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Crossing of specific heat curves in some correlated fermion systems

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Abstract. Specific heat *versus* temperature curves for various pressures, or magnetic fields (or some other external control parameter) have been seen to cross at a point or in a very small range of temperatures in many correlated fermion systems. We show that this behavior is related to the possibility of existence of a quantum critical point. Vicinity to a quantum critical point in these systems leads to a crossover from quantum to classical fluctuation regime at some temperature $T^\star$. The temperature at which the curves cross turns out to be near this crossover temperature. We have discussed the case of the normal phase of liquid Helium three and the heavy fermion systems $CeAl_3$ and UBe_{13} in detail within the spin fluctuation theory, a theory which inherently contains a low energy scale which can be identified with $T^\star$. When the crossover scale is a homogeneous function of these control parameters there is always crossing at a point. We also mention other theories exhibiting a low energy scale near a quantum critical point and discuss this phenomenon in those theories.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 67.55.Cx Thermodynamic properties – 71.28.+d Narrow-band systems; intermediate-valence solids

There has been a surge of interest in correlated fermionic systems for last ten years. This has led to a recognition that the usual mean field or Hartree Fock description of interacting fermionic systems is not enough, in particular when the effective space dimension of the system is low or when the system is near a quantum phase transition due to the effects of characteristic low energy quantum fluctuations [1–3]. For example, systems near a metal insulator transition or near a magnetic instability, high temperature superconductors, heavy fermions and liquid ^{3}He, all show temperature dependence of their properties at low temperatures which differs from that expected in a normal Fermi liquid [4,5].

One interesting observation which has drawn attention recently [6] is that in some systems the specific heat *versus* temperature curves cross at a point or at least within a very narrow regime of temperature, when they are plotted for various values of some external parameter (*e.g.* pressure, magnetic field). This was initially observed in ^{3}He by Brewer *et al.* [7] and has been seen later on, in a variety of systems ranging from systems close to metal-insulator transition to heavy fermions [8–10]. The variety of materials in which this phenomenon has been observed leads one to believe that there is some kind of universality in this behavior. In a recent publication, Vollhardt [6] has given a thermodynamic interpretation to this universality. The argument given there relies on a smooth crossover between behavior of entropy at temperatures low compared to degeneracy temperature and the high temperature classical limit. As such, the question of why such crossings are prominently seen in systems with highly enhanced magnetic susceptibility or effective mass remains unanswered. Here we propose that the operative cause is the proximity to a quantum critical point. In quantum phase transitions, the coupling constant tunes the transition. For example, the Stoner Criteria, $1 - UN(\epsilon_{\rm F}) > 0$ gives instability towards ferromagnetism. Similarly, $1 - U\chi^0(Q) > 0$ gives antiferromagnetic instability corresponding to wave vector Q and $n^{1/3}a_{\rm H} > 0.26$ describes metal insulator transition due to Coulomb correlation as suggested by Mott (here the notations used are standard). These are essentially zero temperature transitions, however, in general, the transition temperature $T_{\rm c} \ll T_{\rm F}$, the degeneracy temperature. Vicinity to a quantum critical point is usually marked by enhancement in the effective mass, and in spin or density (charge) response in a system at low temperatures. This in turn introduces a low energy scale, [11] which marks a crossover from quantum to a classical behavior in the temperature dependence of various physical properties. For example, in the vicinity of a ferromagnetic transition this scale is given by $\alpha(0)T_{\rm F}$, where, $\alpha(0) = 1 - UN(\epsilon_{\rm F})$.

