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Transport properties in antiferromagnetic quantum Griffiths phases

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Abstract – We study the electrical resistivity in the quantum Griffiths phase associated with the antiferromagnetic quantum phase transition in a metal. The resistivity is calculated by means of the semi-classical Boltzmann equation. We show that the scattering of electrons by locally ordered rare regions leads to a singular temperature dependence. The rare-region contribution to the resistivity varies as T^λ with temperature T , where λ is the usual Griffiths exponent which takes the value zero at the critical point and increases with distance from criticality. We find similar singular contributions to other transport properties such as thermal resistivity, thermopower and the Peltier coefficient. We also compare our results with existing experimental data and suggest new experiments.

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Introduction. – Quantum phase transitions [1] occur at zero temperature when an external parameter such as magnetic field, pressure or chemical composition, is varied. They are driven by quantum rather than thermal fluctuations. At continuous quantum phase transitions, *i.e.*, quantum critical points, the quantum fluctuations driving the transition diverge and become scale invariant in space and time. These fluctuations dominate the material's properties in the vicinity of the quantum critical point at low but non-zero temperatures. In metallic systems, they can cause strong deviations from the conventional Fermi-liquid behavior of normal metals [2].

Impurities, defects or other kinds of quenched disorder can significantly modify the low-temperature behavior of quantum many-particle systems. The interplay between dynamic quantum fluctuations and static disorder fluctuations leads to much more dramatic effects at quantum phase transitions than at classical thermal phase transitions, including quantum Griffiths singularities [3–5], infinite-randomness critical points featuring exponential instead of power-law scaling [6,7] and the smearing of the phase transition [8]. These unconventional phenomena are caused by large spatial regions (rare regions) that are devoid of impurities and can show local order even if the bulk system is in the disordered phase. The fluctuations of these rare regions are very slow because

they require changing the order parameter in a large volume. Griffiths showed that this leads to a singular free energy in a whole parameter region which is now known as the Griffiths phase. The probability $\mathcal{P}(L^d)$ for finding an impurity-free rare region with linear size L in a disordered system is exponentially small in its volume L^d , $\mathcal{P}(L^d) \sim \exp(-cL^d)$ with c being a constant that depends on the disorder strength. In systems in which the characteristic energy ϵ of such a rare region decays exponentially with its volume, $\epsilon \sim \exp(-bL^d)$, the resulting density of states is of power-law type, $\rho(\epsilon) \propto \epsilon^{\lambda-1}$, where $\lambda = c/b$ is the non-universal Griffiths exponent. It varies systematically within the Griffiths phase and vanishes at the critical point. The power-law density of states $\rho(\epsilon)$ leads to non-universal power-law quantum Griffiths singularities of several thermodynamical observables including the specific heat, $C \sim T^\lambda$, and the magnetic susceptibility, $\chi \sim T^{\lambda-1}$. The zero-temperature magnetization-field curve behaves as $M \sim H^\lambda$ (for reviews, see refs. [9,10]).

Quantum Griffiths phases have been predicted to occur not only in localized magnets but also in metallic systems [11–13], but clear-cut experimental verifications have been absent for a long time. Only recently, quantum Griffiths phases have been observed in experiment in a number of systems such as magnetic semiconductors [14–16], Kondo lattice ferromagnets [17,18] and

transition metal ferromagnets [19]. The lack of experimental evidence for quantum Griffiths phases in metals may be (at least partially) due to the theories being incomplete: while the thermodynamics in quantum Griffiths phases is comparatively well understood, very little is known about the experimentally important and easily accessible transport properties.

In this letter we therefore study the electrical resistivity in the quantum Griffiths phase of an antiferromagnetic metal by means of the semi-classical Boltzmann equation approach. In the same manner, we also investigate other transport properties such as the thermal resistivity, the thermopower and the Peltier coefficient. We find that the scattering of the electrons by spin fluctuations in the rare regions leads to singular temperature dependences not just at the quantum critical point but in the entire antiferromagnetic quantum Griffiths phase. The rare-region contribution to the resistivity varies as $\Delta\rho \propto T^\lambda$ with temperature T , the contribution to thermal resistivity behaves as $\Delta W \propto T^{\lambda-1}$, and the thermopower and the Peltier coefficient behave as $\Delta S \propto T^{\lambda+1}$ and $\Delta\Pi \propto T^{\lambda+2}$, respectively.

