Ubiquity of linear resistivity at intermediate temperature in bad metals

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Ubiquity of Linear Resistivity at Intermediate Temperature in Bad Metals

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Bad metals display transport behavior that differs from what is commonly seen in ordinary metals. One of the most significant differences is a resistivity that is linear in temperature and rises to well above the Ioffe-Regel limit (where the mean-free path is equal to the lattice spacing). Using an exact Kubo formula, we show that a linear resistivity naturally occurs for many systems when they are in an incoherent intermediate-temperature state. First, we provide a simple analytic model to give intuition for this phenomenology. Then, we verify the analytic arguments with numerical calculations for a simplified version of the Hubbard model which is solved with dynamical mean-field theory. Similar features have also been seen in Hubbard models, where they can begin at even lower temperatures due to the formation of resilient quasiparticles.

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I. INTRODUCTION

Transport properties of strongly correlated materials, such as oxides in the families of vanadates [1], cobaltates[2] or cuprates[3], Kondo semiconductors such as FeSi[4,5], $FeSb_2$[6] CeB_6[7] or SmB_6[8], and organic charge transfer salts[9] are poorly understood, despite an overwhelming amount of experimental work which established non-Fermi-liquid behavior for these systems[10,11]. In particular, a resistivity which rises linearly with temperature above the Mott-Ioffe-Regel limit[12] has become a hallmark for non-Fermi liquid behavior[13]. One common feature of these vastly different materials is that they are formed by doping away from a Mott-Hubbard insulating state. Starting from this observation, and the ubiquity of quasi-linear non-Fermi liquid materials, we provide a simple explanation of the experimental data at moderate to high temperature.

We begin by deriving the transport coefficients using an analytic approach, in the spirit of Mahan and Sofo's work on the best thermoelectrics[14], where the optimization of transport properties was calculated based on a simplified ansatz for the (vertex-corrected) transport relaxation time which then allowed one to perform the optimization. Here, we work in a similar vein, but consider the temperature dependence of the resistivity based on a general discussion of the properties of the transport relaxation time for a strongly correlated metal. By modeling this simplest form for correlated transport, the results should hold for a wide range of materials, and thereby explain the ubiquity of the linear resistivity at intermediate temperature. In the second part, we substantiate the phenomenological results by calculating the resistivity of a non-trivial model of strongly correlated electrons propagating on a d-dimensional lattice. We use the Falicov-Kimball model which, like the Hubbard or periodic Anderson model, has a gap in the excitation spectrum and, unlike these other models, admits an exact solution for the resistivity at arbitrary doping and temperature.

II. MODEL-INDEPENDENT PHENOMENOLOGY

Our starting point is the Kubo formula for the conductivity which reads[15],

$$\sigma_{dc}(T) = \sigma_0 \sum_\sigma \int d\omega \left(-\frac{df(\omega)}{d\omega}\right) \tau_\sigma(\omega) \ , \qquad (1)$$

where σ_0 is a material specific constant with units of conductivity, $(-df(\omega)/d\omega)$ is the derivative of the Fermi function that is sharply peaked around the chemical potential μ, so that the integral is cut-off outside the Fermi window $|\omega| \geq k_B T$. The summation is over the spin states σ and $\tau_\sigma(\omega)$ is the exact transport relaxation time which includes the velocity factors, averaged over the Fermi surface, and all the effects of vertex corrections, if present. We set $k_B = \hbar = 1$ and measure all energies with respect to μ.

