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Non-Fermi liquid transport and “universal” ratios in quantum Griffiths phases

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Abstract. We use the semi-classical Boltzmann equation to investigate transport properties such as electrical resistivity, thermal resistivity, thermopower, and the Peltier coefficient of disordered metals close to an antiferromagnetic quantum phase transition. In the quantum Griffiths phase, the electrons are scattered by spin-fluctuations in the rare regions. This leads to singular temperature dependencies not just at the quantum critical point, but in the entire Griffiths phase. We show that the resulting non-universal power-laws in transport properties are controlled by the same Griffiths exponent λ which governs the thermodynamics. λ takes the value zero at the quantum critical point and increases throughout the Griffiths phase. We also study some of the “universal” ratios commonly used to characterize Fermi-liquid behavior.

1. Introduction

In recent years, quantum phase transitions [1] have attracted a lot of attention in condensed matter theory. Quantum phase transitions happen at absolute zero temperature. They are induced by the change of an external parameter (pressure, chemical composition, and magnetic field) and are driven by quantum fluctuations. A number of metallic systems show strong deviations from conventional Landau Fermi-liquid properties when they are tuned through a quantum critical point [2].

Significant attention has also been attracted by phase transitions in the presence of quenched disorder. It has become clear that at low temperatures, strongly correlated materials can show a surprising sensitivity to imperfections and randomness. The interplay between large-scale quantum fluctuations and random fluctuations due to disorder leads to exotic phenomena such as quantum Griffiths singularities [3, 4, 5], infinite randomness critical points featuring exponential instead of power-law scaling [6, 7] and the smearing of the phase transition [8]. The Griffiths effects 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 locally ordered rare regions are not static but retain their quantum dynamics. Griffiths showed that these rare regions can lead to a singularity in the free energy in a whole parameter region which is now known as the Griffiths phase. In a *quantum* Griffiths phase, the rare-region low-energy density of states follows a power law, $\rho(\epsilon) \propto \epsilon^{\lambda-1}$, where λ is the non-universal Griffiths exponent. λ varies systematically within the Griffiths phase and vanishes at the critical point. This kind of density of states leads to power-law dependencies of several observables on the temperature T , including specific heat, $C \sim T^\lambda$, and 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]). While the thermodynamics of

quantum Griffiths phases is comparatively well understood, much less is known about transport properties.

We showed in Ref. [11] that the rare-region contributions to electrical resistivity, thermal resistivity, thermopower, and the Peltier coefficient in the quantum Griffiths phase associated with an antiferromagnetic quantum phase transition are characterized by non-universal power-laws in T which are controlled by the same Griffiths exponent λ which also governs the thermodynamics. Here, we summarize these results. We then investigate the behaviors in the antiferromagnetic quantum Griffiths phase of some of the “universal” ratios commonly used to characterize Fermi-Liquid behavior in metals. Our paper is organized as follows. In Sec. 2, we briefly discuss the model and method of solution. In Sec. 3, we then summarize the derivations of the transport properties and find that the scattering of the electrons by spin-fluctuations in the rare regions leads to singular temperature dependencies not just at the quantum critical point but in the entire antiferromagnetic quantum Griffiths phase. In Sec. 4, we present the behaviors of various “universal” ratios. Finally, we conclude in Sec. 5.

2. Model

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 [12, 13]. The Hamiltonian has the form

$$H = H_s + H_d + H_{s-d}, \quad (1)$$

where H_s and H_d are the Hamiltonians of s and d electrons, respectively. 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

$$H_{s-d} = g \int d\mathbf{r} \mathbf{s}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}), \quad (2)$$

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.