In most materials the abovementioned crossing of specific heat occurs near this crossover energy scale. This scenario is quite general and holds for transitions involving conserved (for example, the ferromagnetic) as well as

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nonconserved (the anti-ferromagnetic) order parameters. The examples discussed in the present work have been chosen to represent both of these order parameter fluctuations. We use the microscopic spin fluctuation theory [11,12] to discuss the behavior in detail. In this theory, the system is considered near a magnetic instability. The temperature variation of various physical quantities is governed by transverse and longitudinal spin fluctuations. Though the actual transition does not take place, the effect of fluctuations is observable over a wide temperature range at low temperatures [11,13]. This theory has the low energy scale ($\alpha(0)T_{\mathrm{F}}$) inherently built in it.

Consider first the case of liquid ^{3}He. It is a Fermi system with a degeneracy temperature of about 5 K. It has some interesting normal state properties. For example, it behaves like a dense classical liquid down to 0.5 K and like a degenerate Fermi liquid below 0.2 K. It has a large (nuclear) spin susceptibility, about 10 to 25 times the free Fermi gas or Pauli susceptibility χ_P, depending on pressure. The coefficient of the linear term in specific heat is also large. Because of the largeness of spin susceptibility, the liquid can be regarded to be near a ferromagnetic instability within the spin fluctuation theory.

In the following we use some results from our earlier work [5,11,13] to discuss the crossing point in the specific heat curves. The spin fluctuation contribution to the free energy within the mean fluctuation field approximation (or quasi harmonic approximation) at temperature T for systems near a ferromagnetic instability is given by [13],

$$\Delta\Omega = \frac{3T}{2}\sum_{q,m}\ln\left\{1 - U\chi^0(q,m) + \lambda T\sum_{q',m'}D(q'm')\right\}. \tag{1}$$

Here $D(q,m)$ is the fluctuation propagator which is related to inverse dynamical susceptibility, $\chi^0(q,m)$ is the free Fermi gas (Lindhard) response function, and λ is the fluctuation coupling constant. Considering only the thermal part of the integral and ignoring the zero point part, we perform the frequency summation and obtain,

$$\Delta\Omega_{Th} = \frac{3}{\pi}\sum_q\int_0^\infty \frac{\mathrm{d}\omega}{\mathrm{e}^{\omega/\tau}-1}\arctan\left\{\frac{\pi\omega/4q}{\alpha(\tau)+\delta q^2}\right\}, \tag{2}$$

where $\alpha(\tau)$ is the inverse of spin susceptibility in units of the Pauli susceptibility. The denominator and numerator in the argument of the arctan function are the real and imaginary part of the inverse RPA response function $\chi(q,\omega)$. The wavevector q is given in units of Fermi momentum k_{F} and the energy is in units of Fermi energy ($\tau = T/T_{\mathrm{F}}$). For a free Fermi gas $\gamma = 1/2$, $\delta = 1/12$. The correction to the specific heat is given by,

$$\frac{\Delta C}{k_{\mathrm{B}}} = -3\tau^2\sum_q\left[\left(\frac{2}{\tau}\frac{\partial y}{\partial\tau} + \frac{\partial^2 y}{\partial\tau^2}\right)\phi(y) + \left(\frac{\partial y}{\partial\tau}\right)^2\frac{\partial\phi(y)}{\partial y}\right]. \tag{3}$$

The function $\phi(y)$ is $\ln y - 1/2y - \psi(y)$ and $\psi(y)$ is the digamma function where, $y = q(\alpha(\tau)+\delta q^2)/(\pi^2\gamma\tau)$. $\phi(y)$ is related to the fluctuation self energy summed over frequency. It varies as $1/2y$ for $y \ll 1$ and as $1/12y^2$ for $y \gg 1$.