Model and method of solution. – Let us now sketch the derivation of these results. The transport properties of the itinerant antiferromagnetic systems we are interested in can be described by a two-band model consisting of s and d electrons [20,21]. The Hamiltonian has the form $H = H_s + H_d + H_{s-d}$, where H_s and H_d are the Hamiltonians of s and d electrons, respectively. H_{s-d} corresponds to the exchange interaction between s and d electrons. Only the s electrons contribute to the transport properties. They are scattered by the spin fluctuations of the d electrons which are assumed to be in the antiferromagnetic quantum Griffiths phase. The contribution to the resistivity from the scattering by the spin fluctuations stems from the s - d exchange interaction term of the Hamiltonian

$$H_{s-d} = g \int d\mathbf{r} \mathbf{s}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}), \quad (1)$$

where g is the coupling between s and d electrons. \mathbf{s} and \mathbf{S} are the spin densities of the s and d electrons, respectively.

Close to an antiferromagnetic transition in three-dimensional space, transport properties can be treated within a semi-classical approach using the Boltzmann equation because quasiparticles are still (marginally) well defined. For simplicity, we also assume that the spin fluctuations are in equilibrium, *i.e.*, we neglect drag effects. This approximation is valid if the system can lose momentum efficiently by Umklapp or impurity scattering as is the case in a dirty antiferromagnetic system. The linearized Boltzmann equation in the presence of an electric field \mathbf{E} and a temperature gradient ∇T , but zero magnetic field can be written as [22]

$$-\mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial T} \nabla T - \mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \mathbf{E} = \left(\frac{\partial f_{\mathbf{k}}}{\partial t} \right)_{scatt}, \quad (2)$$

where $f_{\mathbf{k}}^0$ is the equilibrium Fermi-Dirac distribution function. The first and second terms correspond to the rate changes of the electron distribution function $f_{\mathbf{k}}$ due to the diffusion and electric field \mathbf{E} , respectively. The last one is the collision term. Let the stationary solution of the Boltzmann equation be $f_{\mathbf{k}} = f_{\mathbf{k}}^0 - \Phi_{\mathbf{k}}(\partial f_{\mathbf{k}}^0 / \partial \varepsilon_{\mathbf{k}})$, where $\Phi_{\mathbf{k}}$ is a measure of the deviation of the electron distribution from equilibrium. Then the linearized scattering term due to the spin fluctuations has the form [21,23]

$$\begin{aligned} \left(\frac{\partial f_{\mathbf{k}}}{\partial t} \right)_{scatt} &= \frac{2g^2}{T} \sum_{\mathbf{k}'} f_{\mathbf{k}'}^0 (1 - f_{\mathbf{k}}^0) n(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) \\ &\quad \times \text{Im} \chi(\mathbf{k} - \mathbf{k}', \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'}), \\ &= \frac{1}{T} \sum_{\mathbf{k}'} \mathcal{P}_{\mathbf{k}'}(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'}) \end{aligned} \quad (3)$$

where $n(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})$ is the Bose-Einstein distribution function and χ is the total dynamical susceptibility of the spin fluctuations of the d electrons.

Electrical resistivity. – In order to calculate the electrical resistivity we consider Ziman's variational principle [22]. The resistivity ρ is given as the minimum of a functional of $\Phi_{\mathbf{k}}$ [22]¹

$$\rho[\Phi_{\mathbf{k}}] = \min \left[\frac{1}{2T} \frac{\iint (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})^2 \Gamma_{\mathbf{k}}^{\mathbf{k}'} d\mathbf{k} d\mathbf{k}'}{\left(\int v_{\mathbf{k}} \Phi_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} d\mathbf{k} \right)^2} \right], \quad (4)$$

where

$$\Gamma_{\mathbf{k}}^{\mathbf{k}'} = \int_0^\infty d\omega \mathcal{P}_{\mathbf{k}'}(\omega) \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} + \omega). \quad (5)$$

Quantum Griffiths effects in disordered metallic systems are realized both in Heisenberg magnets [13,14] and in Ising magnets. In the latter case, they occur in a transient temperature range where the damping is unimportant [11]. In the following, we consider both cases.

