

Transport properties in correlated systems: An analytical model

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Several studies have so far investigated transport properties of strongly correlated systems. Interesting features of these materials are the lack of resistivity saturation well beyond the Mott-Ioffe-Regel limit and the scaling of the resistivity with the hole density in underdoped cuprates. Due to the strongly correlated nature of these materials, mainly numerical techniques have been employed. A key role in this regard is thought to be played by the continuous transfer of spectral weight from coherent to incoherent states. In this paper we employ a simple analytical expression for the electronic Green's function to evaluate both quasiparticle and transport properties in correlated systems. Our analytical approach permits us to enlighten the specific role of the spectral transfer due to the correlation on different features. In particular we investigate the dependence of both quasiparticle and transport scattering rate on the correlation degree and the criterion for resistivity saturation.

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I. INTRODUCTION

The study of transport properties in high temperature superconductors represents a still open issue. Among other debated anomalous features, such as the linear behavior of the resistivity $\rho(T)$ as a function of the temperature for optimally doped compounds, the resistivity saturation presents interesting analogies between the cuprates and the alkali-doped fullerenes. The concept of resistivity saturation derives from a semiclassical picture. The basilar argument is that the electronic mean free path l cannot be lower than the interatomic distance a . In a Drude-like picture this simple consideration implies that the conductivity, which is proportional to the mean free path l , cannot be smaller than a limiting value $\sigma_{\text{sat}} = \sigma(l=a)$, and a saturating value for the resistivity $\rho_{\text{sat}} = 1/\sigma_{\text{sat}}$.¹ This condition, usually known as the Ioffe-Regel criterion, is often connected with the Mott limit associated with the disorder induced metal-insulator transition $k_{\text{F}}l \sim 1$.²

From the experimental point of view, the mostly known materials displacing resistivity saturation are the A15 compounds, where the Ioffe-Regel limit is rapidly achieved in the physical range of temperature due to the strong electron-phonon coupling. Coherently with this picture, A15 materials show a pronounced deviation of $\rho(T)$ from the linear behavior at high temperature when the mean free path is expected to become comparable with the interatomic distance.³ However, both in cuprates and in alkali-doped fullerenes the theoretical prediction of the resistivity saturation at the Ioffe-Regel limit seems to fail.^{4,5} Experimental measurements in lightly doped cuprates show a resistivity greater than the saturation value ρ_{sat} estimated by the simple quasiparticle picture,^{4,6,7} and also transport measurements in the alkali-doped compounds would predict at high temperatures a mean free path smaller than the intermolecular distance.⁵

Although these two classes of materials present significant differences, an interesting common trait which is shared by both families is the relevant role of a strong electronic

correlation. The presence of strong correlation effects questions the simple Drude-like picture based on the quasiparticle concept, and the above criterion for the resistivity saturation is needed to be revised in these materials. On the theoretical ground, the lack of resistivity saturation in cuprates and alkali-doped fullerenes has been recently investigated in detail in Refs. 8–12 by means of the numerical quantum Monte Carlo and dynamical mean-field theory techniques. A simple analytical criterion, alternative to the Ioffe-Regel one, has been in addition proposed. In this alternative framework the resistivity saturation is achieved when the electron scattering rate Γ , inversely proportional to the electron lifetime τ , becomes comparable with the electron bandwidth W . In this regime the quasiparticle concept is clearly meaningless, the Drude peak is lost, and the optical conductivity $\sigma(\omega)$ is almost structureless up to energies $\omega \ll W$. By considering a general sum-rule (SR)¹³ and an opportune model for the optical conductivity $\sigma(\omega)$, Gunnarsson and co-workers^{10,12} estimated thus

