Thermoelectric behavior near the magnetic quantum critical point

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(Received 9 April 2001; revised manuscript received 13 June 2001; published 18 October 2001)

We use the coupled two-dimensional spin–three-dimensional fermion model proposed by Rosch *et al.* [Phys. Rev. Lett. **79**, 159 (1997)] to study the thermoelectric behavior 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 $YbRh_2Si_2$ and $CeCu_{6-x}Au_x$, with a typical two-dimensional ordering wave vector and three-dimensional 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 a logarithmic temperature dependence in thermopower. This has been observed in $CeCu_{6-x}Au_x$. We expect to see the same behavior from future experiments on $YbRh_2Si_2$.

DOI: 10.1103/PhysRevB.64.184414 PACS number(s): 72.15.Jf, 71.27.+a

I. INTRODUCTION

Understanding the behavior of a system close to the 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. Recently several materials have been discovered where it has been possible to demonstrate the existence of magnetic QCP's.[1–3] This has made the problem exciting, where the 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 spin 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.[4,5]

In this paper we will discuss two experimentally well-studied heavy-fermion materials, $CeCu_{6-x}Au_x$ (Ref. 1) and $YbRh_2Si_2$ (Ref. 2), which exhibit antiferromagnetic QCP. In doped $CeCu_6$, replacing Cu with larger Au atoms, favors the formation of long-range magnetic order.[1] Beyond a critical doping $x_c=0.1$, the ground state of the system is antiferromagnetic with finite Néel temperature (T_N).[6] At the critical doping T_N is zero and the system has a QCP. On the other hand, $YbRh_2Si_2$ is undoped and atomically well ordered.[2] It is a much cleaner material than $CeCu_{6-x}Au_x$, with residual resistivity (ρ_0) smaller by a factor of about 10. At ambient pressure it develops long-range magnetic order at a very low temperature of $T_N \simeq 65$ mK.[2] The ordering temperature can be suppressed to practically zero (less than 20 mK) by applying a magnetic field of only 45 mT.[2] Both these materials show pronounced deviations from Fermi liquid (FL) behavior, which is believed to be due to closeness to the QCP. For instance, the dependence of electrical resistivity $\Delta\rho=\rho-\rho_0$ on temperature T is $\Delta\rho \propto T$, while that of specific heat C is $C/T \propto -\ln T$.[1,2] This is in contrast with FL behavior, which predicts $\Delta\rho \propto T^2$ and $C/T=\text{const}$. The low-temperature NFL behavior is observed over a decade of temperature, up to about 1 K for $CeCu_{6-x}Au_x$,[1,6] and up to as high as 10 K for $YbRh_2Si_2$.[2] The source of the interesting physics in these materials is the localized $4f$ electrons[4] 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, if 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 nonmagnetic. 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[4] regarding the nature of the system in the nonordered 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 temperatures 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 favor of this mechanism, that the data on magnetic susceptibility show nontrivial scaling with temperature.[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 that 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,[6] is motivated by inelastic neutron scattering data on $CeCu_{5.9}Au_{0.1}$, which show that the nearly critical spin fluctuations are two-dimensional.[8] But the origin of the quasi-two-dimensional behavior of spin fluctuations is not well understood. However, the same feature is probably also present in $YbRh_2Si_2$, where the structure of the lattice provides a more natural explanation for the spin fluctuations to be two-dimensionl (2d).[2] Besides the nature of the magnetic correlations, there are different opinions regarding the dynamics of the spin fluctuations. It has been argued[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.[6] Following the method of Hertz[10] and Millis,[11] in which the system is described entirely in terms of the spin fluctuations, after a formal Hubbard-Stratanovich transformation to integrate the fermion modes, it also explains the logarithmic temperature dependence of specific heat.[6,11] In an alternative description,[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 $\eta \sim 1/4$.[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 behavior of a system in the paramagnetic phase and close to antiferromagnetic QCP. For $CeCu_{5.9}Au_{0.1}$ it is known that the thermopower (S_t) has a dependence similar to specific heat over the same range of temperature,[14,15] i.e, $S_t/T \propto -\ln T$. We will show that scattering with nearly critical spin fluctuations give rise to the 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 $YbRh_2Si_2$, and so we expect to see the same behavior for thermopower from future experiments.

