Theory of the ac Hall response of a model with X-ray edge Singularities in infinite dimensions

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We study the ac magnetotransport in a non-Fermi liquid metal, which possesses explicit x-ray edge singularities in \( d = \infty \). Specifically, we compute the ac conductivity tensor in a formalism that becomes exact in this limit. The ac Hall constant and Hall angle reveal features that are in striking qualitative agreement with those observed in optical transmission experiments carried out on \( YBa_2Cu_3O_7 \) thin films. Our results provide a concrete realization of the two-relaxation time picture proposed to explain magnetotransport anomalies in the normal state of cuprate superconductors.

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1. INTRODUCTION

Discovery of cuprate superconductors has renewed interest in the physics of strongly correlated electronic systems. Extensive experimental work \([1,2]\) performed by several groups demonstrates that the normal state physical properties are not understandable in terms of the Landau theory of the Fermi liquid (FL) \([3]\), which has been the mainstay of the conventional theory of metals.

In particular, dc transport in the \( ab \) plane in the normal state has been cited as evidence for the non-FL nature of these systems. The inplane resistivity is linear in \( T \) from temperatures as low as 10K to above room temperature with no sign of saturation. Hall measurements have provided more striking evidence of the anomalous charge transport; the inverse Hall angle has a quadratic temperature dependence over a wide range in many materials \([4]\). The ac conductivity derived from optical reflectivity experiments shows a distinctly non-Drude like behavior above 200cm\(^{-1}\). Thus the normal state transport reveals two qualitatively different relaxation rates associated with the decay of the usual transport and Hall currents in the system.

Quite a number of ideas have been proposed to explain these unusual observations. Very early on, almost seven years ago, Anderson proposed the "two-relaxation-rates" scenario to understand these results. In his theory \([5]\), the different relaxation rates arise as a consequence of spin-charge separation; the \( T \)-linear resistivity results from holons scattering off the thermally excited spinons, whose number \( \approx T \), while spinon-spinon scattering in a magnetic field (which is like a fermion scattering process), gives rise to the quadratic Hall relaxation rate. Carrington et al. have proposed an alternative explanation in terms of differing relaxation rates and effective masses associated with the anisotropic 2d Fermi surfaces in these materials \([6]\). However, as argued convincingly by Coleman \([7]\), the FL-based theory suffers from a serious drawback; addition of impurities or underdoping changes the Fermi surface topology and results in a change in the \( T \)-dependence of \( \theta_H^{-1} \). This is not what is observed; these changes are observed to lead to a change in the \( T \)-dependence of the resistivity, but the \( T^2 \)-dependence of the Hall angle is unchanged \([4]\). Theories based on the concept of singular skew-scattering in a marginal Fermi liquid \([8]\) share the above difficulty.

Drew et al. \([9]\) have recently measured the far-infrared (FIR) transmission from thin films of \( YBa_2Cu_3O_7 \). Their experimental results are consistent with a simple finite-frequency generalization of the Anderson-Ong equation previously used to describe dc Hall effect \([5]\). However, the underlying hypothesis of the tomographic Luttinger liquid behavior in the metallic phase of the 2d Hubbard model is still open, inspite of intense importance of the issue.

Theoretically, the problem of computing the transport coefficients for a strongly correlated fermionic system in a controlled way is a rather hard task. The problem is even harder in the case of magnetotransport; to compute the Hall conductivity tensor, one has to evaluate explicitly three-point functions. In finite spatial dimensions, vertex corrections, which may be important, cannot be evaluated satisfactorily in any controlled approximation. The above difficulties make it imperative to search for controlled approximation schemes where some of the above difficulties can be circumvented without sacrificing essential correlation effects.

The dynamical mean-field approximation (DMFA or \( d = \infty \)) has proved to be a successful tool to investigate transport in strongly correlated systems in a controlled way \([10]\). This is because the vertex corrections entering in the Bethe-Salpeter eqn for the two-particle propagator for the conductivity vanish rigorously in \( d = \infty \). To evaluate the conductivity tensor, one needs only to compute the fully interacting local self-energy of the given model, following which the Kubo formalism can be employed \([11]\). Given that DMFA captures the nontrivial local dynamics exactly, one expects that it provides an adequate physical description in situations where local fluctuations are dominant.
Lange [12] has employed the Mori-Zwanzig projection formalism to study dc magnetotransport in the Hubbard model. The actual evaluation of the complicated equations is, however, actually carried out in the Hubbard I approximation. This is known to lead to spurious instabilities (like ferromagnetism, which is washed away when local quantum fluctuations are included). Moreover, only the dc Hall constant is evaluated explicitly. The Hubbard I approximation does not correctly capture the transfer of high-energy spectral weight to low energy upon hole doping, a feature characteristic of correlated systems, and so one expects that it will be inadequate when one attempts to look at the ac conductivity. Majumdar et al. [13] have computed the Hall constant in the $d = \infty$ Hubbard model with next-nearest neighbor (nnn) hopping. It is known, however, that the quantum paramagnetic metallic phase of the Hubbard model is always a Fermi liquid in $d = \infty$ [10], and so their results should be applicable only at temperatures above $T_{coh}$, below which local FL behavior sets in. The computation of the ac magnetotransport for a non-FL in $d = \infty$ has not been attempted at all; only the ac conductivity has been computed [14].

