Thermoelectric Behaviour Near Magnetic Quantum Critical Point

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(Dated: October 29, 2018)

We use the coupled 2d-spin-3d-fermion model proposed by Rosch et. al. (Phys. Rev. Lett. 79, 159 (1997)) to study the thermoelectric behaviour of a heavy fermion compound when it is close to an antiferromagnetic quantum critical point. When the low energy spin fluctuations are quasi two dimensional, as has been observed in YbRh$_2$Si$_2$ and CeCu$_{6-x}$Au$_x$, with a typical 2d ordering wavevector and 3d Fermi surface, the “hot” regions on the Fermi surface have a finite area. Due to enhanced scattering with the nearly critical spin fluctuations, the electrons in the hot region are strongly renormalized. We argue that there is an intermediate energy scale where the qualitative aspects of the renormalized hot electrons are captured by a weak-coupling perturbative calculation. Our examination of the electron self energy shows that the entropy carried by the hot electrons is larger than usual. This accounts for the anomalous logarithmic temperature dependence of specific heat observed in these materials. We show that the same mechanism produces logarithmic temperature dependence in thermopower. This has been observed in CeCu$_{6-x}$Au$_x$. We expect to see the same behaviour from future experiments on YbRh$_2$Si$_2$.

I. INTRODUCTION

Understanding the behaviour of a system close to antiferromagnetic quantum critical point (QCP) is currently an area of active research. The problem is interesting both in the context of high temperature superconductors as well as heavy-fermion materials, especially to understand metallic phases that show non-Fermi liquid (NFL) properties. In recent times several materials have been discovered where it has been possible to demonstrate the existence of magnetic QCP. This has made the problem an exciting ground where theoretical understanding of electrons with strong correlations can be verified experimentally. One central issue in this problem is an appropriate theoretical treatment of electrons interacting with magnetic fluctuations close to the QCP where magnetic correlation length diverges. A second central issue, is whether the spin fermion model describes the relevant degrees of freedom, or whether a more basic model, allowing for the disintegration of the binding of local moments to the quasiparticles, is necessary for describing this transition.

In this paper we will discuss two experimentally well-studied heavy fermion materials, CeCu$_{6-x}$Au$_x$ and YbRh$_2$Si$_2$, that exhibit antiferromagnetic QCP. In doped CeCu$_6$, replacing Cu with larger Au atoms, favours the formation of long range magnetic order.

Beyond a critical doping $x_c = 0.1$, the ground state of the system is antiferromagnetic with finite Néel temperature ($T_N$). At the critical doping $T_N$ is zero and the system has a QCP. On the other hand YbRh$_2$Si$_2$ is undoped and atomically well-ordered. It is a much cleaner material than CeCu$_{6-x}$Au$_x$, with residual resistivity ($\rho_0$) smaller by a factor of about 10. At ambient pressure it develops long range magnetic order at a very low temperature of $T_N \approx 65$ mK. The ordering temperature can be suppressed to practically zero (less than 20 mK) by applying a magnetic field of only 45 mT. Both these materials show pronounced deviations from Fermi liquid (FL) behaviour, which is believed to be due to closeness to the QCP. For instance, the dependence of electrical resistivity $\Delta \rho = \rho - \rho_0$ to temperature $T$ is $\Delta \rho \propto T$, while that of specific heat $C$ is $C/T \propto -\ln T$. This is in contrast with FL behaviour which predicts $\Delta \rho \propto T^2$ and $C/T = \text{constant}$. The low temperature NFL behaviour is observed over a decade of temperature, up to about 1 K for CeCu$_{6-x}$Au$_x$ and up to as high as 10 K for YbRh$_2$Si$_2$. The source of the interesting physics in these materials is the localized 4f electrons of Ce$^{3+}$ (in 4f$^1$ electronic configuration) and Yb$^{3+}$ (in the configuration 4f$^{13}$), and their interaction with the relatively delocalized s, p and d orbital electrons that form a conduction band with a well defined Fermi surface at low temperature. The conduction electrons and the localized 4f electrons carrying magnetic moment are coupled by exchange interaction ($J$). Below a certain critical value of exchange interaction ($J_c$), the local moments interact with each other, mediated by conduction electrons, and at sufficiently low temperature form long range antiferromagnetic order. On the other hand, at the exchange coupling is strong ($J > J_c$), the local moments are quenched below a certain temperature (lattice Kondo temperature). The quenched moments hybridize with the conduction electrons and they participate in the formation of the Fermi sea. The ground state of such a system is non-magnetic. The exchange coupling is usually tuned experimentally by either doping the material or by applying external pressure or external magnetic field.