II. 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

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{g_0}{2} \sum_{\mathbf{k},\mathbf{q},\alpha,\beta} c^\dagger_{\mathbf{k}+\mathbf{q},\alpha} c_{\mathbf{k},\beta} \sigma_{\alpha,\beta} \mathbf{S}_{-\mathbf{q}} + \sum_{\mathbf{q}} [\chi^{-1}(\mathbf{q}) \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}} + \mathbf{\Pi}_{\mathbf{q}} \cdot \mathbf{\Pi}_{-\mathbf{q}}] + \frac{u_0}{4} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} (\mathbf{S}_{\mathbf{k}_1} \cdot \mathbf{S}_{\mathbf{k}_2})(\mathbf{S}_{\mathbf{k}_3} \cdot \mathbf{S}_{\mathbf{k}_4}) \delta(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4). \tag{1}$$

Here $c^\dagger_{\mathbf{k},\sigma}$ is the electron creation operator, $\mathbf{S}_{\mathbf{q}}$ is the operator for the spin fluctuations, $\mathbf{\Pi}_{\mathbf{q}} = \partial_t \mathbf{S}_{\mathbf{q}}$ is the conjugate momentum field for the spin fluctuations, and $\chi(\mathbf{q})$ 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.[12] Thus the typical energies of the spin fluctuations $\omega_s \sim W$, the bandwidth of the conduction electrons. The system is close to an antiferromagnetic instability with ordering wave vector $\mathbf{Q}$. 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[10,11]

$$\chi^{-1}(\mathbf{q},\omega) = \delta + \omega_s (\mathbf{q} - \mathbf{Q})^2_{\parallel} - i\gamma|\omega|. \tag{2}$$

Here δ is the mass of the spin fluctuations and measures 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.[10,11] The main contribution of this term is to renormalize the mass of the spin fluctuations (δ) and make it temperature dependent. Within a Gaussian approximation, δ is linearly dependent on temperature, up to logarithmic corrections.[6,11] We will ignore other effects of the u_0 term in our discussion, and will consider only the quadratic term with a temperature-dependent mass of the spin fluctuations. To simplify the calculation we will assume a spherical Fermi surface for the noninteracting electrons, with the ordering wave vector $\mathbf{Q} = (\alpha, 0, 2k_F \cos\theta_0)$. Here $\theta_0 \neq 0$ (i.e., not $2k_F$ ordering), and $\theta_0 \neq \pi/2$ (i.e., not ferromagnetic ordering). We have chosen $\hat{\mathbf{x}}$ as the direction along which the spin fluctuations are uncorrelated, and α, the ordering in the x direction, varies from one plane of magnetic correlation to another. Since the spectrum of spin fluctuations is 2D, those carrying momentum of the form $\mathbf{Q}+a\hat{\mathbf{x}}$, where a 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 sensitive 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 worthwhile to estimate the fraction of the Fermi surface that is hot, theoretically it is a daunting task. In our calculation 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[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 σ,

$$\sigma \propto \langle \tau_{\mathbf{k}} \rangle_{\mathrm{FS}} \propto \frac{x}{T/\epsilon_F} + \frac{1-x}{(T/\epsilon_F)^2}.$$

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 $CeCu_{6-x}Au_x$, which is a dirtier material, the above estimation is more involved. It was recently shown[17] that the effect of disorder is to favor isotropic scattering and thereby reduce the effectiveness of the Hlubina-Rice mechanism. Thus, one should expect a smaller fraction, than estimated above, enough to make the contribution of the hot carriers significant for $CeCu_{6-x}Au_x$.