Clearly the calculation of specific heat correction involves the temperature dependence of spin susceptibility. A self consistent equation for the temperature dependence of $\alpha(T)$ within one spin fluctuation approximation has been derived in [5,11]. The result is,

$$\alpha(\tau) = \alpha(0) + \frac{\lambda}{\pi}\sum_q q\phi(y). \tag{4}$$

For a finite $\alpha(0)$ there are two regions of temperature [11]. For $\tau < \alpha(0)$, (which corresponds to $y \gg 1$), one gets an enhanced Pauli susceptibility with standard paramagnon theory corrections, $\alpha(\tau) = \alpha(0) + a\tau^2/\alpha(0)$, where a turns out to be 0.44. At higher temperatures, $\alpha(0) < \tau < 1$, $\alpha(\tau) \sim \tau^n$ with the exponent $1 \le n \le 4/3$. This result for the susceptibility mimics the classical Curie Weiss behavior. Notice that even in a degenerate regime ($\tau < 1$), the susceptibility for a Fermi system behaves like the one for a collection of classical spins. This behavior agrees well [11] with experimental results of Thompson *et al.* [14]. The parameter $\alpha(0)T_{\mathrm{F}}$ is the low energy scale which arises in the spin fluctuation theory naturally. The corresponding low temperature ($\tau \le \alpha(0)$) correction to the specific heat is,

$$\frac{\Delta C}{k_{\mathrm{B}}} = -\sum_q\frac{\pi^2\tau}{4q(\alpha+\delta q^2)}\,\cdot \tag{5}$$

The phase space integral reproduces the standard paramagnon mass enhancement result, $\tau\ln\alpha$ for ΔC. In the classical regime, $\alpha(0) \le \tau \ll 1$, where the small y approximation holds and $\alpha(\tau)$ varies as τ, ΔC falls as $1/\tau^2$ and vanishes at higher temperatures.

The main point of the above discussion is that there are two regimes for specific heat similar to the regimes in the susceptibility variation. The behavior of the specific heat in these two regimes is qualitatively different. At low temperature there is an enhanced linear rise of specific heat correction with temperature leading to a peak and thereafter a slow fall as the temperature increases. The peak marks a transition from quantum to classical spin fluctuation regimes corresponding to one observed in the susceptibility behavior. Considered as a function of $\alpha(0)T_{\mathrm{F}}$, the temperature dependence of specific heat is more revealing (see Fig. 1). The figure shows the calculated curves for various temperatures in the case of antiferromagnetic spin fluctuations (to be discussed later). The parameters correspond to those used for $\mathrm{CeAl_3}$. As seen in the figure, below a certain temperature T_{cr}, specific heat decreases as $\alpha(0)T_{\mathrm{F}}$ increases, while above it the behavior is reversed. T_{cr} clearly marks the crossing and is of the order of $\alpha(0)T_{\mathrm{F}}$. Similar features have also been obtained for the ferromagnetic transition and seem to be generic to all systems which show crossing of specific heat curves. The spin fluctuation theory has only one parameter, that is, $\alpha(0)T_{\mathrm{F}}$. The pressure or magnetic field dependence of quantities is realized through the dependence of $\alpha(0)T_{\mathrm{F}}$ on

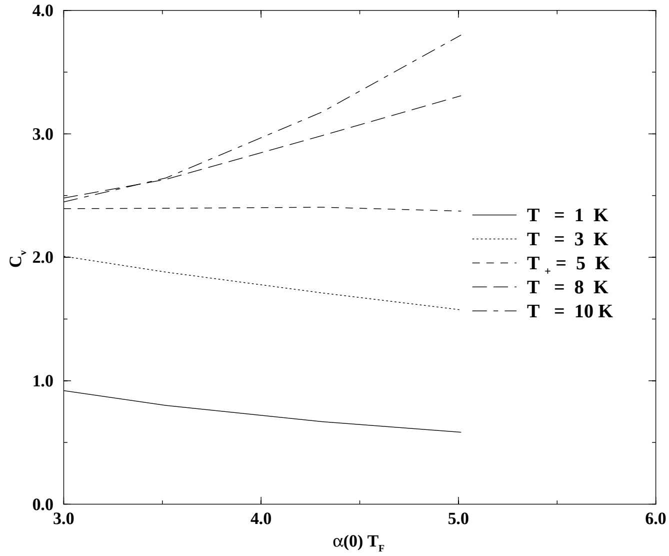

Fig. 1. Specific Heat as a function of $\alpha(0)T_F$ for $CeAl_3$ (to be discussed later in the text) for various temperatures calculated from the spin fluctuation theory. A similar behavior is obtained for ^{3}He.