Since $\tau_\sigma(\omega)$ is nonnegative and vanishes for energies outside the band, it must have at least one maximum within the band. In a Fermi liquid, $\tau_\sigma(\omega)$ diverges as $T \to 0$ and $\omega \to 0$, and the resistivity, $\rho(T) = 1/\sigma_{dc}(T)$, follows a T^2 law at low temperature. If there is residual scattering, due to disorder for example, the divergence gets cut-off and the Fermi-liquid form no longer holds. In a pure strongly correlated metal, for temperatures *above*

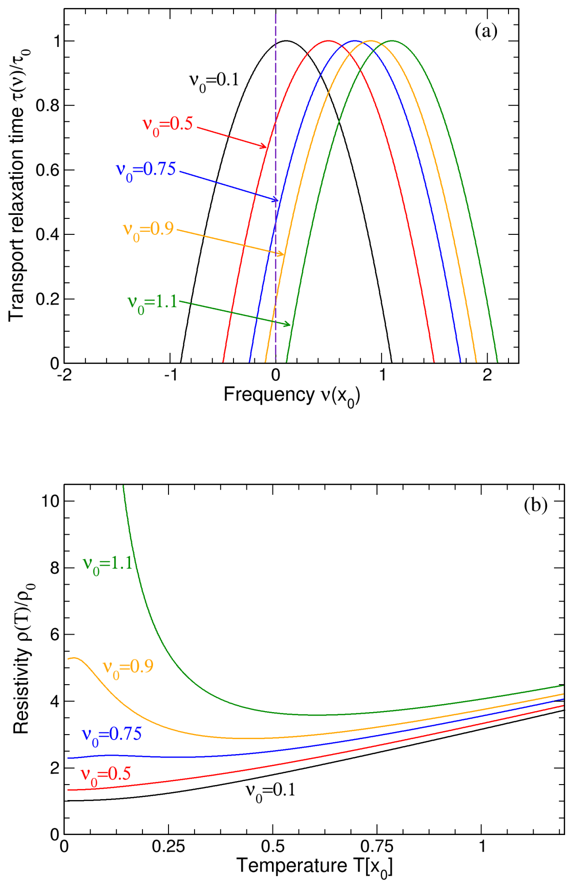

FIG. 1. (color online) Panel (a): Rescaled relaxation time $\tilde{\tau}_\sigma(\nu)$ plotted as a function of rescaled frequency $\nu = \omega/x_0$ relative to the chemical potential, μ, which is indicated by the vertical line at $\nu = 0$. (For definition of the scaling factors see the text.) The different curves show $\tau_\sigma(\nu)$ shifted with respect to μ by $\nu_0 = 0.1$, 0.5, 0.75, 0.9, and 1.1, respectively. Curve (a) corresponds to a dirty metal, curves (b), (c), and (d) to a bad metal, and curve (e) to a slightly doped Mott insulator. Panel (b): The rescaled resistivity obtained from Eq. (3) plotted as a function of rescaled temperature $\tilde{T} = T/x_0$. The different curves are obtained for $\tilde{\tau}_\sigma(\nu)$ as defined in the panel (a).

the low-temperature coherence scale, the transport relaxation time typically has two maxima, located in the upper and the lower Hubbard bands, and neither the shape nor the position of these broad maxima, relative to $\mu(T)$, change appreciably with temperature. The transport relaxation time of the Hubbard model, Falicov-Kimball model, Anderson model, and other effective models of strong correlations, exhibits these features. Since the chemical potential of a strongly correlated metal is within one of the two Hubbard bands, we calculate the resistivity focusing on $\tau_\sigma(\omega)$ with just a single broad maximum at ω_0, neglecting the excitations across the gap.

The conductivity given by Eq. (1) crucially depends on the overlap between $(-df/d\omega)$ and $\tau_\sigma(\omega)$, i.e., on temperature and doping. Temperature broadens the Fermi window where the integrand is appreciable, while doping changes the number of carriers, so that μ gets shifted with respect to ω_0. The value and the shape of $\tau_\sigma(\omega)$ around ω_0 can also be doping dependent.