For CeCu$_{6-x}$Au$_x$ there are two different views regarding the nature of the system in the non-ordered phase and the corresponding mechanism by which the critical instability occurs. In the first picture, the lattice Kondo temperature ($T_K$) becomes zero exactly at the critical point ($J = J_c$). The local moments of the 4f electrons survive at all finite temperature close to the critical point. At the transition point they are critically quenched. The local
moments produce the critical magnetic fluctuations that destabilize the Fermi sea. It has been argued, in favour of this mechanism, that the data on magnetic susceptibility shows non-trivial scaling with temperature.\textsuperscript{7} At the critical point the susceptibility has the scaling form $\chi = T^{-\alpha} f(\omega/T)$ with an anomalous exponent $\alpha \simeq 0.75$, which is different from conventional insulating magnets which have $\alpha = 1$. The alternative picture suggests that $T_K$ is finite at the critical point. Well below this temperature, and close to the critical point, the local moments are quenched by Kondo mechanism. The $4f$ electrons become part of the Fermi sea. Then, the phase transition occurs by the usual spin-density wave instability of the Fermi surface. In this picture the local moments do not play any role in the phase transition. This theoretical viewpoint, proposed by Rosch and collaborators,\textsuperscript{6} is motivated by inelastic neutron scattering data on CeCu$_{15.9}$Au$_{0.1}$ which show that the nearly critical spin fluctuations are two dimensional.\textsuperscript{8} But the origin of the quasi 2d behaviour of spin fluctuations is not well understood. However, the same feature is probably also present in YbRh$_2$Si$_2$, where the structure of the lattice provides a more natural explanation for the spin fluctuations to be 2d.\textsuperscript{2} Besides the nature of the magnetic correlations, there are different opinions regarding the dynamics of the spin fluctuations. It has been argued\textsuperscript{9} that if the ordering wave-vector spans different points of the Fermi surface, then the dynamics of the spin fluctuations is overdamped, with dynamic exponent $z = 2$. This model of spin fluctuations with $d = 2$ and $z = 2$, coupled with three-dimensional electrons, was used to explain the linearity of resistivity with temperature.\textsuperscript{6} Following the method of Hertz,\textsuperscript{10,11} in which the system is described entirely in terms of the spin fluctuations, after a formal Hubbard-Stratonovich transformation to integrate the fermion modes, it also explains the logarithmic temperature dependence of specific heat.\textsuperscript{6,11} In an alternative description,\textsuperscript{12} in terms of low energy electrons interacting with spin fluctuations, it has been suggested recently that both the frequency and momentum dependence of the spin fluctuation propagator undergo singular corrections such that the propagator acquires an anomalous dimension $\eta \sim 1/4$.\textsuperscript{13} Thus, after nearly a decade, there is still no clear understanding regarding the appropriate model that describes the quantum phase transition.

In this paper we will study the thermoelectric behaviour of a system in the paramagnetic phase and close to antiferromagnetic QCP. For CeCu$_{15.9}$Au$_{0.1}$ it is known that thermopower ($S_t$) has a dependence similar to specific heat over the same range of temperature,\textsuperscript{14,15} i.e, $S_t/T \propto -\ln T$. We will show that scattering with nearly critical spin fluctuations give rise to temperature dependent quasiparticle mass ($m^*$) over much of the Fermi surface. The signature of this can be seen in static response (specific heat) and in transport (thermopower). Finally we will argue that the same mechanism should be relevant for YbRh$_2$Si$_2$, and so we expect to see the same behaviour for thermopower from future experiments.

\section{Model}

Our model is motivated by the second picture as described above. It assumes that $T_K^*$ defines a high energy parameter. For $T \sim T_K^*$ the local nature of the spins of the $4f$ electrons is important as they participate in some lattice Kondo phenomenon. For $T < T_K^*$, the $4f$ electrons become part of the hybridized conduction band. In this regime the nearly critical spin fluctuations of the conduction electrons is important. It is an intermediate temperature range where the system is described by low energy conduction electrons interacting with quasi 2d spin fluctuations. Within the spin-fermion description, at sufficiently low temperature, the 3d nature of the spin fluctuations is retrieved and the model used here ceases to be valid. In this regime, the model predicts, in pure systems, a crossover to an electronic Fermi liquid with a finite mass. However the physics governing this dimensional crossover, has not been investigated.