In three space dimensions, the clean critical theory is above its upper critical dimension [14, 15]; moreover the concept of quasiparticles is still (marginally) well defined. Therefore, transport properties can be treated within a semi-classical Boltzmann approach in the Griffiths phase (note that the method may break down sufficiently close to the actual quantum critical point [11]). The linearized Boltzmann equation in the presence of a temperature gradient ∇T , and an electric field \mathbf{E} but zero magnetic field can be written as [16]

$$-\mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial T} \nabla T - \mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \mathbf{E} = \left. \frac{\partial f_{\mathbf{k}}}{\partial t} \right|_{\text{scatt}}, \quad (3)$$

where $f_{\mathbf{k}}^0$ is the equilibrium Fermi-Dirac distribution function. The first and second terms describe changes of the electron distribution function $f_{\mathbf{k}}$ due to diffusion and electric field \mathbf{E} , respectively. The last one is the collision term which comprises elastic impurity scattering as well as magnetic scattering due to the spin fluctuations. In the following, we focus on the magnetic part of the scattering. 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 [13, 17]

$$\left. \frac{\partial f_{\mathbf{k}}}{\partial t} \right|_{\text{scatt}} = \frac{2g^2}{T} \sum_{\mathbf{k}'} f_{\mathbf{k}'}^0 (1 - f_{\mathbf{k}}^0) n(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) \text{Im} \chi(\mathbf{k} - \mathbf{k}', \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})$$

$$= \frac{1}{T} \sum_{\mathbf{k}'} \mathcal{P}_{\mathbf{k}'}(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'}), \quad (4)$$

where the second line defines the transition rates $\mathcal{P}_{\mathbf{k}}$. The symbol $n(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})$ denotes the Bose-Einstein distribution function, and χ is the total dynamical susceptibility of the spin-fluctuations (d electrons). In the above equation, the spin-fluctuations are assumed to be in equilibrium. This approximation is valid if the system can lose momentum efficiently by Umklapp or impurity scattering.

Quantum Griffiths effects in disordered metallic systems are realized in both Heisenberg magnets [18] and Ising magnets. In the latter case, they occur in a transient temperature range where the damping is unimportant [19]. In the following, we consider both cases.

In order to study the rare-region contribution to the transport properties in the Griffiths phase, we need to find the total rare-region dynamical susceptibility. To get it, we can simply sum over the susceptibilities of the individual clusters (rare regions). The imaginary part of the dynamical susceptibility of a single cluster of characteristic energy ϵ of a disordered itinerant quantum Heisenberg antiferromagnet in the quantum Griffiths phase is given by [20]

$$\text{Im}\chi_{\text{cl}}(\mathbf{q}, \omega; \epsilon) = \frac{\mu^2 \gamma \omega}{\epsilon^2(T) + \gamma^2 \omega^2} F_{\epsilon}^2(\mathbf{q}), \quad (5)$$

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 $\gamma T \ll \epsilon$, $\epsilon(T) \approx \epsilon$. $F_{\epsilon}(\mathbf{q})$ is the form factor of the cluster which encodes the spatial magnetization profile.

The imaginary part of the dynamical susceptibility of a single cluster in random quantum Ising models is given by [19]

$$\text{Im}\chi_{\text{cl}}(\mathbf{q}, \omega; \epsilon) = \pi \frac{\mu^2}{4} \tanh\left(\frac{\epsilon}{2T}\right) [\delta(\epsilon - \omega) - \delta(\epsilon + \omega)] F_{\epsilon}^2(\mathbf{q}). \quad (6)$$

The precise functional form of $F_{\epsilon}(\mathbf{q})$ is not known, but we can find it approximately by analyzing the Fourier transform of a typical local magnetization profile of the rare region. We find $F_{\epsilon}^2(\mathbf{q}) = X[(\mathbf{q} - \mathbf{Q})^3 \log(\epsilon^{-1})]$, where X and \mathbf{Q} are a scaling function and the ordering wave vector, respectively [11].