III. ELECTRON SELF-ENERGY

To calculate the effect of the low-energy spin fluctuations on the hot electrons, we will examine the electron self-energy. The lowest-order term in perturbation gives

$$\Sigma(\mathbf{p},\omega) = -\frac{g_0^2}{V}\sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi i} \chi(\mathbf{k},\Omega) G(\mathbf{p}+\mathbf{k},\omega+\Omega), \tag{3}$$

where $G(\mathbf{p},\omega)$ is the free-electron propagator given by,

$$G(\mathbf{p},\omega) = \frac{n_p}{\omega - \epsilon_p - i\eta} + \frac{1-n_p}{\omega - \epsilon_p + i\eta}.$$

Here n_p is the electron occupation of the momentum state $\mathbf{p}$ at $T=0$. As expected, the above expression has different behavior in the hot and cold regions. But within each region the self-energy is practically momentum independent. The imaginary part of the self-energy gives the quasiparticle lifetime as determined by scattering with the spin fluctuations. For $\omega > 0$ we have

$$\mathrm{Im}\,\Sigma(\mathbf{p},\omega) = -\frac{g_0^2}{V} \sum_{0<\epsilon_k<\omega} \frac{(\omega - \epsilon_{\mathbf{k}+\mathbf{p}})}{[\delta + \omega_s(\mathbf{k}-\mathbf{Q})_\parallel^2]^2 + (\omega - \epsilon_{\mathbf{k}+\mathbf{p}})^2}.$$

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 $\mathbf{k} = \mathbf{Q} + a\hat{\mathbf{x}}$. 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

$$\mathrm{Im}\,\Sigma(\mathbf{p},\omega) \propto -\left(\frac{g_0^2}{\epsilon_F \omega_s}\right) \frac{\omega^2}{\max[\delta,\omega]}. \tag{4}$$

For $\omega > \delta$ the lifetime of the hot electrons is much smaller than that given by Fermi liquid behavior $[\mathrm{Im}\,\Sigma(\omega) \propto \omega^2]$. As we have mentioned above, this is due to more effective scattering with the spin fluctuations in this region. For the cold electrons the behavior is Fermi-liquid-like.

Next, we will examine the real part of the self-energy. The dependence of $\mathrm{Re}\,\Sigma$ on frequency is more important than the dependence on momentum. We get

$$-\lim_{\omega\to 0} \frac{\partial}{\partial\omega} \mathrm{Re}\,\Sigma(\mathbf{p},\omega) = \frac{g_0^2}{\pi V} \sum_{\mathbf{k}} \left\{ \frac{1}{\gamma_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}+\mathbf{p}}^2} - \frac{(\gamma_{\mathbf{k}}^2 - \epsilon_{\mathbf{k}+\mathbf{p}}^2)}{(\gamma_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}+\mathbf{p}}^2)^2} \ln\left|\frac{\gamma_{\mathbf{k}}}{\epsilon_{\mathbf{k}+\mathbf{p}}}\right| + \frac{\pi(2n_{\mathbf{k}+\mathbf{p}} - 1)\gamma_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{p}}}{(\gamma_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}+\mathbf{p}}^2)^2} \right\}.$$

Here $\gamma_{\mathbf{k}} = \delta + \omega_s(\mathbf{k}-\mathbf{Q})_\parallel^2$. If $\mathbf{p}$ 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,

$$-\lim_{\omega\to 0} \frac{\partial}{\partial\omega} \mathrm{Re}\,\Sigma(\mathbf{p},\omega) \propto \left(\frac{g_0^2}{\pi \epsilon_F \omega_s}\right) \ln\left(\frac{\omega_s}{\delta}\right). \tag{5}$$

