{2}\Sigma_{\boldsymbol{p}}(i\omega_n) \right] G_{\boldsymbol{p}}(i\omega_n)$$
$$\simeq -T \sum_{\boldsymbol{q}, i\nu_n} \Gamma_{\boldsymbol{q}}(i\nu_n) \left[T\frac{\partial}{\partial T}\Pi_{\boldsymbol{q}}(i\nu_n) + \mu\frac{\partial}{\partial \mu}\Pi_{\boldsymbol{q}}(i\nu_n) \right], \qquad (8)$$

where we have retained only terms to $O(\Sigma_{\boldsymbol{p}}(i\omega_n))$, so as to be consistent with the NSR Green's function in Eq. (3). In evaluating (7) and (8), we need the value of the chemical potential $\mu(T)$, which is obtained from the equation for the number N of Fermi atoms,

$$N = 2T \sum_{\boldsymbol{p}, i\omega_n} G_{\boldsymbol{p}}(i\omega_n). \qquad (9)$$

Equation (9) is also used in self-consistently determining the superfluid phase transition temperature T_c from the T_c-equation [20],

$$\frac{m}{4\pi a_s} = -\sum_{\boldsymbol{p}} \left[\frac{1}{2\xi_{\boldsymbol{p}}} \tan h\frac{\xi_{\boldsymbol{p}}}{2T_c} - \frac{1}{2\varepsilon_{\boldsymbol{p}}} \right], \qquad (10)$$

which is obtained from the Thouless criterion [21], which states that the superfluid instability occurs when the particle-particle scattering matrix $\Gamma_{\boldsymbol{q}}(i\nu_n)$ has a pole at $\boldsymbol{q} = \boldsymbol{0}$ and $\nu_n = 0$.

In our numerical calculations, we tune the interaction strength by adjusting the value of the dimensionless parameter $(k_F a_s)^{-1}$. We briefly note that, in the unitarity limit ($(k_F a_s)^{-1} = 0$), the interaction effect formally disappears in Eqs. (5) and (10), in the sense that the factor $m/(4\pi a_s)$ in these equations vanishes.

3 Specific Heat in the BCS–BEC Crossover Region Above T_c

Figure 2a shows the specific heat C_V in a unitary Fermi gas above T_c. Starting from the high temperature region, C_V decreases from the classical result $C_V^{cl} = (3/2)N$, with decreasing temperature. Since this high temperature behavior is well described by the case of a free Fermi gas (C_V^F), this temperature dependence may be simply attributed to the Fermi statistical effect. While the free Fermi gas result C_V^F monotonically decreases with decreasing temperature, the specific heat C_V at the unitarity is enhanced in the low temperature region, $T_c \leq T \lesssim 2T_c$. As seen in Fig. 2a, this enhancement semi-quantitatively agrees with the recent experiment on a ^{6}Li Fermi gas [16].[1] Since

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[1] We note that the difference between the calculated C_V and experimental result seen in Fig. 2a could be due to an inherent uncertainty in the temperature resolution of the experiment, because the temperature cannot be directly measured [17]. The inclusion of such effects to the calculation of CV is left as our future work.
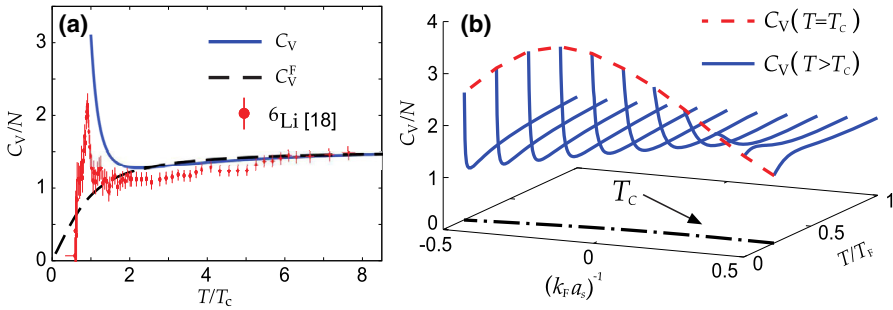
Fig. 2 a Comparison of our result with the recent experiment on a ^{6}Li unitary Fermi gas [17]. C_V^F shows the specific in a free Fermi gas. **b** Calculated specific heat C_V in the BCS–BEC crossover regime of an ultracold Fermi gas above T_c (see footnote 2) (Color figure online)

the physical properties of a unitary Fermi gas are known to be dominated by strong pairing fluctuations near T_c [8–11,16,20,22], this anomaly in C_V is also considered as a strong-coupling phenomenon associated with strong fluctuations in the Cooper channel. Indeed, as shown in Fig. 2b, this enhancement is remarkable in the unitary regime.