To estimate the resistivity we expand $\tau_\sigma(\omega)$ around its maximum at ω_0,

$$\tau_\sigma(\omega) \approx \tau_0 - \tau_1(\omega - \omega_0)^2 \ , \tag{2}$$

where $\tau_0 = \tau_\sigma(\omega_0)$, $\tau_1 = -d^2\tau_\sigma(\omega)/2d\omega^2\Big|_{\omega\to\omega_0}$, and we use a simple model in which $\tau_\sigma(\omega)$ is approximated by the parabolic form in Eq. (2) for $\Lambda_- < \omega < \Lambda_+$ and $\tau_\sigma(\omega) = 0$ otherwise; this form properly has a maximum, and shows linear behavior as one approaches the band edges, as expected for a three-dimensional material. The cutoffs $\Lambda_\pm$ are obtained by setting $\tau_\sigma(\omega) = 0$ in Eq. (2). This yields $\Lambda_\pm = \omega_0 \pm x_0$, where $x_0^2 = \tau_0/\tau_1$ is inversely proportional to the curvature of $\tau_\sigma(\omega)$ at ω_0 and x_0 has dimensions of energy. Since the high-energy part of $\tau_\sigma(\omega)$ does not contribute much to the conductivity, $x_0 = \omega_0 - \Lambda_-$ often defines an effective bandwidth relevant for transport of a doped Mott insulator.

To evaluate the integral in Eq. (1), we introduce dimensionless variables, $\nu = \omega/x_0$ and $\tilde{T} = T/x_0$, and write the relaxation time as, $\tau_\sigma(\nu)/\tau_0 = 1 - (\nu - \nu_0)^2$, where $\nu_0 = \omega_0/x_0$. Integrating by parts, and using $\tau_\sigma(\Lambda_-) = \tau_\sigma(\Lambda_+) = 0$, yields

$$\sigma_{dc}(\tilde{T}) = 2\tau_0\sigma_0 \int_{\nu_0-1}^{\nu_0+1} d\nu \ f(\nu) \ \frac{d\tau(\nu)}{d\nu} \ , \tag{3}$$

where $f(\nu) = 1/[1 + \exp(\nu/\tilde{T})]$, $d\tau_a/d\nu = -2(\nu - \nu_0)$, and we took the spin degeneracy into account. The integrand is a regular function and the numerical evaluation is straightforward. The renormalized resistivity, $\rho(\tilde{T})/\rho_0$, where $\rho_0 = 1/(\sigma_0\tau_0)$, is shown in panel (b) of Fig. 1 for several characteristic values of ν_0. Panel (a) shows $\tau_\sigma(\nu)/\tau_0$ used for each of the resistivity curves. The data indicate three types of behavior, depending on the relative position of μ and ω_0. Here μ is fixed as a function of T, but as seen below, fixing the density instead, produces similar results.

For $\nu_0 \geq 1$, when the chemical potential is close to the band-edge, the resistivity decreases rapidly as temperature increases from $T = 0$. At about $T \simeq \omega_0/2$, the resistivity drops to a minimum and, then, increases with temperature, assuming at about $T \simeq \omega_0$ a linear form. Such a behavior is typical of lightly doped Mott insulators. For $\nu_0 \leq 1$, when the chemical potential is just above the band edge, the low-temperature resistivity is metallic. It starts from a finite value, at $T = 0$, and grows to a well pronounced maximum, which is reduced and shifted to lower temperature as ν_0 is reduced. The minimum still occurs at about $T \simeq \omega_0/2$ and, for $T \geq \omega_0$, the resistivity becomes a linear function in a broad temperature range. Such a behavior is typical of bad metals. For $\nu_0 \ll 1$, the chemical potential is close to the maximum of $\tau_\sigma(\nu)$ and $\rho(T)$ increases parabolically