Due to scattering, the noninteracting 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

$$Z^{-1} = 1 - \lim_{\omega\to 0} \frac{\partial}{\partial\omega} \mathrm{Re}\,\Sigma(\mathbf{p},\omega)$$

defines the quasiparticle residue. Since δ, 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 Γ 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,[18]

$$\frac{S}{N}=\sum_{\mathbf{p}} \frac{1}{\pi T}\int_{-\infty}^{\infty} d\omega\left(-\frac{\partial f}{\partial \omega}\right)\omega \tan^{-1}\left(\frac{\tau(\omega)}{\epsilon_p-\omega/Z}\right).$$

Here $f(\omega)$ is the Fermi function, and $\tau(\omega)$ is quasiparticle lifetime obtained from the inverse of imaginary part of self-energy. From the above expression it is easy to see that $S/N \propto 1/Z$. Over the hot region, keeping only the leading term, $Z^{-1}\sim \ln(1/\delta)$. Then,

$$S/N \propto \mathcal{N}(0)T\left(\frac{g_0^2}{\epsilon_F\omega_s}\right)\ln\left(\frac{\omega_s}{\delta}\right), \tag{6}$$

where $\mathcal{N}(0)$ is the density of states of the noninteracting 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 behavior ($S\propto T$). This gives rise to the anomalous logarithmic temperature dependence of specific heat. In the past[11,6] this behavior 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 $\ln(1/T)$ behavior 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. 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,[19] i.e,

$$S_t=\frac{L_{12}}{eTL_{11}},$$

where

$$L_{12}=\lim_{\omega\to 0}\frac{1}{\omega V}\mathrm{Im}\int_0^{\beta} d\tau\, e^{i\omega\tau}\langle T_\tau \mathbf{j}_Q(\tau)\cdot \mathbf{j}(0)\rangle$$

is the correlation function between heat current ($\mathbf{j}_Q$) and particle current ($\mathbf{j}$), and

$$L_{11}=\lim_{\omega\to 0}\frac{1}{\omega V}\mathrm{Im}\int_0^{\beta} d\tau\, e^{i\omega\tau}\langle T_\tau \mathbf{j}(\tau)\cdot \mathbf{j}(0)\rangle$$

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

$$\mathbf{j}_Q=\frac{i}{2}\sum_{\mathbf{p},\sigma} \mathbf{v}_{\mathbf{p}}(c^{\dagger}_{\mathbf{p},\sigma}\dot{c}_{\mathbf{p},\sigma}-\dot{c}^{\dagger}_{\mathbf{p},\sigma}c_{\mathbf{p},\sigma}).$$

In principle, the heat current will have a second term of the form $(i/2)\Sigma_{\mathbf{k},\sigma}\nabla_k U(\mathbf{k})(\dot{n}_{\mathbf{k},\sigma}n_{-\mathbf{k},\sigma}-\dot{n}_{-\mathbf{k},\sigma}n_{\mathbf{k},\sigma})$, where $U(\mathbf{k})$ 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 reexpressed in a more transparent form as

$$L_{12}=\sum_{\mathbf{p}} v_{\mathbf{p}}^2\int_{-\infty}^{\infty} d\omega\left(-\frac{\partial f}{\partial \omega}\right)\omega A^2(\mathbf{p},\omega),$$

$$L_{11}=\sum_{\mathbf{p}} v_{\mathbf{p}}^2\int_{-\infty}^{\infty} d\omega\left(-\frac{\partial f}{\partial \omega}\right)A^2(\mathbf{p},\omega).$$

Here $\mathbf{v}_{\mathbf{p}}=\partial\epsilon_p/\partial\mathbf{p}$ is the quasiparticle velocity, and $A(\mathbf{p},\omega)$ is the spectral function defined as

$$A(\mathbf{p},\omega)=\frac{\tau(\omega)^{-1}}{(\omega/Z-\epsilon_p)^2+\tau(\omega)^{-2}}.$$

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

$$L_{11}=v_F^2\mathcal{N}(0)\int_{-\infty}^{\infty} d\omega\left(-\frac{\partial f}{\partial \omega}\right)\tau(\omega).$$