At a glance, the anomalous enhancement of the specific heat C_V seen in Fig. 2a resembles the case of liquid ^{4}He [19], where stable atoms constituting this Bose liquid are responsible for the famous λ-structure in the temperature dependence of the specific heat near the superfluid instability. Since pairing fluctuations in a unitary Fermi gas are accompanied by preformed Cooper pairs, it is an interesting problem whether or not the observed enhancement of C_V can be understood by regarding a unitary Fermi gas as a "Bose gas" of stable preformed Cooper pairs.

To examine this, it is convenient to divide the number equation (9) into the sum of the free fermion part,

$$N_F = 2T \sum_{\boldsymbol{p},i\omega_n} G_{\boldsymbol{p}}^0(i\omega_n) = 2\sum_{\boldsymbol{p}} f(\xi_{\boldsymbol{p}}), \tag{11}$$

and the fluctuation contribution coming from the second term in Eq. (3),

$$N_{FL} = -T \sum_{\boldsymbol{q},i\nu_n} \Gamma_{\boldsymbol{q}}(i\nu_n) \frac{\partial}{\partial\mu} \Pi_{\boldsymbol{q}}(i\nu_n) = \int_{-\infty}^{\infty} d\omega n_B(\omega) \rho_B(\omega). \tag{12}$$

Here, $n_B(\omega)$ is the Bose distribution function, and

$$\rho_B(\omega) = \sum_{\boldsymbol{q}} \frac{-1}{\pi} \text{Im}\left[\Gamma_{\boldsymbol{q}}(i\nu_n \to \omega + i\delta) \frac{\partial}{\partial\mu} \Pi_{\boldsymbol{q}}(i\nu_n \to \omega + i\delta)\right] \tag{13}$$

can be interpreted as the "molecular density of states" (where δ is an infinitesimally small positive number). Equation (12) implies that N_{FL} is related to the bosonic character of the system. Evaluating the contribution from *real* poles ($\Omega_{\boldsymbol{q}}$'s) of the

analytic-continued particle-particle scattering matrix $\Gamma_{\boldsymbol{q}}(i\nu_n \to \omega + i\delta)$ to Eq. (12) ($\equiv N_{\mathrm{ST}}$), one has [20,21]

$$N_{\mathrm{ST}} = \sum_{\Omega_{\boldsymbol{q}}} \left[\frac{\frac{\partial}{\partial\mu}\Pi_{\boldsymbol{q}}(\Omega_{\boldsymbol{q}})}{\frac{\partial}{\partial\Omega_{\boldsymbol{q}}}\Pi_{\boldsymbol{q}}(\Omega_{\boldsymbol{q}})} \right] n_{\mathrm{B}}(\Omega_{\boldsymbol{q}}), \tag{14}$$

where the summation is taken over real poles ($\Omega_{\boldsymbol{q}}$'s). Apart from the prefactor of the Bose distribution function in Eq. (14), N_{ST} is found to be directly related to the number of stable molecular bosons having the dispersion $\Omega_{\boldsymbol{q}}$. In the extreme BEC limit (where the system is well described by a gas of tightly bound molecules), the prefactor is reduced to two, and the molecular dispersion becomes $\Omega_{\boldsymbol{q}} = q^2/2M$ (where $M = 2m$), as expected. To conclude, the fluctuation contribution $N_{\mathrm{FL}} = N_{\mathrm{ST}} + N_{\mathrm{SC}}$ can be decomposed into twice the number of stable preformed Cooper pair molecules N_{ST} and the so-called scattering part N_{SC} [20,21], the latter of which physically describes the number of *metastable* preformed pairs with a finite lifetime.

As shown in Fig. 3, while the fluctuation contribution N_{FL} at T_{c} is dominated by stable molecules (N_{ST}) in the strong-coupling BEC regime, they are absent in the unitarity limit.[2] This indicates that, although the enhanced specific heat $C_V(T \sim T_{\mathrm{c}})$ shown in Fig. 2a is similar to the λ-structure in the case of liquid ^{4}He, their origins are different from each other. While *stable* ^{4}He atoms are responsible for this anomaly in a liquid ^{4}He, the suppression of the entropy due to the formation of *metastable* preformed pairs, with decreasing temperature, leads to the amplification of the specific heat near T_{c} in a unitary Fermi gas, through the thermodynamic relation,