As we are interested in the rare-region contribution to the resistivity in the Griffiths phase, we need to find the rare-region dynamical susceptibility which is simply the sum over the susceptibilities of the individual rare regions. The imaginary part of the dynamical susceptibility of a single cluster (rare region) of characteristic energy ϵ in the quantum Griffiths phase of a disordered itinerant quantum Heisenberg antiferromagnet is given by

$$\text{Im} \chi_{cl}(\mathbf{q}, \omega; \epsilon) = \frac{\mu^2 \gamma \omega}{\epsilon^2(T) + \gamma^2 \omega^2} F_\epsilon^2(\mathbf{q}), \quad (6)$$

where μ is the moment of the cluster and γ is the damping coefficient which results from the coupling of the spin fluctuations and the electrons. $\epsilon(T)$ plays the role of the local distance from criticality. For high temperatures $\gamma T \gg \epsilon$, $\epsilon(T) \approx T$ and for low temperatures $\gamma T \ll \epsilon$, $\epsilon(T) \approx \epsilon$.

¹We set Planck's constant, electron's charge and Boltzmann constant $\hbar = e = k_B = 1$ in what follows.

$F_\epsilon(\mathbf{q})$ is the form factor of the cluster which encodes the spatial magnetization profile. For random quantum Ising models the imaginary part of the dynamical magnetic susceptibility of a single cluster (rare region) is given by

$$\text{Im}\chi_{cl}(\mathbf{q}, \omega; \epsilon) = \pi \frac{\mu^2}{4} \tanh\left(\frac{\epsilon}{2T}\right) \times [\delta(\epsilon - \omega) - \delta(\epsilon + \omega)] F_\epsilon^2(\mathbf{q}). \quad (7)$$

To get the total rare-region susceptibility, we integrate over all rare regions using the density of states $\rho(\epsilon)$,

$$\text{Im}\chi(\mathbf{q}, \omega) = \int_0^\Lambda d\epsilon \rho(\epsilon) \text{Im}\chi_{cl}(\mathbf{q}, \omega; \epsilon), \quad (8)$$

where Λ is an energy cut-off. The precise functional form of $F_\epsilon(\mathbf{q})$ is not known, since every cluster has a different shape and size. However, we can find it approximately by analyzing the Fourier transform of a typical local magnetization profile of the rare region. Consider a rare region of linear size L (located at the origin). Following Millis *et al.* [24], the order parameter is approximately constant for $r < L$, while for large $r > L$, it decays as $e^{-r/\xi}/r$, where ξ is the bulk correlation length. Taking the Fourier transform we find that $F_\epsilon(\mathbf{q})$ depends on ϵ via the combination $|\mathbf{Q} - \mathbf{q}|^3 \log(\epsilon^{-1})$ only, where \mathbf{Q} is the ordering wave vector. Correspondingly, from eq. (8), we find that the rare-region contribution to the zero-temperature susceptibility in the quantum Griffiths phase can be expressed as

$$\text{Im}\chi(\mathbf{q}, \omega) \propto |\omega|^{\lambda-1} \text{sgn}(\omega) X[|\mathbf{q} - \mathbf{Q}|^3 \log(\omega^{-1})], \quad (9)$$

where X is a scaling function. The precise form of the logarithmic correction is difficult to find and beyond the scope of this paper. For random quantum Ising models, the susceptibility has the same structure as eq. (9) [11]. It is clear that the scaling function X will give only logarithmic corrections to the temperature dependence of the resistivity ρ in our further calculations.