$$\rho_{\text{sat}} \propto W/T_{\text{K}}, \quad (1)$$

where T_{K} is the electron kinetic energy. It is interesting to note that, unlike the Ioffe-Regel criterion which involves the comparison between *length* scales (l and a), Eq. (1) relates the resistivity saturation value to the *energy* scales W, T_{K} . Note also that Eq. (1) is quite general and specific material details, as the source of the electron scattering, are hidden in the evaluation of the electron quantities W, T_{K} . In cuprates, for instance, due to the strong electronic correlation, the amount of charge carriers, and hence of the kinetic energy, is expected to be roughly proportional to the hole doping δ , namely $T_{\text{K}} \sim T_{\text{K}}^0 \delta(1-\delta)$, where T_{K}^0 is the kinetic energy of the uncorrelated system. The limiting value of the resistivity saturation is thus expected to be significantly doping dependent $\rho_{\text{sat}} \sim \rho_{\text{sat}}^0 / \delta(1-\delta)$,¹¹ and it could in particular account for the lack of saturation in the physical range of temperature of the low doping regime.

The aim of this paper is to investigate in a more analytical way the effect of the electronic correlation on the transport properties and on the saturation phenomenon. We note that both the Ioffe-Regel criterion ($l \sim a$) and the simple model introduced by Gunnarsson and coauthors ($\Gamma \sim W/2$) do not rely on the microscopic nature on the electron scattering mechanism (impurities, phonons) or on the specific temperature dependence of it, but they are only related to the absolute magnitude of the scattering channels, parametrized by the quantity Γ . In this perspective, in the following we consider an impurity scattering mechanism where the electrons are elastically scattered by dilute paramagnetic impurities. Although the temperature dependence of the resistivity in this case is of course disregarded, this assumption is, however, sufficient to investigate the phenomenon of the resistivity saturation which, as mentioned above, depends only on the absolute value of ρ more than on its temperature dependence. In our context the impurity scattering rate Γ_0 thus plays the role of ruling the intensity of the quasiparticle scattering, in the same way as the temperature acts within the electron-phonon framework. At a first level of approximation, thus, our analysis as a function of Γ_0 can shed a useful light on the temperature dependence in other scattering mechanisms once the dependence of Γ_0 on the temperature is known ($\Gamma_0 \sim \text{const}$ for impurities, $\Gamma_0 \sim T^2$ for electron-electron scattering, and $\Gamma_0 \sim T^3$ for the electron-phonon one at low temperatures). We introduce also an approximate expression for the one-particle Green's function to take into account, in a self-consistent way, the interplay between the electronic correlation and the impurity scattering. This simple model permits one to evaluate in an analytical way the effects of the electronic correlation on one-particle quantities as the quasiparticle scattering rate Γ , the electron lifetime τ , and the kinetic energy T_K . We evaluate also the resistivity by using Kubo's formula, obtaining the behavior of the resistivity as a function of the correlation degree. We qualitatively confirm the results of Refs. 11 and 12 and we predict a significant difference, in the low doping highly correlated regime, between the quasiparticle lifetime as extracted, for instance, from angle-resolved photoemission spectroscopy and the apparent transport lifetime as extracted from resistivity measurements by using a simple Drude-like formula.

II. THE MODEL

A paradigmatic model to discuss the strong electronic correlation effects in solid state physics is the Hubbard model where propagating electrons described by Bloch-like states strongly interact with each other through a local repulsion. In the case of a single nondegenerate band the Hubbard Hamiltonian reads thus

$$H = \sum_{ij\sigma} [t_{ij} - \mu \delta_{ij}] c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_{i\sigma\sigma'} n_{i\sigma} n_{i\sigma'} \quad (2)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, t_{ij} represents tight-binding hopping elements and U describes an on site Coulomb repulsion. The chemical potential μ rules the electronic band filling n . In the

most interesting case close at half-filling ($n=1$), the complex physics of the Hubbard model can be parametrized in terms of two energy scales: the kinetic energy, which scales with the electronic bandwidth W , and the Hubbard repulsion U . The behavior of the system depends strictly on the ratio U/W , where the $U/W \ll 1$ regime describes a weakly correlated system with strong itinerant quasiparticle character, while in the $U/W \gg 1$ limit the electronic states are almost totally localized.