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

$$\text{Im}\chi(\mathbf{q}, \omega) = \int_0^{\Lambda} d\epsilon \rho(\epsilon) \text{Im}\chi_{\text{cl}}(\mathbf{q}, \omega; \epsilon), \quad (7)$$

where Λ is an energy cut-off. In the Heisenberg case we find that the rare-region contribution to the zero-temperature susceptibility in the quantum Griffiths phase can be expressed as (up to logarithmic corrections)

$$\text{Im}\chi(\mathbf{q}, \omega) \propto |\omega|^{\lambda-1} \text{sgn}(\omega) X[(\mathbf{q} - \mathbf{Q})^3 \log(\omega^{-1})]. \quad (8)$$

The rare-region susceptibility of the random quantum Ising model has the same structure as Eq.(8) [19].

3. Transport properties

3.1. Electrical resistivity

In order to calculate the electrical resistivity we consider Ziman's variational principle [16]. The resistivity ρ is given as the minimum of a functional of $\Phi_{\mathbf{k}}$,¹

$$\rho[\Phi_{\mathbf{k}}] = \min \left[\frac{1}{2T} \frac{\int \int (\Phi_{\mathbf{k}} - \Phi_{\mathbf{k}'})^2 \Gamma_{\mathbf{k}}^{\mathbf{k}'} d\mathbf{k} d\mathbf{k}'}{\left(\int v_{\mathbf{k}} \Phi_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} d\mathbf{k} \right)^2} \right], \quad (9)$$

where

$$\Gamma_{\mathbf{k}}^{\mathbf{k}'} = \int_0^{\infty} d\omega \mathcal{P}_{\mathbf{k}'}(\omega) \delta(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}} + \omega), \quad (10)$$

with $\mathcal{P}_{\mathbf{k}'}(\omega)$ defined in Eq.(4).

By making a suitable ansatz for the distribution function $\Phi_{\mathbf{k}}$ in the functional (9), we can find the resistivity. Close to the antiferromagnetic quantum phase transition, the susceptibility is strongly peaked around the ordering wave vector \mathbf{Q} . This leads to anisotropic scattering processes. However, in the presence of a high concentration of impurities, the low temperature resistivity is dominated by elastic impurity scattering which is isotropic. The isotropic scattering redistributes the electrons over the Fermi surface. This allows us to make the standard ansatz

$$\bar{\Phi}_{\mathbf{k}} \propto \mathbf{n} \cdot \mathbf{k}, \quad (11)$$

where \mathbf{n} is a unit vector parallel to the electric field. Note that any constant prefactor in $\bar{\Phi}_{\mathbf{k}}$ is unimportant because it drops out of the resistivity functional (9). Then, following the calculations for the electrical resistivity outlined in Ref. [16], we obtain

$$\Delta\rho \propto T \int d^3\mathbf{q} \frac{(\mathbf{n} \cdot \mathbf{q})^2}{q} \int_0^{\infty} d\omega \frac{\partial n(\omega)}{\partial T} \text{Im}\chi(\mathbf{q}, \omega). \quad (12)$$

Inserting the susceptibility (8), the temperature dependence of the electrical resistivity due to the spin-fluctuations in the Griffiths phase is given by

$$\Delta\rho \propto T^{\lambda}, \quad (13)$$

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

3.2. Other transport properties

In the same way, we study the thermal resistivity W (i.e., the inverse of the thermal conductivity κ). We find that the rare-region contribution to the thermal resistivity in the antiferromagnetic quantum Griffiths phase has the form

$$\Delta W \propto T^{\lambda-1}. \quad (14)$$

The Seebeck effect, the existence of an electric field \mathbf{E} in a metal subject to a thermal gradient ∇T , is characterized by the thermopower S which is defined by the relation $\mathbf{E} = S \nabla T$. To calculate the thermopower, we analyze the Boltzmann equation (3) in the presence of both ∇T and \mathbf{E} . Elastic impurity scattering leads to the usual linear temperature dependence $S_{\text{imp}} \propto T$

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

while the contribution due to the magnetic scattering by the rare regions in the Griffiths phase reads

$$\Delta S \propto T^{\lambda+1}. \quad (15)$$

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 $\Pi = S T$. Correspondingly, the rare-region contribution to the Peltier coefficient has the form

$$\Delta \Pi \propto T^{\lambda+2}. \quad (16)$$

In analogy to the resistivity (13), the results for ΔW , ΔS , and $\Delta \Pi$ are given up to logarithmic corrections only.