The model is described by the Hamiltonian

\begin{equation}
\mathcal{H} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \frac{g_0}{2} \sum_{q,\alpha,\beta} \frac{\chi(q)}{\omega} c_{k+q,\alpha}^\dagger c_{k,\beta} \sigma_{\alpha,\beta} \cdot S_{-q} + \sum_{q} \left[ \chi^{-1}(q) S_q \cdot S_{-q} + \Pi_q \cdot \Pi_{-q} \right] + \frac{u_0}{4} \sum_{k_1, \ldots, k_4} (S_{k_1} \cdot S_{k_2}) (S_{k_3} \cdot S_{k_4}) \delta(k_1 + \ldots + k_4).
\end{equation}

Here $c_{k,\sigma}^\dagger$ is the electron creation operator, $S_q$ is the operator for the spin fluctuations, $\Pi_q = \partial_t S_q$ is the conjugate momentum field for the spin fluctuations, and $\chi(q)$ is the static magnetic susceptibility. $g_0$ is the bare coupling between the electrons and the spin fluctuations, and $u_0$ is the interaction energy of the spin fluctuations. The collective spin fluctuations are formally obtained by integrating out high energy electrons in the band up to a certain cutoff.\textsuperscript{12} Thus the typical energies of the spin fluctuations $\omega_q \sim W$, the bandwidth of the conduction electrons. The system is close to an antiferromagnetic instability with ordering wave-vector $Q$. We will assume that
the dynamics of the spin fluctuations is purely damped with
dynamic exponent $z = 2$. The spectrum of the 2d
spin fluctuations will be described by\textsuperscript{10,11}
\begin{equation}
\chi^{-1}(\mathbf{q}, \omega) = \delta + \omega_s (\mathbf{q} - \mathbf{Q})^2 - i\gamma|\omega|.
\end{equation}
Here $\delta$ is the mass of the spin fluctuations and mea-
sures the deviation from the QCP, the parallel directions
are those along the planes of magnetic correlation, and
$\gamma \sim (g_0/\epsilon_F)^2$ is an estimate of the damping from the
polarization bubble. In the spin fluctuation part of the
Hamiltonian, the interaction term $u_0$ is marginal, since
the scaling dimension is zero.\textsuperscript{10,11} The main contribu-
tion of this term is to renormalize the mass of the spin fluctu-
ations ($\delta$) and make it temperature dependent. Within a
Gaussian approximation, $\delta$ is linearly dependent on tem-
perature, up to logarithmic corrections.\textsuperscript{6,11} We will ig-
nore other effects of the $u_0$ term in our discussion, and
will consider only the quadratic term with temperature
dependent mass of the spin fluctuations. To simplify the
calculation we will assume a spherical Fermi surface for
the non-interacting electrons, with the ordering wave-
vector $\mathbf{Q} = (\alpha, 0, 2k_F \cos \theta_0)$. Here $\theta_0 \neq 0$ (i.e. not
2$k_F$ ordering), and $\theta_0 \neq \pi/2$ (i.e. not ferromagnetic or-
dering). We have chosen $\hat{x}$ as the direction along which
the spin fluctuations are uncorrelated, and $\alpha$, the order-
ing in the $x$-direction, varies from one plane of magnetic
correlation to another. Since the spectrum of spin fluctu-
ations is 2d, those carrying momentum of the form
$\mathbf{Q} + \alpha \hat{x}$, where $\alpha$ is arbitrary, are all nearly critical. Due
to constraints from energy-momentum conservation, only
those points on the Fermi surface that are connected by
the nearly critical spin fluctuations are particularly sen-
tive to the QCP, since electrons at these points undergo
singular scattering with the spin fluctuations. These are
the so-called “hot spots”. It is important to note that
since the spin fluctuations are 2d, there will be a finite
area of the Fermi surface that is hot. Though it is worth-
while to estimate the fraction of the Fermi surface that is
hot, theoretically it is a daunting task. In our cal-
culation we will assume that most of the Fermi surface
is hot. In effect, we are assuming that contribution to
static response and also to transport is mostly from the
hot regions. It was pointed out by Hlubina and Rice\textsuperscript{16}
that in transport the hot carriers are less effective than
the cold ones. This is because the quasiparticle lifetime
of the hot carriers is less than that of the cold carriers,
since the former suffer enhanced scattering with the spin
fluctuations. As we will show below, the lifetime of the
hot electrons $\tau_h \propto 1/T$, while the cold electrons have
Fermi liquid characteristics with $\tau_c \propto 1/T^2$. If $x$ is the
fraction of the Fermi surface (FS) that is hot, then we can
make an estimate of conductivity $\sigma$,
\begin{equation}
\sigma \propto (\tau_k)_{FS} \propto \frac{x}{T/\epsilon_F} + \frac{1 - x}{(T/\epsilon_F)^2}.
\end{equation}