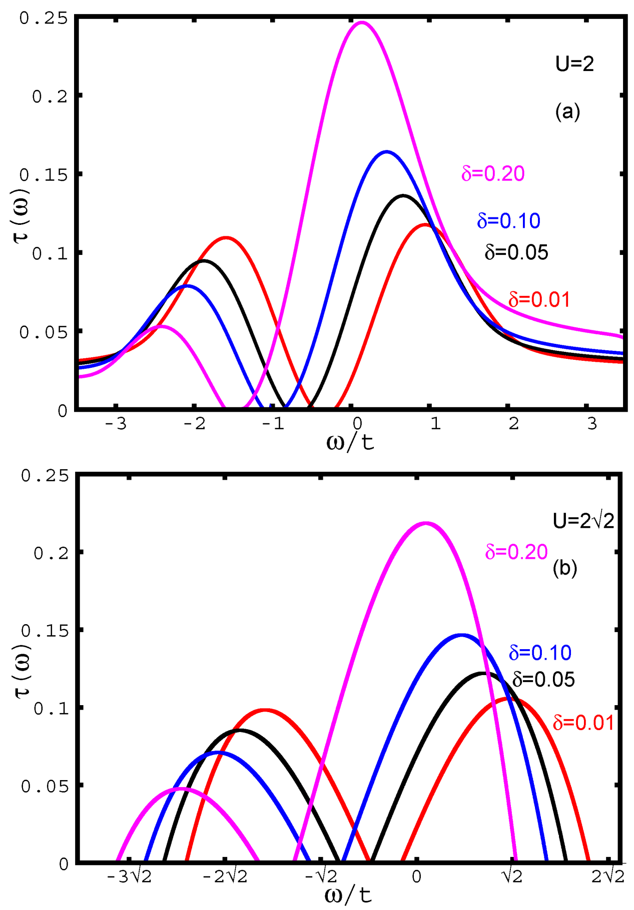

FIG. 2. (color online) Transport lifetimes in the Falicov-Kimball model for $U = 2t^*$ on a hypercubic lattice (a) and $U = 2\sqrt{2}t^*$ on the Bethe lattice (b).

from its zero-temperature value, as found in dirty metals. At higher temperatures, $T > \omega_0$, there is a crossover to the linear behavior. According to this simple model, strongly correlated materials are classified into three distinct groups: lightly doped insulators characterized by a low-temperature resistivity upturn, bad metals characterized by an extended range of quasilinear resistivity, and dirty metals characterized by a *constant plus* T^2 behavior.

III. MODEL-DEPENDENT EXAMPLE

The analytic approach is suggestive of the robustness of the linear resistivity for bad metals due to the general nature of $\tau_\sigma(\omega)$, but we want to go further to obtain similar results with a nontrivial microscopic model. We choose the spin-1/2 Falicov-Kimball model which is closely related to the Hubbard model and leads to similar transport properties (above the coherence temperature of the Hubbard model). The question we primarily want to address is: to what extent can a model for strongly correlated electrons capture the phenomenology of non-Fermi liquid electrical transport with a focus on the linear resistivity? The advantage of the Falicov-Kimball model is that the dynamical mean-field theory (DMFT) provides an exact solution at arbitrary filling[16]. (There have been related studies on the Hubbard model using DMFT[17,18] exploring transport in bad metals as well).

The spin-1/2 Falicov-Kimball Hamiltonian reads

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma}\, c_{j\sigma} + U \sum_{i\sigma} w_i c^\dagger_{i\sigma} c_{i\sigma}, \qquad (4)$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) is the mobile electron creation (annihilation) operator of spin σ and w_i is 1 or 0 and represents the localized electron number operator at site i. (Each lattice site can only be occupied by a single localized electron, because the on-site repulsion between the localized electrons of the opposite spin is assumed infinite.) The interaction of the conduction electrons with localized electrons is U and t^* is the hopping integral scaled so that we can properly take the $d \to \infty$ limit[19]. We work on both a hypercubic and Bethe lattice using units where $t^* = 1$. We maintain the paramagnetic constraint, $\rho_{c\sigma} = \rho_{c\bar{\sigma}} = \rho_c$, by equating the conduction and localized densities. For hole doping, we have $\rho_c = \rho_f = 1 - \delta \leq 1$, where δ is the concentration of the holes in the lower Hubbard band, while for electron doping, $\rho_c = 1 + \delta \geq 1$, where δ is the concentration of electrons in the upper Hubbard band.