4. “Universal” ratios in quantum Griffiths phases

In this section, we investigate the behaviors in quantum Griffiths phases of some of the “universal” ratios commonly used to characterize Fermi-liquid behavior. Two of the ratios, the Wilson ratio $\chi T/C$ [21, 22] and the Grüneisen parameter [23], the ratio between thermal expansion coefficient β and specific heat C , only involve thermodynamics. They have been discussed before. In the Wilson ratio, the Griffiths-phase power-laws of C and χ cancel, leading to a logarithmic temperature dependence [24]

$$R_W = \chi T/C \propto [\log(1/T)]^2. \quad (17)$$

The Grüneisen parameter in the quantum Griffiths phase also diverges logarithmically with vanishing temperature T [25]

$$\Gamma = \beta/C \propto \log(1/T). \quad (18)$$

The knowledge of the transport properties (Sec. 3) allows us to study further ratios. According to the Wiedemann-Franz law [26], the ratio of the electrical resistivity divided by the temperature and the thermal resistivity, the so-called Lorenz number $L = \rho/WT$, takes the universal value L_0 within Fermi-liquid theory. In the Griffiths phase, dominant impurity scattering leads to the universal value L_0 while the rare-region contributions to the Wiedemann-Franz law give a subleading contribution

$$\Delta L \propto T^\lambda. \quad (19)$$

Let us now consider the quasi-universal ratio $q = S/C$ of the Seebeck coefficient to the specific heat [27]. Due to the spin-fluctuations in the Griffiths phase, this ratio strongly deviates from its usual temperature-independent behavior and is given by

$$q \propto T^{1-\lambda}. \quad (20)$$

Another “universal” ratio is the Kadowaki-Woods ratio, normally defined as AT^2/C^2 [28], where A is the coefficient of the T^2 -term of the resistivity. To evaluate it in the Griffiths phase where the leading temperature dependence of the resistivity is not quadratic, we rewrite the definition as $(\rho - \rho_{\text{imp}})/C^2$. Then, we find that the Kadowaki-Woods ratio behaves as

$$R_{KW} = (\rho - \rho_{\text{imp}})/C^2 \propto T^{-\lambda} \quad (21)$$

in the antiferromagnetic quantum Griffiths phase, in contrast to the temperature-independent Fermi-liquid behavior.

5. Conclusions

We have studied the transport properties in antiferromagnetic quantum Griffiths phases. 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 . We have also investigated the behaviors of some “universal” ratios. In antiferromagnetic quantum Griffiths phases, the Kadowaki-Woods ratio and the ratio between Seebeck coefficient and specific heat show strong deviations from the usual Fermi-liquid behavior. In contrast, the Wiedemann-Franz law is fulfilled to leading order in T , but the spin-fluctuations in the rare regions lead to a subleading non-universal power-law in T controlled by the Griffiths exponent. The two ratios involving thermodynamics only, the Wilson ratio and the Grüneisen ratio, show only logarithmic deviations from Fermi-liquid behavior.

Our results have been obtained using the semi-classical Boltzmann equation approach. As discussed in Ref. [11], this approach is valid in the Griffiths phase and may break down sufficiently close to the quantum critical point. We also emphasize that our results have been derived for antiferromagnetic quantum Griffiths phases and may not be valid for ferromagnetic systems. First results on the thermodynamics of ferromagnetic quantum Griffiths phases [29] suggest that the Griffiths singularities take slightly different functional forms than in antiferromagnets. A detailed study of the transport properties remains a task for the future.

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