The first term, which is the contribution from the hot
region, will dominate to give $\Delta \rho \propto T$ only if $x > 1/(1 + T/\epsilon_F)$. This gives a rough estimate of the fraction
necessary for the hot carriers to dominate. In the case of
CeCu$_6$$_{1-x}$Au$_x$, which is a dritier material, the above es-
timation is more involved. It was recently shown\textsuperscript{17} that
the effect of disorder is to favour isotropic scattering and
thereby reduce the effectiveness of Hlubina-Rice mecha-
nism. Thus, one should expect a smaller fraction, than
estimated above, enough to make the contribution of the
hot carriers significant for CeCu$_6$$_{1-x}$Au$_x$.

III. ELECTRON SELF ENERGY

To calculate the effect of the low energy spin fluctua-
tions on the hot electrons, we will examine the electron self-
energy. The lowest order term in perturbation gives,
\begin{equation}
\Sigma (\mathbf{p}, \omega) = -\frac{g_0^2}{V} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi i} \chi (\mathbf{k}, \Omega) G (\mathbf{p} + \mathbf{k}, \omega + \Omega),
\end{equation}
where $G (\mathbf{p}, \omega)$ is the free electron propagator given by,
\begin{equation}
G (\mathbf{p}, \omega) = \frac{n_p}{\omega - \epsilon_p - i\eta} + \frac{1 - n_p}{\omega - \epsilon_p + i\eta}.
\end{equation}
Here $n_p$ is the electron occupation of the momentum state
$\mathbf{p}$ at $T = 0$. As expected, the above expression has dif-
ferent behaviours in the hot and cold regions. But within
each region the self-energy is practically momentum inde-
pendent. The imaginary part of the self-energy gives the
quasiparticle lifetime as determined by scattering with the
spin fluctuations. For $\omega > 0$ we have,
\begin{equation}
\text{Im} \Sigma (\mathbf{p}, \omega) = -\frac{g_0^2}{V} \sum_{0<\epsilon_k<\omega} \frac{(\omega - \epsilon_{k+p})}{(\delta + \omega_s (\mathbf{k} - \mathbf{Q})^2)^2 + (\omega - \epsilon_{k+p})^2}.
\end{equation}
If $\mathbf{p}$ is a point in the hot region, then it is connected to
another hot spot by a wave-vector of the form $\mathbf{k} = \mathbf{Q} + \alpha \hat{x}$.
We linearize the spectrum about this second hot point,
and perform the integral in terms of local coordinates
around it. In the hot region we get,
\begin{equation}
\text{Im} \Sigma (\mathbf{p}, \omega) \propto -\frac{g_0^2}{\epsilon_F \omega_s} \frac{\omega^2}{\max[\delta, \omega]}.
\end{equation}
For $\omega > \delta$ the lifetime of the hot electrons is much smaller
than that given by Fermi liquid behaviour ($\text{Im} \Sigma (\omega) \propto
\omega^2$). As we have mentioned above, this is due to more
effective scattering with the spin fluctuations in this re-
region. For the cold electrons the behaviour is Fermi liquid
like.