In this letter, we address precisely this issue. We study the ac magnetotransport expected in the paramagnetic (non-FL) metallic state of a model which has explicit x-ray edge singularities in $d = \infty$ [15]. Our motivation for the choice of this model is two-fold. Firstly, it has been the first model to have been solved exactly in $d = \infty$ [10], and has an explicit non-FL metal phase. The second motivation comes from the proposal due to Anderson [3], who argues that the non-FL metallic behavior in the normal state of cuprates arises from processes which lead to an effective blocking of the $\downarrow$-spin recoil in the 2d HM near half-filling. The resulting x-ray edge (XRE) singularities drive the non-FL features observed. In view of the above discussion, we expect that an exact (in $d = \infty$) computation of the ac conductivity and Hall response in an appropriate model (the imbedded impurity model with XRE singularities) should capture the essential features if the non-FL behavior is indeed driven by XRE effects.

II. COMPUTATION OF THE AC HALL EFFECT

We start with the simplified Hubbard model (SHM),

$$H = -t \sum_{<ij>} (c_{i\uparrow}^\dagger c_{j\uparrow} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

(1)

where the $\downarrow$-electrons do not hop. A model of a similar type has been proposed by Sire et al. [16] as an effective model derived from a full three-band Hubbard model. Interestingly enough, this is also (locally) equivalent to an effective model obtained from the HM if the $\downarrow$-spin recoil is suppressed. As is known, this model possesses an explicit analytical solution in $d = \infty$. In our work below, we neglect the actual 2d character of the $Cu - O$ planes, and work with a semielliptic unperturbed DOS.

An assumption implicit in the choice here is that band-structure effects are not important, and that the origin of the non-FL behavior is entirely due to strong correlations. As observed by Shastry et al. [4], the Hall constant in a strongly correlated system is dominated by spectral weight far from the Fermi surface, and hence is independent of its shape. This lends good support to the assumption made above. To compute the ac conductivity tensor in $d = \infty$, one needs only the full s.p propagator $G_\uparrow(k, \omega) = 1/(\omega - \epsilon_k - \Sigma_\uparrow(\omega))$, where $\Sigma_\uparrow(\omega)$ is the exact, local self-energy of the model eqn.(1) in $d = \infty$. Since this is already known, we do not repeat the derivation here, but refer the reader to [17]. Given $G_\uparrow(k, \omega)$, one can compute the full interacting DOS. This is the only input to the optical conductivity, calculated within the framework of the Kubo approach [10] in $d = \infty$. The off-diagonal conductivity is, however, harder to compute. The Hamiltonian in a magnetic field is

$$H = - \sum_{<ij>} t_{ij}(A)(c_{i\uparrow}^\dagger c_{j\uparrow} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

(2)

with $<ij>$ denoting nearest neighbors on a Bethe lattice in $d = \infty$. The hopping matrix elements are modified by a Peierls phase factor and are $t_{ij} = \exp(2i\pi/\phi_0 \int^j_A \cdot d l)$, where $A$ is the vector potential and $\phi_0 = hc/e$. The off-diagonal part of the conductivity involves the computation of a three-point function to first order in the external field, as mentioned before [18]. Fortunately, a convenient form has been worked out by Lange [12], so we use the approach developed there. Explicitly, after a somewhat tedious calculation, the imaginary part of $\sigma_{xy}(\omega)$ is given by

$$\sigma_{xy}(\omega) = c_{xy} \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} \int_{-\infty}^{\infty} d\omega_1 d\omega_2 A_\uparrow(\epsilon, \omega_1) A_\uparrow(\epsilon, \omega_2) \frac{1}{\omega} \left[ F(\epsilon, \omega_1; \omega) - F(\epsilon, \omega_2; \omega) + (\omega \rightarrow -\omega) \right]$$

(3)

where

$$F(\epsilon, \omega_1; \omega) = A_\uparrow(\epsilon, \omega_1 - \omega) [f(\omega_1) - f(\omega_1 - \omega)]$$

(4)

and $A_\uparrow(\epsilon, \omega) = -Im[\omega - \epsilon - \Sigma_\uparrow(\omega)]^{-1}/\pi$ is the s.p spectral function in $d = \infty$.

III. RESULTS AND DISCUSSION

We now describe the results of our calculation. The calculations were performed with a semielliptic DOS with an effective half-width $D(= 0.1 ev)$ and $U/D = 20$ which
FIG. 1. Real and Imaginary (in inset) parts of the optical conductivity $\sigma_{xx}$ for $U/D = 20$, $\delta = 0.1$ (continuous) and $\delta = 0.2$ (dotted-dashed). The dotted line shows the case with $U/D = 2$, $\delta = 0.2$. The low-energy behavior is practically unchanged in the two cases. Notice the non-Drude fall-off at intermediate frequency ($\omega \approx 0.2eV$). Inset shows the imaginary part of $\sigma_{xx}(\omega) \approx \omega^7$, $\gamma = 0.9$.

reproduces an insulating solution at half-filling. We specify that this effective bandwidth is not obviously related to the “free” bandwidth taken from spectroscopic estimates, but should be thought of as an independent parameter of our proposed model. We have checked (see fig.1) that decreasing $U$ ($U/D = 2$) does not affect the low energy part of the $\sigma_{xx}(\omega)$, which continues to have the same frequency dependence upto $\omega/D \approx 1$.