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

$$L_{11}\propto\left(\frac{\epsilon_F\omega_s}{g_0^2}\right)\frac{v_F^2\mathcal{N}(0)}{T}. \tag{7}$$

This result[1,6] 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 $\mathcal{N}(\omega)=\mathcal{N}(0)+\omega\mathcal{N}'(0)+O(\omega^2/\epsilon_F^3)$, where $\mathcal{N}'(0)\neq 0$ only if there is particle-hole asymmetry in the bare noninteracting 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. τ is a typical scattering time, and $\omega<\tau^{-1}$. After the energy integral around the Fermi surface we get,

$$L_{12}=v_F^2\int_{-\infty}^{\infty}d\omega\left(-\frac{\partial f}{\partial\omega}\right)\omega\tau(\omega)\mathcal{N}(\omega/Z)$$

$$=\left(\frac{\epsilon_F\omega_s}{g_0^2}\right)v_F^2\{T\mathcal{N}'(0)/Z+T\mathcal{N}(0)\tau\}. \tag{8}$$

The first term in the equation above 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

$$S_t\propto\frac{1}{e}\left(\frac{g_0^2\mathcal{N}'(0)}{\epsilon_F\omega_s\mathcal{N}(0)}\right)T\ln(\omega_s/\delta). \tag{9}$$

In the regime where $T>\Gamma(p-p_c)$, $S_t/T\propto\ln(1/T)$, as has been observed[14,15] in thermopower measurements on $CeCu_{6-x}Au_x$.

V. CONCLUSION

To check the consistency of our model and calculation, we need to estimate the high-energy scale (namely, T_K^*) of $CeCu_{5.9}Au_{0.1}$. 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

$$F(T,H)/k_B=X(T,H)\ln\left[2\cosh\left(\frac{\mu\lambda H}{Y(T,H)}\right)\right], \tag{10}$$

where

$$X(T,H)=T_K^*+C_1\left(\frac{T^2}{T_K^*}\right)-C_2\left(\frac{T^2}{T_K^*}\right)\ln(T^2+C_3H^2),$$

$$Y(T,H)=T_K^*+(T^2+C_3H^2)^{1/2}.$$

Here C_1–C_3 are parameters of the fitting function, μ is the effective magnetic moment of the Ce^{3+} ions in units of the Bohr magneton (μ_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 the renormalization group calculation for 2D spin fluctuations,[11] 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 $4f$ cerium electrons 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 $\chi\sim\mu^2/T_K^*$, down to zero temperature. The fitting function is chosen such that at very low temperature ($T\rightarrow 0$), $\chi(T)-\chi(0)\propto -T$.[20] This limiting behavior 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 the susceptibility

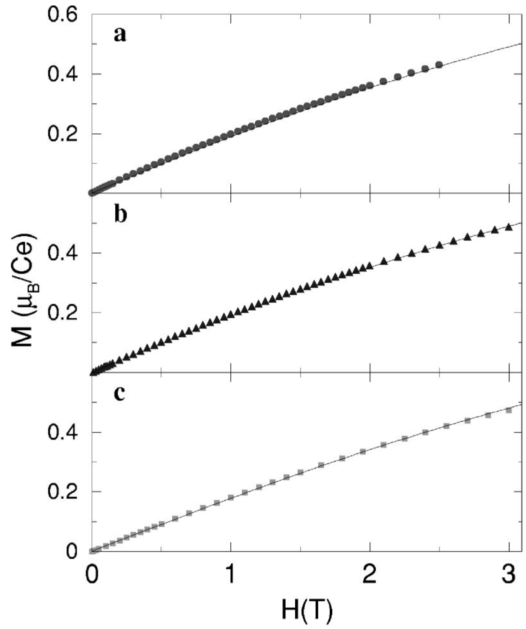

FIG. 1. Magnetization (M) vs external magnetic field (H) at different temperatures: (a) $T=0.15$ K, (b) $T=0.3$ K, and (c) $T=0.8$ K. The discrete points are experimental. The solid lines are fits using Eq. (10).