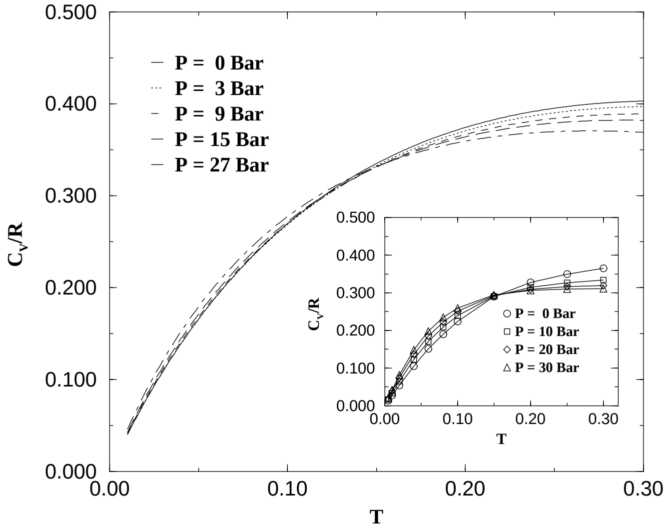

Fig. 2. The calculated curves for $C(P,T)$ of ^{3}He. Here $\alpha(0)T_F$ has been assumed to vary linearly with pressure. The inset shows the experimental curves produced from Table 5 from reference [15]. For a detailed comparison with the experiment over the entire range of temperature see reference [13].

them. Whenever $\alpha(0)T_F$ is homogeneously increasing or decreasing function of these parameters the specific heat curves will cross at a point. In this case $\partial C/\partial\alpha(0)T_F = 0$ at $T = T_{cr}$ also means $\partial C/\partial X = 0$ at the same temperature, where X is an external control parameter like pressure or magnetic field. The later equation is the condition for crossing of curves at a point.

For liquid ^{3}He the specific heat calculated from spin fluctuation theory is plotted in Figure 2 as a function of temperature for various values of pressure, assuming a linear reduction of $\alpha(0)T_F$ with pressure. The experimental curves show similar behavior [15]. The linear variation of $\alpha(0)T_F$ with pressure is experimentally observed above pressures about 15 kbar. However, at small pressures there is some departure. The peak in $\triangle C(T)$ appears around 0.15 K. In Figure 2 the free Fermi gas part $(\pi^2 T/2T_F)$ has been added to $\Delta C(T)$. The value of $\alpha(\tau)$ has been calculated self consistently using equation (4) and then used as an input in the specific heat calculation. The coupling constant λ has been chosen to be 0.08 and the cutoff for the momentum sum, $1.2k_F$. The crossing temperature is related to $\alpha(0)T_F$ which depends on pressure in general. The crossing point shifts towards high temperature side slightly with increase in cutoff and with decrease in λ but the nature of crossing is not affected.

There are some heavy fermion materials in which the specific heat curves cross. We consider the case of $CeAl_3$ [9] and UBe_{13} [10]. $CeAl_3$ does not undergo either a magnetic or a superconducting transition, while UBe_{13} becomes superconductor at 0.9 K at normal pressure. The present discussion pertains to their normal state properties only. Heavy fermions are characterized by a large linear temperature dependent term in the specific heat and a large low temperature spin susceptibility [16]. In this regime the resistivity also shows a T^2 behavior characteristic of a Fermi liquid. Above a certain temperature $T^\star$, the susceptibility starts showing a Curie Weiss behavior, indicating the existence of interacting local moments on the f-shells. The local moment to Pauli like behavior of the susceptibility, as temperature reduces, marks the onset of coherence in these systems. In UBe_{13} this coherence regime is less visible because of the onset of superconductivity, but once the superconductivity is suppressed on application of pressure the coherence is restored [17]. At present a clear microscopic understanding of the behavior of heavy fermions is lacking, one has to take recourse to various levels of phenomenology. It is possible that the unusual low temperature dependence of physical properties in UBe_{13} for example, is due to its being a non-Fermi liquid of as yet unknown origin. We take the point of view here that this behavior can be described in terms of proximity to a quantum critical point which is also known to lead to temperature dependences different from Fermi liquid theory (see for example [5]).