Next, we will examine the real part of the self-energy.
The dependence of $\text{Re} \Sigma$ on frequency is more important
than the dependence on momentum. We get,
The temperature dependence of entropy is
\[ \tau_c \propto T \ln(1/\delta). \]

Here \( \gamma_k = \delta + \omega_s(k - Q)^2 \). If \( p \) is a point within the hot region, each of the three terms in the above expression is logarithmic. As before, after linearizing the spectrum near the second hot spot, we get
\[
-\lim_{\omega \to 0} \frac{\partial}{\partial \omega} \text{Re} \Sigma(p, \omega) \propto \left( \frac{g_0^2}{\pi \epsilon_p \omega_s} \right) \ln \left( \frac{\omega_s}{\delta} \right). \tag{6}
\]

Due to scattering, the non-interacting electron mass \( m \) is renormalized to the quasiparticle mass \( m^* = m/Z \) (in the absence of any momentum dependence of the electron self-energy), where
\[
Z^{-1} = 1 - \lim_{\omega \to 0} \frac{\partial}{\partial \omega} \text{Re} \Sigma(p, \omega)
\]
defines the quasiparticle residue. Since \( \delta \), which measures the deviation from the critical point, can be written as \( \delta = \Gamma(p - p_c) + T \), the quasiparticle mass becomes temperature dependent. Here \( p \) is an experimental parameter that can be tuned to the critical value \( p_c \), and \( \Gamma \) is an appropriate energy parameter. As a consequence the entropy of each hot quasiparticle becomes anomalously large. This can be seen from the expression for entropy (\( S \)) per particle,
\[
\frac{S}{N} \propto N(0)T \left( \frac{g_0^2}{\epsilon_\tau \omega_s} \right) \ln \left( \frac{\omega_s}{\delta} \right), \tag{7}
\]

where \( N(0) \) is the density of states of the non-interacting system at the Fermi energy. For \( T > \Gamma(p - p_c) \), the temperature dependence of entropy is \( S \propto T \ln(1/T) \), which is different from Fermi liquid behaviour \( (S \propto T) \). This gives rise to the anomalous logarithmic temperature dependence of specific heat. In the past, this behaviour has been understood from a purely bosonic point of view following the formalism of Hertz and Millis. For the spin fluctuations the Gaussian part of the action gives a free energy \( F \propto T^2 \ln T \), which explains the \( \ln(1/T) \) behaviour of \( C/T \). Thus, here we find that there is agreement between the results of the spin-fermion model and the pure bosonic model.

\[ IV. \ \text{THERMOPOWER} \]

From our discussion on entropy, it is natural to expect that this entropy enhancement should be seen in the measurement of thermopower \( (S_t) \). This is because one can think of thermopower as proportional to the correlation function between the heat current and the particle current, and heat current involves the transport of entropy due to temperature and electric potential gradients in the system. Strictly speaking, thermopower is defined as a ratio of two correlation functions,
\[
S_t = \frac{L_{12}}{eTL_{11}},
\]

where
\[
L_{12} = \lim_{\omega \to 0} \frac{1}{\omega V} \int_0^\beta d\tau e^{i\omega\tau} \langle T_{\tau} j_Q(\tau) \cdot j(0) \rangle,
\]
is the correlation function between heat current \( (j_Q) \) and particle current \( (j) \), and
\[
L_{11} = \lim_{\omega \to 0} \frac{1}{\omega V} \int_0^\beta d\tau e^{i\omega\tau} \langle T_{\tau} j(\tau) \cdot j(0) \rangle,
\]
is the correlation function between particle currents. \( L_{11} \) is a measure of electrical conductivity \( (\sigma = e^2L_{11}) \). Here we are ignoring the tensor nature of \( L_{11} \) and \( L_{12} \), and assuming that temperature and potential gradients and the thermal current are along the major symmetry directions of the lattice so that the tensors are diagonal. We express the single particle energies with respect to the chemical potential and assume that chemical potential in the sample is uniform. The expression for heat current is given by,
\[
j_Q = \frac{i}{2} \sum_{p, \sigma} \vec{v}_p \left( \epsilon_p^{\dagger} c_{\sigma}^{\dagger} c_{\sigma}^{\dagger} - \epsilon_p c_{\sigma} c_{\sigma}^{\dagger} \right).
\]

In principle, heat current will have a second term of the form \( \frac{i}{2} \sum_{k, \sigma} \nabla_k U(k) \left( \hat{n}_{k, \sigma} n_{-k, \sigma} - \hat{n}_{-k, \sigma} n_{k, \sigma} \right) \), where \( U(k) \) is the Fourier transform of the interaction term between the electrons. However, such a term is quartic in fermionic operators and generates only subleading contributions in our calculation. We will also ignore corrections to the particle current and heat current vertices due to exchange of spin fluctuations. These vertex corrections are nonsingular, and change only the numerical prefactor (which we do not attempt to calculate) of our leading term, because the spin fluctuations are peaked around...
a finite wave-vector. With these approximations the expressions for the correlation functions can be re-expressed in a more transparent form as

\[ L_{12} = \sum_p v_p^2 \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \omega A^2(p, \omega), \]

\[ L_{11} = \sum_p v_p^2 \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) A^2(p, \omega). \]

