Crossing of Specific Heat Curves in some correlated Fermion systems

Suresh G. Mishra and P.A. Sreeram
Institute of Physics, Sachivalaya Marg, Bhubaneswar 751 005, India.

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 vicinity of a quantum critical point in these systems which leads to a crossover at some temperature $T^*$ from quantum to classical fluctuation regime. The temperature at which the curves cross turns out to be near $T^*$. 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. When the crossover scale is any homogeneous function of these control parameters there is always crossing at a point.

PACS numbers: 71.27.+a, 67.55.Cx, 71.28.+d

There has been a surge of interest in correlated fermionic systems for the past 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. 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 [1].

One phenomenon which had been observed long ago is that in some systems the specific heat curves as a function of temperature, for various values of external parameters (e.g. pressure, magnetic field) cross at a point or at least within a very narrow regime of temperature. This phenomenon was initially observed for $^3$He by Brewer et. al [2] and has been seen later on, in a variety of materials ranging from systems close to metal-insulator transition to heavy fermions. 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 [3] has given a thermodynamic interpretation to this universality. The argument 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 (or $T = 0$ critical point). 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 which marks a crossover from quantum to a classical behavior in the temperature dependence of various physical properties. In most materials the abovementioned crossing of specific heat occurs near this crossover temperature. This scenario is quite general and holds for transitions involving conserved (for example, the ferromagnetic) as well as nonconserved (the anti-ferromagnetic) order parameters. The examples discussed in the present letter have been chosen to represent both of these order parameter fluctuations. We use the microscopic spin fluctuation theory [4] to discuss the behavior in detail. This theory has the low energy scale 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 $\chi_P$, depending on pressure. The coefficient of the linear term in specific heat is also large. In the spin fluctuation theory presented below, the liquid is regarded as near a ferromagnetic instability. In this theory 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 [5].

In the following we use some results from our earlier works [6,7] to discuss the crossing point in the specific heat curves. We consider first fluctuation above the transition to a ferromagnetic phase. 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 [8].
\[ \Delta \Omega = \frac{3T}{2} \sum_{q,m} \ln \{1 - U_{\chi_{qm}}^0 + \lambda T \sum_{q',m'} D_{q'm'} \}. \]  

(1)

Here \( D_{q,m} \) is the fluctuation propagator which is related to inverse dynamical susceptibility, \( \chi_{qm}^0 \) is the free Fermi gas (Lindhardt) response function, and \( \lambda \) 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,

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

(2)

where \( \alpha(\tau) \) is the inverse of spin susceptibility in units of the Pauli susceptibility. The wavevector \( q \) is given in units of Fermi momentum \( k_F \) and the energy is in units of Fermi energy \((\tau = T/T_F)\). For a free Fermi gas \( \gamma = 1/2, \delta = 1/12 \). The correction to the specific heat is given by,

\[ \frac{\Delta C}{k_B} = -3\tau^2 \sum_q \left[ \left( \frac{\partial y}{\partial \tau} \frac{\tau}{\partial^2 y} + \frac{\partial^2 y}{\partial^2 \tau} \right) \phi(y) + \left( \frac{\partial y}{\partial \tau} \right)^2 \frac{\partial \phi(y)}{\partial y} \right] \]  

(3)

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

\[ \alpha(\tau) = \alpha(0) + \frac{\lambda}{\pi} \sum_q q \phi(y). \]  

(4)

For a finite \( \alpha(0) \) there are two regions of temperature. 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 \( 1 < n < 4/3 \). 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 with experimental results of Thompson et. al. [8]. The parameter \( \alpha(0)T_F \) is the low energy scale which arises in the spin fluctuation theory naturally. The corresponding low temperature \( (\tau \leq \alpha(0)) \) correction to the specific heat is,

\[ \frac{\Delta C}{k_B} = -\sum_q \frac{\pi^2 \tau}{4q(\alpha + \delta q^2)}. \]  

(5)

The phase space integral reproduces the standard paramagnon mass enhancement result, \( \tau \ln \alpha \) for \( \Delta C \). In the classical regime, \( \alpha(0) \leq \tau \ll 1 \), where the small \( y \) approximation holds and \( \alpha(\tau) \) varies as \( \tau, \Delta C \) 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. Considered as a function of \( \alpha(0)T_F \), the temperature dependence of specific heat is more revealing. Below a certain temperature \( T_{cr} \), specific heat decreases as \( \alpha(0)T_F \) increases, while above it the behavior is reversed (see Fig. 1). \( T_{cr} \) clearly marks the crossing and is of the order of \( \alpha(0)T_F \). The spin fluctuation theory has only one parameter, that is, \( \alpha(0)T_F \). The pressure or magnetic field dependence of quantities is realized through the dependence of \( \alpha(0)T_F \) on 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 \( ^3\text{He} \) the specific heat is plotted in Fig. 2 as a function of temperature for various values of pressure, assuming a linear reduction of \( \alpha(0)T_F \) with pressure. The linear scaling is experimentally observed above pressures about 15 kbar. However, at small pressures there is some departure. The peak in \( \Delta C(T) \) appears around 0.15K. To calculate the specific heat, 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 Eq. (4) and then used as an input in the specific heat calculation. The coupling constant \( \lambda \) has been chosen to be 0.08 and the cutoff for the momentum sum, \( 1/15 \) has been chosen to be 0.08 and the cutoff for the momentum sum, \( 1/15 \) has been chosen to be 0.08 and the cutoff for the momentum sum, \( 1/15 \). 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 \( \lambda \) 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.
present discussion pertains to their normal state properties only. Heavy fermions are characterised by a large linear temperature dependent term in the specific heat and a large low temperature spin susceptibility \(\tau/\alpha\). 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 \(\text{UBe}_{13}\), 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 \([12]\). 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 \(\text{UBe}_{13}\) 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 (for example \([13]\)).