A standard way to describe electronic properties in interacting systems is by means of the Green's function formalism in the context of the quantum field theory. Single-particle properties are thus taken into account by Green's function $G(\mathbf{p}, \omega)$ which describes the propagation of a one-particle electronic excitation with momentum \mathbf{p} and energy ω . From a generic point of view, the interacting Green's function $G(\mathbf{p}, \omega)$ is usually described in terms of a *coherent* and an *incoherent* part:¹⁴

$$G(\mathbf{p}, \omega) = G_{\text{coh}}(\mathbf{p}, \omega) + G_{\text{inc}}(\mathbf{p}, \omega), \quad (3)$$

where $G_{\text{coh}}(\mathbf{p}, \omega)$ describes quasiparticle Bloch-like electrons for which \mathbf{p} is a good quantum number, and $G_{\text{inc}}(\mathbf{p}, \omega)$ corresponds to the incoherent background with a weak dependence on the electronic momentum: $G_{\text{inc}}(\mathbf{p}, \omega) \approx G_{\text{inc}}(\omega)$.

Different analytical approaches have been employed to deal with the Hubbard model, according to whether the main interest is paid on the coherent or the incoherent part in the strong correlated regime. An example of the first case is the Gutzwiller method,¹⁵ reproduced by the mean-field solution of the slave-boson techniques, which describes a coherent quasi-particle state with reduced spectral weight $Z (Z < 1)$ and reduced bandwidth $W^{\text{eff}} = ZW$. In the half-filling case and for U larger than a critical value $U \geq U_c$, Z vanishes describing a metal-insulator Brinkmann-Rice transition.¹⁶ From the opposite point of view, the Hubbard I (Hub-I) approximation,¹⁷ which is exact in the atomic limit, is mainly aimed at a schematic representation of the localized states, described by an upper and a lower Hubbard band spaced by an energy gap of width U . A comprehensive description of the system should account in a mixed way for both these features, as it is confirmed by numerical calculations based on the dynamical mean-field theory.¹⁸ The actual predominance of itinerant quasiparticle states or of almost localized incoherent excitations is ruled by their respective spectral weights, Z_{coh} and $Z_{\text{inc}} = 1 - Z_{\text{coh}}$, which depend on the microscopic parameters U and n . Physical properties are expected to be strongly dependent on the amount of the coherent and incoherent spectral weight.

In this paper we introduce a simple analytical model to describe the transfer of spectral weight from coherent to incoherent states, and its effects on transport properties. In explicit terms, we approximate the (unknown) coherent part $G_{\text{coh}}(\mathbf{p}, \omega)$ with the Gutzwiller solution and the incoherent term with the Hubbard I solution. The retarded Green's function reads thus¹⁹

$$G_{\text{coh}}(\mathbf{p}, \omega) = \frac{Z}{\omega - Z\epsilon_{\mathbf{p}} + \mu}, \quad (4)$$

$$G_{\text{inc}}(\omega) = \frac{1-Z}{N_s} \sum_{\mathbf{p}} \left[\frac{n/2}{\omega - \epsilon_{\mathbf{p}} n/2 + \mu + U/2} + \frac{1-n/2}{\omega - (1-n/2)\epsilon_{\mathbf{p}} + \mu - U/2} \right], \quad (5)$$

where Z is the quasiparticle spectral weight evaluated by the Gutzwiller solution for generic U and n ,²⁰ N_s is the total number of sites, and where the factor $(1-Z)$ has been explicitly introduced in the incoherent term in order to preserve the conservation of the total spectral weight. In addition, due to the quasilocated picture of the electronic states in the Hubbard bands, we have also approximated the incoherent Green's function with its local contribution, so that $G_{\text{inc}}(\omega) \simeq (1-Z)/N_s \sum_{\mathbf{p}} G_{\text{Hub-I}}(\mathbf{p}, \omega)$. We want to stress that the model introduced in Eqs. (3)–(5) is not meant to be exhaustive of all the complex phenomenology of correlated systems. However, it has the advantage to account in the simplest and analytical way for the transfer of spectral weight, here ruled by the parameter $Z(U, n)$, from coherent to incoherent states by increasing the rate of the electronic correlation. This simple model was recently employed to study the reduction of the screening properties in strongly correlated systems, leading to a predominance of forward scattering, and its interplay with the nonadiabatic superconducting pairing.²⁰ Simple arguments to understand the reduction of the screening properties in correlated systems come from the fact that the metallic screening of charge fluctuations requires the momentum \mathbf{p} to be a good quantum number and it is mainly related to the coherent states. As we are going to see, similar argumentations hold true also for transport properties.