FIG. 2. $ReR_H(\omega)$ for $U/D = 20$, $\delta = 0.1$ (continuous) and $\delta = 0.2$ (dotted-dashed). The full frequency dependence is shown in the inset. $ReR_H(\omega)$ falls off much faster with $\omega$ in comparison to $Re\sigma_{xx}(\omega)$ and is qualitatively in agreement with the experimental results of Ref. [9].

FIG. 3. $ImR_H(\omega)$ for $U/D = 20$, $\delta = 0.1$ (continuous) and $\delta = 0.2$ (dotted-dashed). The full frequency dependence is shown in the inset. Notice the qualitative agreement with the experimental results of Ref. [9].

All calculations were performed at a temperature $T = 0.01D$. The computed optical conductivity $\sigma_{xx}(\omega)$ has a distinctly non-Drude fall off at intermediate frequencies, while $Im\sigma_{xx}(\omega) \approx \omega^7$ at small $\omega$ with $\gamma = 0.9$ for both $n = 1 - \delta = 0.9, 0.8$ with our parameters (Fig. 3). More interesting, however, is the result of the computation of the ac Hall effect. In Fig. 4 we show the real part of the ac Hall constant as a function of frequency. The corresponding imaginary part is depicted in Fig. 5. The results show striking similarities to the thin-film data of Drew et al.. It is interesting to notice that the frequency dependence of the $R_H(\omega)$ is much faster ($\approx \omega^{2\gamma}$) than that of $\sigma_{xx}(\omega)$, and thus our results show that in this frequency regime, the ac transport is indeed characterized by two relaxation rates describing relaxation of longitudinal and Hall currents in the system. Additional support is provided by results for the ac Hall angle. We show the real part of $\cot\theta_H(\omega)$ in Fig. 6, the frequency dependence of the real and the imaginary parts of $\cot\theta_H(\omega)$ observed experimentally is qualitatively reproduced by our calculation. Finally, the real part of $\tan\theta_H(\omega)$ is depicted in Fig. 7. Clearly, Retan$\theta_H(\omega)$ falls off much faster ($\approx \omega^{2\gamma}$) with $\omega$ than does $\sigma_{xx}(\omega)$, providing additional evidence [7] in favor of the two-relaxation time scenario. Calculation of the dc Hall effect [19] using the FKM shows that near $n = 1$, the resistivity goes linearly with $T$, while $cot\theta_H(T) \approx aT^2 + b$ as one would expect if the ”two-relaxation time” scenario were valid. Additionally, these distinct behaviors persist as a function of hole doping; the curves are qualitatively similar for $\delta = 0.1, 0.2$. Thus, our calculation shows unambiguously that an exact (in $d = \infty$) treatment of the local dynamical fluctuations in a model with infrared singularities qualitatively reproduces the essential features of ac magnetotransport observed in
The agreement with experimental results of Ref. [9] is striking.

In view of the qualitative agreement of our obtained results with the experimental results of Drew et al., we conclude that the charge dynamics is that consistent with a picture where FL theory is invalidated near half-filling in a model with low-energy XRE singularities. In this model, the low-energy response is scale-invariant, in contrast to what is found in the $d = \infty$ Hubbard model (a FL for $T < T_{coh}$); in fact the only scale is the temperature, as in the marginal FL theory.

It is interesting to inquire about a possible link with Anderson’s ideas. To see this, we notice that the impurity version of the model eqn.(1) is precisely the x-ray edge model. This was bosonized many years ago by Schotte et al. [20], and the resulting low energy behavior was found to be the same as that of a Tomonaga-Luttinger model defined on a half-line. Upon refermionization, the resulting model is effectively one-dimensional in each radial direction around the “impurity” (recall that in $d = \infty$, the lattice model is mapped onto a selfconsistently embedded single impurity model). This is very similar to Anderson’s tomographic Luttinger liquid ideas, and the link is suggestive. We have solved the selfconsistently embedded (lattice) version of the XRE model to study the effects of low-energy singularities on the charge dynamics. Our results indicate that the anomalous features observed in ac magnetotransport are understandable in terms of the dynamics of the non-FL metallic state in a model characterized by XRE singularities.

To conclude, we have presented, we believe, the first controlled calculation of the ac magnetotransport for a non-FL metal in $d = \infty$. Our calculated results reveal that the longitudinal and transverse responses in a non-FL are governed by distinct relaxation time-scales, in agreement with the two-relaxation time picture pro-
posed to explain the dc magnetotransport in cuprates. Qualitative agreement with published far-infrared data on YBCO thin films is seen, and so our results are also an evidence for the importance of X-ray edge-like effects in the “normal” non-FL metallic state of the doped cuprate superconductors.

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