Because of the similarity to liquid ^{3}He, at the phenomenological level it is tempting to apply the spin fluctuation theory to these materials also, with $\alpha(0)T_F$ playing the role of the crossover temperature $T^\star$. However, there is a difference. While ^{3}He can be considered close to a ferromagnetic transition, most heavy fermion materials seem to be close to an antiferromagnetic instability. In the present work, we therefore consider the heavy fermions in the coherence regime as nearly antiferromagnetic Fermi liquid. We have calculated the specific heat corrections by writing the equations for the susceptibility enhancement and specific heat near an antiferromagnetic instability. The formalism remains same except that the factor ω/q in equation (2) is replaced by ω to take care of

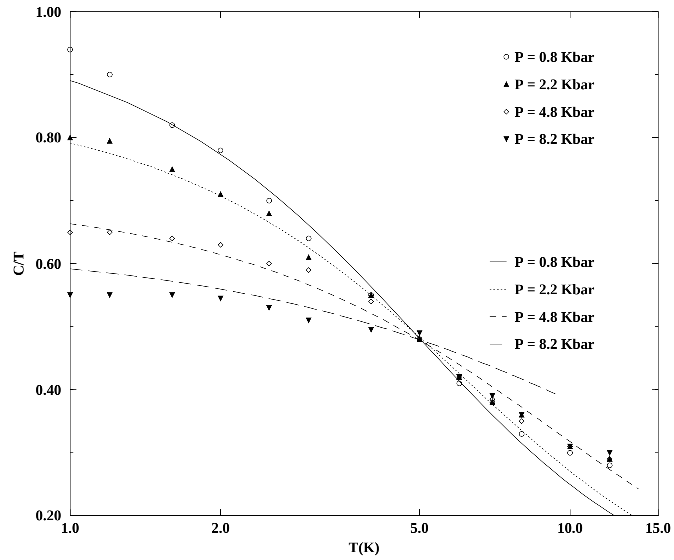

Fig. 3. Semilog plot of $C(P,T)/T$ as a function of T for $CeAl_3$ for various pressures. The symbols are experimental points (Ref. [12]) and the lines are results from the spin fluctuation theory.

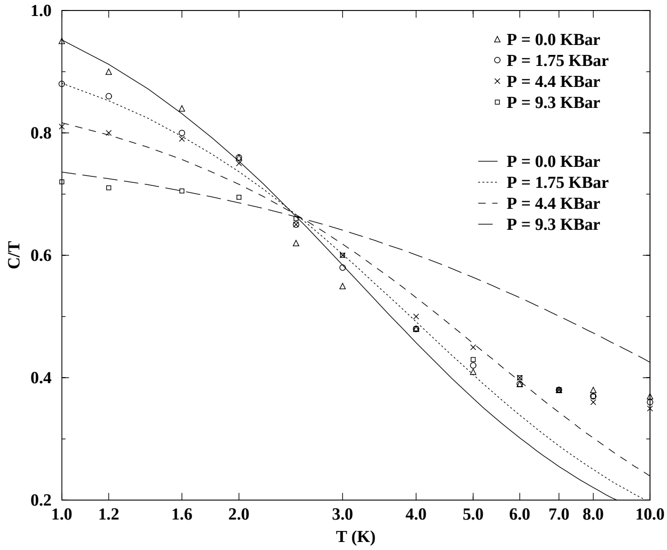

Fig. 4. Semilog plot of $C(P,T)/T$ as a function of T for UBe_{13}, above the superconducting transition temperature, for various pressures. The symbols are experimental points (Ref. [12]) and the lines are results from the spin fluctuation theory.