In the following we are going to employ the model described by Eqs. (3)–(5) to investigate correlation effects on the transport properties induced by impurity scattering. As a first step toward this aim we need therefore to generalize Eqs. (3)–(5) in the presence of impurities. A phenomenological way to take into account scattering by nonmagnetic impurities is by introducing an impurity “self-energy” term $\Sigma_{\text{imp}}(\omega)$ which renormalizes the bare electronic frequency ω :

$$\omega \rightarrow \omega - \Sigma_{\text{imp}}(\omega). \quad (6)$$

The explicit expression of the electron Green's function in the presence of impurity reads thus

$$G_{\text{coh}}(\mathbf{p}, \omega) = \frac{Z}{\omega - Z\epsilon_{\mathbf{p}} + \mu - \Sigma_{\text{imp}}(\omega)}, \quad (7)$$

$$G_{\text{inc}}(\omega) = \frac{1-Z}{N_s} \sum_{\mathbf{p}} \left[\frac{n/2}{\omega - \epsilon_{\mathbf{p}} n/2 + \mu + U/2 - \Sigma_{\text{imp}}(\omega)} + \frac{1-n/2}{\omega - (1-n/2)\epsilon_{\mathbf{p}} + \mu - U/2 - \Sigma_{\text{imp}}(\omega)} \right]. \quad (8)$$

Note that, generally speaking, taking into account the impurity scattering through a “self-energy” term as done in Eqs. (6)–(8) is not formally correct since it assumes: (i) that each contribution of the Green's function (coherent part, upper and lower Hubbard band) conserves the same structure as in the absence of impurities with a simple replacing

$\omega \rightarrow \omega - \Sigma_{\text{imp}}(\omega)$; and (ii) that the “self-energy” term is the same for each of those contributions. In this way we are neglecting then the interferences between impurity and Coulomb scattering and between coherent and incoherent terms which can in principle take place. In our approach we assume Eq. (6) thus to be valid *as an approximation*. We note, however, that Eqs. (7) and (8), although approximate, are expected to work well both in the uncorrelated limit $U=0$, where the impurity self-energy $\Sigma_{\text{imp}}(\omega)$ is related to the resummation of the T -matrix of the impurity scattering, and in the highly correlated limit $W=0$ where no electronic hopping is allowed, the electrons are localized, and impurity scattering does not give rise to any decay processes [$\Sigma''_{\text{imp}}(\omega)=0$].

III. ONE-ELECTRON SELF-ENERGY AND QUASIPARTICLE LIFETIME

In the previous section we have introduced an analytical model for the electron Green's function in the presence of both electronic correlation and impurity scattering. An important feature of this model is to account in a simple way for the transfer of spectral weight between itinerant and localized states as a function of the degree of correlation. In this section we employ the model to estimate the effect of the electronic correlation on the finite quasiparticle lifetime due to the impurity scattering. In order to evaluate the impurity self-energy we assume the T -matrix resummation,²¹ which is exact for uncorrelated systems in the dilute impurity regime ($n_{\text{imp}} \ll 1$), to be valid even in the presence of electronic correlation, namely,

$$\Sigma_{\text{imp}}(\omega) = \frac{n_{\text{imp}} V_{\text{imp}}}{1 - V_{\text{imp}} G_{\text{loc}}(\omega)}, \quad (9)$$