Here \( v_p = \partial \epsilon_p / \partial p \) is the quasiparticle velocity, and \( A(p, \omega) \) is the spectral function defined as

\[ A(p, \omega) = \frac{\tau(\omega)^{-1}}{\left( \omega - \epsilon_p \right)^2 + \tau(\omega)^{-2}}. \]

The evaluation of \( L_{11} \) is more straightforward and we will examine it first. The momentum sum can be converted into an integral over various energy surfaces. The dominant contribution is from the Fermi level, and we get

\[ L_{11} = v_F^2 N(0) \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \tau(\omega). \]

We have already noted that over the hot region \( \tau(\omega) \propto \omega^{-1} \). For the frequency integral since \( \omega \sim T \), we get

\[ L_{11} \propto \left( \frac{\epsilon_F \omega_s}{g_0} \right) v_F^2 N(0) \frac{T}{T}. \]  \hspace{1cm} (8)

This result simply reiterates what we had noted before, that when the hot carriers dominate transport, \( \Delta \sigma \propto 1/T \). Now for \( L_{12} \), we first notice that the expression is odd in frequency. This is because \( L_{12} \) is a measure of particle-hole asymmetry in the system. In our calculation we will consider as phenomenological input two different sources of such asymmetry. One such source is from the density of states, so that \( N(\omega) = N(0) + \omega N'(0) + \omega^2/\epsilon_p^2 \), where \( N'(0) \neq 0 \) only if there is particle-hole asymmetry in the bare non-interacting system of electrons. The second source of asymmetry will be from the quasiparticle lifetime which, for the hot carriers, we write as \( \tau^{-1}(\omega) = (g_0^2/\epsilon_F \omega_s) |\omega| (1 + \tau \omega) \). Here the second term is a possible particle-hole asymmetric term in scattering lifetime. \( \tau \) is a typical scattering time, and \( \omega < \tau^{-1} \). After the energy integral around the Fermi surface we get,

\[ L_{12} = v_F^2 \int_{-\infty}^{\infty} d\omega (-\frac{\partial f}{\partial \omega}) \omega \tau(\omega) N(\omega/Z) \]

\[ = \left( \frac{\epsilon_F \omega_s}{g_0} \right) v_F^2 \{ T N'(0)/Z + TN(0)\tau \}. \]  \hspace{1cm} (9)

The first term in the above equation is from the asymmetry in density of states, and the second term is from the asymmetry in quasiparticle lifetime. We note that the factor of \( 1/Z \), which leads to entropy enhancement, is associated with the asymmetry in density of states. Thus, the first term is the dominant one and eventually gives anomalous temperature dependence to thermopower. For this leading term we can write

\[ S_t \propto \frac{1}{e} \left( \frac{g_0^2 N'(0)}{\epsilon_F \omega_s N(0)} \right) T \ln(\omega_s/\delta). \]  \hspace{1cm} (10)

In the regime where \( T > \Gamma(p - p_c) \), \( S_t/T \propto \ln(1/T) \), as has been observed in thermopower measurement on CeCu\textsubscript{5-\(x\)}Au\textsubscript{\(x\)}.

\[ F(T, H)/k_B = X(T, H) \ln \left[ 2 \cosh \left( \frac{\mu \lambda H}{Y(T, H)} \right) \right]. \]  \hspace{1cm} (11)

FIG. 1: Magnetization (M) vs external magnetic field (H) at different temperatures: a) T=0.15K, b) T=0.3K and c) T=0.8K. The discrete points are experimental. The solid lines are fits using equation (10).