The model is solved using DMFT[20] in the infinite dimensional limit $d \to \infty$, such that the self-energy $\Sigma(\omega)$ is a functional of the local conduction electron Green's function, $G_{loc}(\omega)$, and the full lattice problem is equivalent to a single-site model with an electron coupled self-consistently to a time-dependent external field. Several reviews, whose notation we adopt, now exist both on DMFT generally[21] and on the exact DMFT for the Falicov-Kimball model[16]. We find $\Sigma(\omega)$, $G_{loc}(\omega)$, and the local density of conduction states $\rho_{loc}(\omega) = -\mathrm{Im}\, G_{loc}(\omega)/\pi$ numerically using methods described elsewhere[22] .

For $\rho_c = 1$, $\rho_{loc}(\omega)$ is symmetric and, for large enough U, we have a Mott insulator in which a filled lower Hubbard band is separated from an empty upper Hubbard band by a band gap with the chemical potential in the middle of the gap ($U_c = \sqrt{2}$ for the hypercubic lattice and $U_c = 2$ for the Bethe lattice). Away from half-filling, $\rho_{loc}(\omega)$ is asymmetric and for electron doping, which is the case we consider, the chemical potential is in the upper Hubbard band. Its distance from the lower band edge Λ_- is determined by charge conservation $\delta = 2\int d\omega f(\omega)\rho_{loc}(\omega) - 1$.

For $d \to \infty$, the vertex corrections to the conductivity vanish[23] and explicit formulas can be found for the relaxation time. On the Bethe lattice, this yields[24]:

$$\tau_\sigma(\omega) = \frac{1}{3\pi^2}\mathrm{Im}^2[\mathrm{G_{loc}}(\omega)] \left(\frac{|\mathrm{G_{loc}}(\omega)|^2 - 3}{|\mathrm{G_{loc}}(\omega)|^2 - 1}\right) . \qquad (5)$$

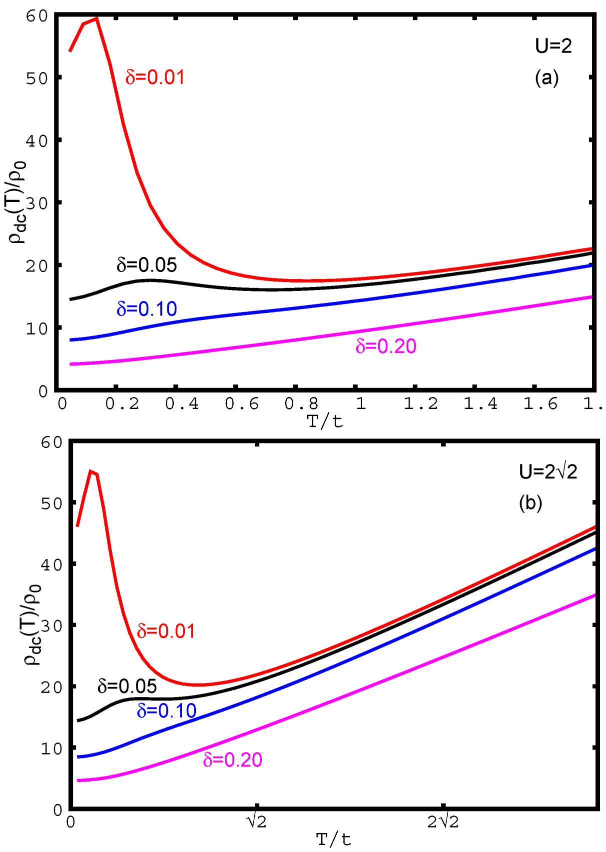

FIG. 3. (color online) Resistivity for (a) $U = 2t$ on the hypercubic lattice and (b) $U = 2\sqrt{2}t$ on the Bethe lattice

while on the hypercubic lattice, we have[16]:

$$\tau_\sigma(\omega) = \frac{1}{4\pi^2}\frac{\text{Im } G_{loc}(\omega)}{\text{Im } \Sigma(\omega)} + \frac{1}{2\pi^2}\left\{1 - \text{Re}\left[\left(\omega+\mu-\Sigma(\omega)\right)G_{loc}(\omega)\right]\right\} . \tag{6}$$