low energy behavior of the fluctuation propagator [5]. The difference is due to the fact that in this case the order parameter does not remain a conserved quantity. Further, to reproduce the huge effective mass observed, fluctuation modes are essentially dispersionless in heavy fermions [18], namely the coefficient of the q^2 term in y, *i.e.*, $\delta \approx 0$. This leads to the specific heat varying as $\tau/\alpha(0)$ at low temperatures and the leading temperature correction to zero temperature susceptibility varying as $\tau^2/\alpha^2(0)$. Here $\alpha(0)$ corresponds to inverse staggered susceptibility in units of the susceptibility $\chi^0(Q)$ of the non-interacting system.

In Figures 3 and 4 the specific heat curves for $CeAl_3$ and UBe_{13} have been plotted as a function of temperature for various pressures. The value of γ has been taken to be 0.185 and the cutoff q_c is 2.0. The fluctuation coupling λ is 5×10^{-4} for $CeAl_3$ and 2×10^{-4} for UBe_{13}, and decreases slightly with pressure. The parameter $\alpha(0)T_F$ is of the order of the crossing temperature with a weak linear pressure dependence. The variation with pressure is within 10%. In contrast to ^{3}He, here $\alpha(0)T_F$ increases with pressure. This is because in ^{3}He pressure brings the atoms closer and thereby increasing the interaction, while in heavy fermions the reduction in the lattice parameter enhances the hybridization between conduction electrons and f-electrons thereby the antiferromagnetic exchange between local moment and the conduction electron will be enhanced leading to a non magnetic ground state. It is seen that the curves cross within a small regime close to the experimental crossing point. Beyond the crossing point the deviation from the experimental curves is large. In fact, in heavy fermions, the curves cross at two points, the second point being away from the crossover temperature $T^\star$, though still at temperatures far below T_F. The reason for the second crossing cannot be found in a single parameter theory like the present one. It might be due to some other low lying modes like crystal field excitations or phonons [6].

So far we have discussed the ferro- and antiferromagnetic quantum critical points within the spin fluctuation theory. This result does not seem to be specific to the spin fluctuation theory and the type of transition involved. For example, in a phenomenological model attempting to incorporate some aspects of strong correlations near the Mott transition Rice *et al.* generalized the Brinkman-Rice theory to finite temperatures by introducing an extra ansatz for the entropy. It was applied to the case of UBe_{13} [19] and later to liquid ^{3}He [20]. At a low energy scale which is related to reducing double occupancy there is crossover between Pauli to Curie behavior for the susceptibility. The specific heat curves [20] for liquid ^{3}He at various pressures do cross (however, over a wide range of temperatures unlike the experimental findings [15]). Recently, the metal insulator transition has been discussed within the single band Hubbard model for infinite dimension by Georges and Krauth [8]. Again a low energy scale, related to the vanishing quasiparticle weight, arises in the metallic side of the transition. The specific heat curves cross at temperature around this scale. However, the theory gives a second crossing around the energy scale U.

We have used the terms quantum and classical in the discussion above, because, the temperatures below $\alpha(0)T_F$ essentially define a regime where one gets a Fermi liquid behavior whereas at high temperatures, fluctuations get correlated resulting in the classical behavior for the susceptibility. The distinction, quantum *versus* classical, becomes clear when one takes the limit $\alpha(0) \rightarrow 0$ (the quantum critical point). In that case the Curie law for susceptibility is obtained down to zero degree [5], while in the opposite limit $(\alpha(0) \rightarrow 1)$ one gets the Pauli susceptibility; in either of these limits the curves for specific heat do not cross.

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