V. CONCLUSION

To check the consistency of our model and calculation, we need to estimate the high energy scale (namely, \( T_K \)) of CeCu\textsubscript{5-\(x\)}Au\textsubscript{\(x\)}. For this purpose, we have fitted an approximate form of the free energy function (\( F \)) that will match with the experimental results at low temperature and in the presence of magnetic field (\( H \)). The function that matches well with the experiment has the form,
the effective magnetic moment of the Ce

The uniform

where

Here $C_1 - C_3$ are parameters of the fitting function, $\mu$ is the effective magnetic moment of the Ce$^{3+}$ ions in units of Bohr magneton ($\mu_B$) and $\lambda = \mu_B/k_B = 0.67$. We have chosen a simple possible form of the free energy which, at low temperatures ($T \ll T_K^*$), is consistent with the critical form of free energy that is suggested by renormalization group calculation for 2d spin fluctuations,\(^1\) namely $F \propto T^2 \ln(T_0/T)$. At high temperatures ($T \gg T_K$) it matches smoothly to an impurity model where the 4$f$ cerium ions act as Kondo impurities. The uniform magnetic susceptibility in this regime is Curie-Weiss like, with $\chi(T) \propto \mu^2/T$. This temperature dependence is cut-off at $T_K^*$, below which $\chi \sim \mu^2/TK^*$, down to zero temperature. The fitting function is chosen such that at very low temperature ($T \to 0$), $\chi(T) - \chi(0) \propto -T$.\(^20\) This limiting behaviour agrees with the form $\chi \approx a_0 + 1/(a_1 + a_2T)$ which Rosch et al.\(^6\) used to fit susceptibility data up to 1.4 K. We also find that susceptibility derived from equation (10) can describe reasonably well (with a difference of at most twenty percent) the data\(^7\) up to 6 K. The variation of entropy and magnetization as functions of temperature and magnetic field that one expects from the above free energy matches well with the experiments (Figures 1,2). From the fit we estimate $T_K^*$ to be around 15 K, and $\mu \sim 2.6$. In the absence of magnetic field the specific heat coefficient ($\gamma = C/T$) can be written as $\gamma = a \ln(T_0/T)$. From the fit we estimate $a = 0.5$ J/mol-K$^2$ and $T_0 = 9.4$ K, which have comparable order of magnitudes with the experimentally measured values $a = 0.6$ J/mol-K$^2$ and $T_0 = 5.3$ K.\(^1\) The logarithmic behaviour in specific heat and thermopower in CeCu$_6-x$Au$_x$ is observed around 1 K, which is well below $T_K^*$. The experimental fits and the estimates suggest that the spin-fermion model that we have been considering is consistent with the experimental data.

We now discuss the limitations of our calculation. We have completely ignored the interaction between the spin fluctuations (the $u_0$ term). This is justified since this term is marginally irrelevant. In our calculation we considered only the lowest order diagram in the perturbation series in terms of the spin-fermion coupling. However, we have examined the lowest order spin-fermion vertex correction, and found that it is well-behaved close to the QCP (described in the appendix). So we believe that the qualitative features of our calculation will not be modified by including higher order terms of the series. This is very different from what is found in the 2d-spin-2d-fermion model, where the spin-fermion vertex is singular indicating a potential breakdown of the approach.\(^12\) So, if the 2d-spin 3d-fermion model breaks down, there is no trace of this breakdown in perturbation theory.

From our calculation we see that irrespective of whether the system is clean or dirty, if there is a large enough hot region in the system, then both specific heat and thermopower should show anomalous logarithmic temperature dependence.

Since the microscopic origin of the 2d spin fluctuations is not known, our model seem to be a fine tuned one rather than one that is expected intuitively. It would be interesting to investigate the origin of the 2d magnetic coupling, and why most of the Fermi surface is hot by means of microscopic first principles calculations. This study should be supplemented by an investigation of the 2d-3d dimensional crossover, to estimate the energy scale at which it is expected to occur. We notice that specific heat and resistivity measurements on YbRh$_2$Si$_2$ seem to indicate that the model, with most of the Fermi surface hot, is quite valid for it. From this we can conclude that we expect to see the behaviour $S_1/T \propto \ln(1/T)$ from thermopower measurement on YbRh$_2$Si$_2$, probably over a wider range of temperatures than the Ce-material.

VI. ACKNOWLEDGEMENTS

We are very happy to thank A. Rosch for many useful insights and suggestions. We thank A. Schroeder, G.
get $\Gamma \propto$ tal data on CeCu$_3$Au$_4$, and O. Trovarelli for a useful discussion about the structure of YbRh$_2$Si$_2$. This research was supported by the Petroleum Research Fund of the American Chemical Society, under grant ACS-PRF #33495-AC5, and by the Division of Materials Research of the National Science Foundation under grant DMR-0096462.