To minimize the resistivity functional (4), we need to make an ansatz for the distribution Φ . Close to an antiferromagnetic quantum phase transition, the magnetic scattering is highly anisotropic because $\chi(\mathbf{q}, \omega)$ peaks around the ordering wave vector \mathbf{Q} . However, since we are interested in a strongly disordered system, the low-temperature resistivity will be dominated by the elastic impurity scattering which is isotropic and redistributes the electrons over the Fermi surface. Correspondingly, we can use the standard ansatz

$$\Phi_{\mathbf{k}} \propto \mathbf{n} \cdot \mathbf{k}. \quad (10)$$

where \mathbf{n} is a unit vector parallel to the electric field. Note that any constant prefactor in $\Phi_{\mathbf{k}}$ is unimportant because it drops out in the resistivity functional (4) and in the corresponding thermal resistivity functional (13). Then,

after applying standard techniques [22] the magnetic part of the resistivity given in eq. (4) becomes

$$\Delta\rho \propto T \int d^3\mathbf{q} \frac{(\mathbf{n} \cdot \mathbf{q})^2}{q} \int_0^\infty d\omega \frac{\partial n(\omega)}{\partial T} \text{Im}\chi(\mathbf{q}, \omega). \quad (11)$$

Inserting the susceptibility (9) yields the rare-region contribution to the resistivity in the antiferromagnetic quantum Griffiths phase as

$$\Delta\rho \propto T^\lambda. \quad (12)$$

Thus, the temperature dependence of the resistivity follows a non-universal power law governed by the Griffiths exponent λ .

Other transport properties. – In the same way, we study other transport properties such as the thermal resistivity, the thermopower, and the Peltier coefficient. The variational principle for the thermal resistivity has the form [22]

$$W[\Phi_{\mathbf{k}}] = \min \left[\frac{\int \int (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})^2 \Gamma_{\mathbf{k}}^{\mathbf{k}'} d\mathbf{k} d\mathbf{k}'}{\left(\int v_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) \Phi_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} d\mathbf{k} \right)^2} \right], \quad (13)$$

where μ is the chemical potential of the s electrons. As long as impurity scattering dominates, we can use the standard ansatz for the variational function,

$$\Phi_{\mathbf{k}} \propto (\varepsilon_{\mathbf{k}} - \mu) \mathbf{n} \cdot \mathbf{k}. \quad (14)$$

Then, following the calculation for the thermal resistivity outlined in ref. [22] we obtain

$$\Delta W \propto \frac{1}{T^2} \int d^3\mathbf{q} \int d\omega \frac{\partial n(\omega)}{\partial T} \text{Im}\chi(\mathbf{q}, \omega) \times \left[\omega^2 \left(\frac{1}{q} - \frac{q}{6k_F^2} \right) + \frac{\pi^2 q}{3k_F^2} T^2 \right]. \quad (15)$$

where k_F is the Fermi momentum of the s electrons². Inserting the susceptibility (9) into (15), the temperature dependence of the thermal resistivity due to the spin fluctuations in the Griffiths phase from the above equation is given by

$$\Delta W \propto T^{\lambda-1}. \quad (16)$$

The existence of an electric field \mathbf{E} in a metal subject to a thermal gradient ∇T is called Seebeck effect and is characterized by the thermopower S which is defined via $\mathbf{E} = S\nabla T$. To calculate the thermopower, we analyze the Boltzmann equation (2) in the presence of both \mathbf{E} and ∇T using the trial function,

$$\phi_{\mathbf{k}} \propto \eta_1 \mathbf{n} \cdot \mathbf{k} + \eta_2 (\varepsilon_{\mathbf{k}} - \mu) \mathbf{n} \cdot \mathbf{k}, \quad (17)$$

²Here, we have averaged over all directions of the vector \mathbf{n} ; this is sufficient to get the temperature dependence.