For fixed ρ_f, the shape of $\tau_\sigma(\omega)$ is independent of temperature. In a Fermi liquid, where one can approximate[15] $\tau_\sigma(\omega) \simeq \text{Im } G_{loc}(\omega)/\text{Im } \Sigma(\omega)$ with $\text{Im}\Sigma(\omega \to 0) \to 0$, the relaxation time $\tau_\sigma(\omega)$ diverges as $\omega \to 0$. In the Falicov-Kimball model, however, Im $\Sigma(0)$ does not vanish and $\tau_\sigma(0)$ remains finite. For large U, the width of the single-particle excitations exceeds their energy leading to overdamped excitations rather than with quasiparticles, such that the Fermi liquid description is not applicable.

The transport relaxation time of the Falicov-Kimball model due to such overdamped excitations, obtained for a fixed value of U and several values of δ, is shown in Fig. 2. The left and right panel show the results for the hypercubic and Bethe lattice, respectively. Note the similarity to the inverse quadratic approximation used in the first part. The transport relaxation time vanishes below the band edge Λ_- and has a peak at the energy ω_0, in the upper Hubbard band (for electron doping). As δ increases, ω_0 and Λ_- decrease but the difference $\omega_0 - \Lambda_-$ remains approximately constant. The resistivity obtained for the same set of parameters is shown in Fig. 3. The doping dependence of $\rho(T)$ follows from the observation that δ reduces ω_0 and that, for $\Lambda_- < \mu < \omega_0$, the Fermi window removes the contribution of the high-energy part of $\tau_\sigma(\omega)$. Close to half-filling (very small δ), where $\mu \simeq \Lambda_- \ll \omega_0$, the resistivity exhibits a low-temperature peak, then, drops to a minimum at about $T \simeq \omega_0/2$ and, eventually, becomes a linear function of T, for $T \geq \omega_0$. An increase of δ brings ω_0 closer to μ, which reduces the resistivity maximum and brings the onset of the linear region to lower temperatures. For a sufficiently large δ, the maximum is completely suppressed and the resistivity is a monotonically increasing function of temperature. For $\delta \simeq 0.2$, we find $\omega_0 \simeq \mu$ and obtain a resistivity with a well defined T^2 term at the lowest temperatures. Note, the crossover between different regimes can also be induced by pressure which modifies the hopping integrals and shifts ω_0 with respect to μ.

IV. CONCLUSIONS

The results obtained for the Falicov-Kimball model are in complete agreement with the phenomenological theory presented in the first part of the paper. Hence, the analytic model is verified as providing the generic behavior of a doped Mott insulator at intermediate T. The central result of this paper is that the linear resistivity seen in strongly correlated materials at intermediate T is governed by the appearance of a maximum in $\tau_\sigma(\omega)$ above the chemical potential. The slope of the linear resistivity does not vary much for a range of chemical potentials near the maximum, so the temperature dependence of $\mu(T)$ does not change this behavior. In other correlated models like the Hubbard model, the linear resistivity will disappear when T is reduced below the renormalized Fermi-liquid scale, but it appears that the resilient quasiparticle picture[25] allows the linear region to be brought down to even lower T's than seen in the Falicov-Kimball model. In the very high T limit, where T is bigger than the bandwidth, general arguments[26] show that the resistivity is linear for the Bethe lattice, but saturates at a constant for the hypercubic lattice. Those results are complementary to the general linear resistivity here, found for temperatures much less than the bandwidth.

V. ACKNOWLEDGEMENTS

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