**APPENDIX A: SPIN-FERMION VERTEX**

Here we describe the calculation of the spin-fermion vertex and show that at the QCP ($\delta \to 0$) the vertex is not singular. This is important because otherwise our perturbative calculation will break down at low temperature near the QCP. With a singular vertex, the coupling constant between the electrons and the spin fluctuations will get strongly renormalized at low energy. The qualitative features of the theory will change, in particular the electron self energy. We will express the lowest order correction to the bare spin-fermion coupling as $g = g_0(1 + \Gamma)$. Since we are interested only in the hot electrons and their low energy interaction with the spin fluctuations, we will calculate the vertex $\Gamma$ with all external frequency zero. The expression for the vertex will then be,

$$\Gamma = ig_0^2 \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G(p_1 + k, \omega) G(p_2 + k, \omega) \chi(Q + a\hat{x} + k, \omega). \quad (A1)$$

Here $p_1$ and $p_2$ are two hot points that are connected by wave-vector $Q + a\hat{x}$. Expressing the linearized spectrum near the two hot points as $\epsilon_{1k}$ and $\epsilon_{2k}$, we can rewrite the above expression as

$$\Gamma = 4g_0^2 \sum_k \int_0^{\infty} \frac{d\omega}{\pi} \frac{\omega^2}{\epsilon_{1k}^2 + \omega^2} \frac{\epsilon_{2k}^2}{\epsilon_{2k}^2 + \omega^2} \frac{1}{\epsilon_{1k}^2 + \omega^2} \frac{1}{\epsilon_{2k}^2 + \omega^2}.$$  

It is easy to check by simple dimensional analysis that as $\delta \to 0$, the above expression is finite. As an estimate we get $\Gamma \propto g_0^2 \Lambda^{1/2} / (\epsilon_p^{3/2} \omega_s^{1/2})$, where $\Lambda$ is a dimensionless cutoff in the momentum space.

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1. H.v. Löhneysen, T. Pietrus, G. Portisch, H. G. Schlager, A. Schröder, M. Sieck, and T. Trappmann, Phys. Rev. Lett 72, 3262 (1994).
2. O. Trovarelli, C. Geibel, S. Mederle, C. Langhammer, F. M. Grosche, P. Gegenwart, M. Lang, G. Sparn, and F. Steglich, Phys. Rev. Lett 85, 626 (2000).
3. N. D. Mathur, F. M. Grosche, S. R. Julian, I. R. Walker, D. M. Freye, R. K. W. Haselwimmer, and G. G. Lonzarich, Nature (London) 394, 39 (1998).
4. A. Schröder, G. Aeppli, P. Coldea, M. Adams, O. Stockert, H.v. Löhneysen, E. Bucher, R. Ramazashvili, and P. Coleman, Nature 407, 351 (2000).
5. Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, cond-mat/0011477.
6. A. Rosch, A. Schröder, O. Stockert, and H.v. Löhneysen, Phys. Rev. Lett 79, 159 (1997).
7. A. Schröder, G. Aeppli, E. Bucher, R. Ramazashvili, and P. Coleman, Phys. Rev. Lett 80, 5623 (1998).
8. O. Stockert, H.v. Löhneysen, A. Rosch, N. Pyka, and M. Loewenhaupt, Phys. Rev. Lett 80, 5627 (1998).
9. S. Sachdev, A. V. Chubukov, and A. Sokol, Phys. Rev. B 51, 14874 (1995).
10. J. A. Hertz, Phys. Rev. B 14, 1165 (1976).
11. A. J. Millis, Phys. Rev. B 48, 7183 (1993).
12. Ar. Abanov, and A. V. Chubukov, Phys. Rev. Lett 84, 5608 (2000).
13. A. V. Chubukov, Private communications.
14. J. Benz, C. Pfleiderer, O. Stockert, and H.v. Löhneysen, Physica B 259-261, 380 (1999).
15. C. Pfleiderer, Private communications.
16. R. Hlubina, and T. M. Rice, Phys. Rev. B 14, 9253 (1995).
17. A. Rosch, Phys. Rev. Lett 82, 4280 (1999).
18. A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, Methods of Quantum Field Theory in Statistical Physics, 171 (Dover Publications, New York, 1963).
19. G. D. Mahan, Many-Particle Physics, 232 (Plenum Press, New York, 1990).
20. L. B. Ioffe, and A. J. Millis, Phys. Rev. B 51, 16115 (1995).