Because of the similarity to liquid \(^3\text{He}\), at the phenomenological level it is tempting to apply the spin fluctuation theory to these materials, with \(\alpha(0)T_F\) playing the role of the crossover temperature \(T^\star\). However, there is a difference. While \(^3\text{He}\) can be considered close to a ferromagnetic transition, most heavy fermion materials seem 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 \(\omega/q\) in Eq. 3 is replaced by \(\omega\) to take care of low energy behavior of the fluctuation propagator \([14]\). The difference is due to the fact that 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 \([15]\), namely the coefficient of the \(q^2\) term in \(y\), i.e., \(\delta \approx 0\). In this case, the leading contribution to specific heat is \(\tau/\alpha(0)\) at low temperatures. In the same range of temperatures the leading temperature correction to zero temperature susceptibility is \(\tau^2/\alpha^2(0)\).

In Fig.3 and 4 the specific heat curves for CeAl\(_3\) and \(\text{UBe}_{13}\) have been plotted as a function of temperature for various pressures. The value of \(\gamma\) has been taken to be 0.185 and the cutoff \(q_c\) is 2.0. The fluctuation coupling \(\lambda\) is \(5 \times 10^{-4}\) for CeAl\(_3\) and \(2 \times 10^{-4}\) for \(\text{UBe}_{13}\), 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 \(^3\text{He}\), here \(\alpha(0)T_F\) increases with pressure. This is because in \(^3\text{He}\) 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 \([3]\).

So far we have discussed the ferro- and antiferromagnetic quantum critical points. 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 \(\text{UBe}_{13}\) \([14]\) and later to liquid \(^3\text{He}\) \([15]\). At a low energy scale which is related to reducing double occupancy there is crossover between Pauli to Curie behavior for the susceptibility. However, the specific heat curves \([15]\) for liquid \(^3\text{He}\) at various pressures seem to cross over a wide range of temperatures unlike the experimental findings \([16]\). Recently, the metal insulator transition has been discussed within the single band Hubbard model for infinite dimension by Georges and Krauth \([17]\). 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 \( \alpha(0) \to 0 \) (the quantum critical point). In that case the Curie law for susceptibility is obtained down to zero degree, while in the opposite limit \( (\alpha(0) \to 1) \) one gets the Pauli susceptibility; in either of these limits the curves for specific heat do not cross.

Acknowledgement: We are grateful to Prof. T. V. Ramakrishnan for critical reading of the manuscript.

[1] See for example, J. Phys.: Condens. Matter 8(48) (1996), special issue on non-Fermi-liquid behavior in metals, edited by P. Coleman, B. Maple, and A. Millis.

[2] D. F. Brewer, J. G. Daunt and A. K. Sreerdh, Phys. Rev. 115 (1959) 836.

[3] D. Vollhardt, Phys. Rev. Letts. 78 1307 (1997).

[4] S. G. Mishra and T. V. Ramakrishnan, Phys Rev. B18, 2308 (1978).

[5] T. Moriya, Spin Fluctuation in Itinerant Electron Magnetism (Springer, Heidelberg, 1985).

[6] S. G. Mishra and T.V. Ramakrishnan, Phys. Rev. B31 2825 (1985).

[7] S. G. Mishra and P. A. Sreeram, Phys. Rev. B 57 2188 (1998).

[8] J. R. Thompson, Jr., H. Ramm, J. F. Jarvis and Horst Meyer, Jour. Low. Temp. Phys., 2 521,539 (1970).

[9] G.E. Brodale, R.A. Fisher, N.E. Phillips and J. Flouquet, Phys. Rev. Lett. 56 390 (1986).

[10] N.E. Phillips, R.A. Fisher, J. Flouquet, A.L. Giorgi, J.A. Olsen and G.R. Stewart, J. Mag. Magnetic Materials 63 & 64 332 (1987).

[11] For a review see N. Grewe and F. Steglich, Handbook on the Physics and Chemistry of Rare Earths Vol 14, Eds. K.A. Gschneidner Jr., and L. Eyring Amstardem Elsevier p. 343 (1991).

[12] M. C. Aronson, J. D. Thompson, J. L. Smith, Z. Fisk and M. W. McElfresh, Phys. Rev. Lett. 63 2311 (1989).

[13] M.A. Continentino, Phys. Rev. B 57 5966 (1998).

[14] T.M. Rice, K. Ueda, H.R. Ott, and H. Rudigier, Phys. Rev.B 31 594 (1985).

[15] K. Seiler, C. Gros, T.M. Rice, K. Ueda, and D. Vollhardt, J. Low Temp. Phys. 64 195 (1986).

[16] D.S. Greywall, Phys. Rev. B27 2747 (1983).

[17] A. Georges and W. Krauth, Phys.Rev. B 48 7167.

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. $C(P, T)$ for $^3$He with \( \alpha(0)T_F \) assumed to vary linearly with pressure.

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.
\[ \alpha(0) T_F \]

\[ C_v = \begin{cases} 
1 & T = 1 \text{ K} \\
3 & T = 3 \text{ K} \\
5 & T = 5 \text{ K} \\
8 & T = 8 \text{ K} \\
10 & T = 10 \text{ K} 
\end{cases} \]
The graph shows the relationship between temperature (T) and concentration (C) at different pressures. The pressures indicated are:

- $P = 0$ Bar
- $P = 3$ Bar
- $P = 9$ Bar
- $P = 15$ Bar
- $P = 27$ Bar