derived from Eq. (10) can describe reasonably well (with a difference of at most 20%) 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 free energy above matches well with the experiments (Figs. 1 and 2). From the fit we estimate T_K^* to be around 15 K, and μ

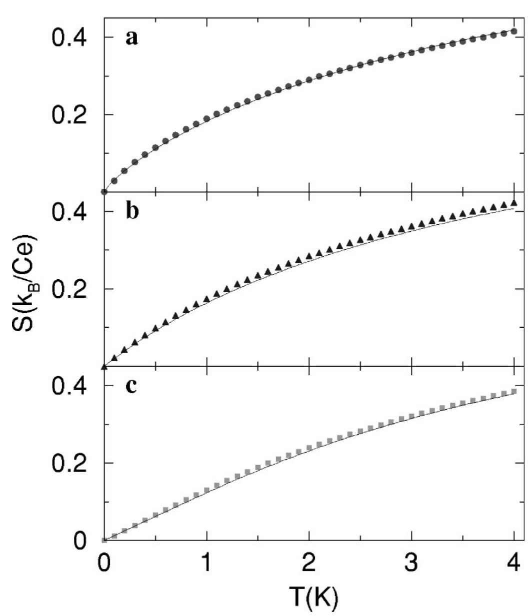

FIG. 2. Entropy (S) per Ce atom vs temperature (T) at different magnetic fields: (a) $H=0$ T, (b) $H=1.5$ T and (c) $H=3$ T. The discrete points are experimental, obtained by numerically integrating data from specific heat measurement. The solid lines are fits using Eq. (10).

$\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 orders of magnitudes with the experimentally measured values $a = 0.6$ J/mol K^2 and $T_0 = 5.3$ K.[1] The logarithmic behavior 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 seems 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 $YbRh_2Si_2$ (Ref. 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 behavior $S_t/T \propto \ln(1/T)$ from thermopower measurement on $YbRh_2Si_2$, probably over a wider range of temperatures than the Ce material.

ACKNOWLEDGMENTS

We are very happy to thank A. Rosch for many useful insights and suggestions. We thank A. Schroeder, G. Aeppli, C. Pfleiderer, and A. Rosch for files of experimental data on $CeCu_{6-x}Au_x$, and O. Trovarelli for a useful discussion about the structure of $YbRh_2Si_2$. This research was supported by the Petroleum Research Fund of the American Chemical Society, under Grant No. ACS-PRF 33495-AC5, and by the Division of Materials Research of the National Science Foundation under Grant No. DMR-0096462.

APPENDIX: 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 $g = g_o(1+\Gamma)$. Since we are interested only in the hot electrons and their low-energy interaction with the spin fluctuations, we will calculate the vertex Γ with all external frequency zero. The expression for the vertex will then be

$$\Gamma = i g_0^2 \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G(\mathbf{p}_1+\mathbf{k},\omega) G(\mathbf{p}_2+\mathbf{k},\omega)\chi \times(\mathbf{Q}+a\hat{\mathbf{x}}+\mathbf{k},\omega). \tag{A1}$$

Here $\mathbf{p}_1$ and $\mathbf{p}_2$ are two hot points that are connected by the wave vector $\mathbf{Q}+a\hat{\mathbf{x}}$. Expressing the linearized spectrum near the two hot points as $\epsilon_{1\mathbf{k}}$ and $\epsilon_{2\mathbf{k}}$, we can rewrite the above expression as

$$\Gamma = 4 g_0^2 \sum_{\mathbf{k}} \int_0^{\infty} \frac{d\omega}{\pi} \times \frac{\omega^2}{(\gamma_{\mathbf{Q}+\mathbf{k}}^2+\omega^2)(\epsilon_{1\mathbf{k}}+\epsilon_{2\mathbf{k}})(\omega+\epsilon_{1\mathbf{k}})(\omega+\epsilon_{2\mathbf{k}})}.$$

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

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