$$C_V = T \left(\frac{\partial S}{\partial T} \right)_{V,N}. \tag{15}$$

We see in Fig. 3 that the number N_{SC} of metastable Cooper pairs at T_{c} first increases, as one approaches the unitarity regime from the weak-coupling BCS side. Since the increase of this fluctuation contribution suppresses the entropy $S(T \sim T_{\mathrm{c}})$, the specific heat C_V is enhanced near T_{c}, as shown in Fig. 2b. Such a fluctuation effect on the entropy S is, however, suppressed in the strong-coupling BEC regime, because metastable preformed Cooper pairs are replaced by stable tightly bound molecules with a finite binding energy [20] $E_{\mathrm{bind}} = 1/ma_s^2$. (See Fig. 3). This is the reason for the non-monotonic behavior of $C_V(T = T_{\mathrm{c}})$ with respect to the interaction strength seen in Fig. 2b.

In the strong-coupling BEC regime, the system is well described by a gas of $N_{\mathrm{B}} = N/2$ tightly bound molecules with the molecular mass $M = 2m$. As a result, C_V increases with decreasing the temperature near T_{c} when $(k_{\mathrm{F}}a_s)^{-1} \gtrsim 0.8$, as in the case of an ideal Bose gas (although we do not explicitly show this in this paper). In

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[2] We briefly note that $N_S C$ in Fig. 3 is slightly negative in the strong-coupling regime when $(k_{\mathrm{F}}a_s)^{-1} \gtrsim 0.3$. This is because, strictly speaking, the molecular picture is not exact, when preformed Cooper pairs have a finite lifetime. Thus, $N_S C$ involves fluctuation effects that cannot be fully understood within the simple particle picture [22].

Fig. 3 Calculated number of stable preformed pairs $N_{ST}(T = T_c)$, as well as and contribution of scattering states $N_{SC}(T = T_c)$. The fluctuation contribution N_{FL} is given by the sum of the two as $N_{FL} = N_{SC} + N_{ST}$ (see footnote 2) (Color figure online)
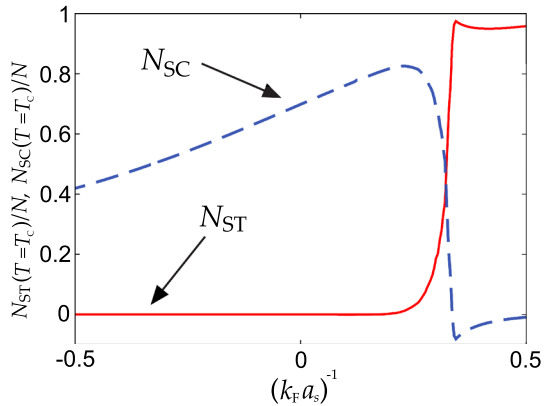
the BEC limit, $C_V(T = T_c)$ just equals the specific heat $C_V^{BEC} \simeq 1.93 N_B$ of an ideal molecular Bose gas at the BEC phase transition temperature [23].

4 Summary

To summarize, motivated by the prospective usefulness of the specific heat C_V as a probe to study effects of strong pairing fluctuations in an ultracold Fermi gas, we have discussed strong coupling corrections to this thermodynamic quantity in the BCS–BEC crossover region. Within the framework of the strong-coupling theory developed by Nozières and Schmitt-Rink, we showed that C_V is enhanced in the unitary regime near T_c. We also showed that this anomalous enhancement is sufficient to explain the recent experiment on a ^{6}Li unitary Fermi gas, where the observed specific heat is amplified with decreasing the temperature near T_c.

Although this behavior looks similar to the λ-structure of the temperature dependence of the specific heat in a liquid ^{4}He near the superfluid phase transition temperature, we pointed out that the origin of the former is fundamentally different from the latter. Indeed, we found that there are no stable preformed Cooper pairs at the unitarity, which is quite different from the latter case, where ^{4}He atoms are always stable. Instead, the bosonic character of a unitary Fermi gas near T_c is dominated by the increase of metastable preformed pairs as the temperature is lowered. This naturally suppresses the entropy near T_c, leading to the amplification of C_V. Our result indicates that the anomalous amplification of the specific heat observed in a ^{6}Li unitary Fermi gas can be fully explained by fluctuating Fermi pairs, without the inclusion of stable bosons.

In this paper, we have only treated the normal state. Since the specific heat has also been observed in the superfluid phase, it is important to extend the present theory to the region below T_c. In addition, since a real Fermi gas is trapped in a harmonic potential, effects of spatial inhomogeneity on the specific heat is also a crucial future problem. Since the specific heat is a fundamental thermodynamic quantity, our results would contribute to the further understanding of thermodynamic properties of an ultracold Fermi gas in the BCS–BEC crossover region.

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