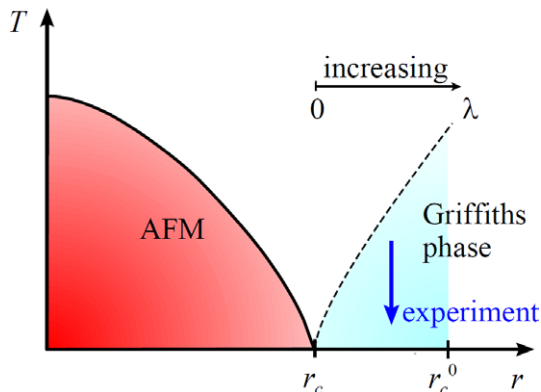


Fig. 1: (Color online) Schematic temperature-control parameter phase diagram of an itinerant antiferromagnet close to the quantum critical point. Our results apply in the Griffiths phase at low temperatures.

where η_1 and η_2 are variational parameters. Elastic impurity scattering leads to the usual linear temperature dependence $S_{imp} \propto T$ while the contribution due to the magnetic scattering by the rare regions in the Griffiths phase reads

$$\Delta S \propto T^{\lambda+1}. \quad (18)$$

Another transport coefficient called the Peltier coefficient Π characterizes the flow of a thermal current in a metal in the absence of a thermal gradient. It is related to the thermopower by $\Pi = ST$. Correspondingly, the rare-region contribution to the Peltier coefficient has the form

$$\Delta \Pi \propto T^{\lambda+2}. \quad (19)$$

Discussion and conclusions. – In summary, we have investigated the transport properties in the quantum Griffiths phase close to an antiferromagnetic quantum phase transition in a metallic system (see fig. 1). The rare-region contributions to electrical resistivity, thermal resistivity, thermopower, and the Peltier coefficient are characterized by non-universal power laws in T which are controlled by the Griffiths exponent λ .

Our results have been obtained using the semi-classical Boltzmann equation approach. This approach is valid in Griffiths phase in which the system consists of a few locally ordered rare regions in a non-magnetic bulk where the quasiparticles are well defined. Sufficiently close to the actual quantum critical point (which is of infinite-randomness type) the quasiparticle description may break down, invalidating our results. A detailed analysis of this question hinges on the fate of the fermionic degrees of freedom at the infinite-randomness quantum critical point. This difficult problem remains a task for the future.

We have used the standard isotropic ansatz (10), (14) for the deviation of the electron distribution from equilibrium. This is justified as long as the rare-region part $\Delta\rho(T)$ of the resistivity is small compared to the impurity part ρ_0 . When $\Delta\rho$ becomes larger, the anisotropy of the scattering

needs to be taken into account. This can be done by adapting the methods of Rosch [25] to the situation at hand.

We emphasize that our results have been derived for antiferromagnetic quantum Griffiths phases and may not be valid for ferromagnetic systems. The problem is that a complete theory of the ferromagnetic quantum Griffiths phase in a metal does not exist. In particular, the dynamical susceptibility still is not known. Correspondingly, the transport properties in ferromagnetic quantum Griffiths phases remain an open problem.

Non-universal power laws in a variety of observables including transport properties can also arise from a different physical mechanism far away from the magnetic quantum phase transition. In Kondo-disordered systems, the existence of a wide distribution of local single-ion Kondo temperatures is assumed; this leads to the power-law singularities [26,27]. This model was used to explain experimental results in some heavy-fermion compounds such as UCu_4Pd and $\text{UCu}_{3.5}\text{Pd}_{1.5}$ [28,29].

Let us now turn to experiment. Unfortunately and somewhat ironically, all clear-cut experimental observations of quantum Griffiths phases are in itinerant ferromagnets rather than in antiferromagnets. However, quantum Griffiths effects have been discussed in the context of the antiferromagnetic quantum phase transition in heavy-fermion systems [30,31]. One of the most striking predictions following from our theory is that the exponent characterizing the electrical resistivity should be less than one sufficiently close to the quantum phase transition. There are several antiferromagnetic systems such as $\text{CeCo}_{1.2}\text{Cu}_{0.8}\text{Ge}_2$ and $\text{Ce}(\text{Ru}_{0.6}\text{Rh}_{0.4})_2\text{Si}_2$ [30,31] that show unusual power-law behavior of the electrical resistivity with an exponent less than unity. The first system's resistivity increases with decreasing temperature. This is incompatible with our prediction and is described by the Kondo model. The resistivity of the second compound decreases with decreasing temperature in agreement with our prediction. However, it is not clear whether this behavior is indeed caused by the quantum Griffiths phase. To establish this, one should measure various thermodynamics quantities as well as the transport properties and relate their low-temperature behavior.

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