where $G_{\text{loc}}(\omega)$ is the local Green's function:

$$G_{\text{loc}}(\omega) = \frac{1}{N_s} \sum_{\mathbf{p}} G(\mathbf{p}, \omega) = G'_{\text{loc}}(\omega) + iG''_{\text{loc}}(\omega), \quad (10)$$

and V_{imp} the electron-impurity matrix element, here assumed to be constant. Note that, unlike the case of retarded interactions, Eq. (9) relates the self-energy evaluated at the frequency ω , $\Sigma_{\text{imp}}(\omega)$, only to the Green's function evaluated at the *same* frequency, $G_{\text{loc}}(\omega)$. This gives a significant advantage because, since we are mainly interested in transport and electronic properties close to the Fermi level, it is sufficient to evaluate, in a self-consistent way, the zero frequency limit of the impurity self-energy $\Sigma_{\text{imp}}(\omega) \simeq \Sigma_{\text{imp}}(\omega=0)$, without involving the full frequency structure of $\Sigma_{\text{imp}}(\omega)$. In this perspective we approximate the impurity self-energy with only two parameters, Δ and Γ , representing, respectively, the real and imaginary part of the impurity self-energy at the Fermi level, $\Sigma_{\text{imp}} = \Delta - i\Gamma$. The impurity parameters Δ and Γ will be thus evaluated in a self-consistent way as a function of the degree of electronic correlation and of microscopic quantities as n , U and the coherent spectral weight $Z(n, U)$. We have

$$\Delta = \frac{n_{\text{imp}} V_{\text{imp}} [1 - V_{\text{imp}} G'_{\text{loc}}]}{[1 - V_{\text{imp}} G'_{\text{loc}}]^2 + [V_{\text{imp}} G''_{\text{loc}}]^2}, \quad (11)$$

$$\Gamma = - \frac{n_{\text{imp}} V_{\text{imp}}^2 G''_{\text{loc}}}{[1 - V_{\text{imp}} G'_{\text{loc}}]^2 + [V_{\text{imp}} G''_{\text{loc}}]^2}. \quad (12)$$

In the absence of electronic correlation, for an infinite bandwidth system, $G'_{\text{loc}}=0$ and $G''_{\text{loc}}=-\pi N(0)$, and we obtain the usual relations, $\Delta(U=0, W \rightarrow \infty) = \Delta_0 / \{1 + [\pi N(0) V_{\text{imp}}]^2\}$, $\Gamma(U=0, W \rightarrow \infty) = \Gamma_0 / \{1 + [\pi N(0) V_{\text{imp}}]^2\}$, where $N(0)$ is electron density of states (DOS) at the Fermi level and where $\Delta_0 = n_{\text{imp}} V_{\text{imp}}$, $\Gamma_0 = n_{\text{imp}} \pi N(0) V_{\text{imp}}^2$, are, respectively, the weak-coupling mean impurity potential and the weak-coupling impurity scattering rate.

In the following, in order to provide an analytical evaluation of the correlation effects on the impurity scattering, we employ a constant DOS model with $N(\epsilon) = N(0)$ for $|\epsilon| \leq W/2$, for which case the critical Hubbard energy is $U_c = 2W$. This constant DOS model is here meant to be representative of three-dimensional systems with structureless DOS (as the fullerenes) and also of two-dimensional systems as the cuprates provided the chemical potential are not too close to the logarithmic Van Hove singularity. Several energy scales can be identified in the system, among which the Hubbard repulsion U , the bare electron bandwidth W , the “effective” bandwidth of the coherent states $W^{\text{eff}} = ZW$, the bare impurity scattering rate $\Gamma_0 = \pi N(0) n_{\text{imp}} V_{\text{imp}}^2$, and the effective impurity scattering rate $\Gamma (\leq \Gamma_0)$ will be introduced in the following. The aim of this paper is to focus on the effects on the impurity scattering of the spectral weight transfer induced by the electronic correlation. In this perspective we consider a system where in the absence of correlation the impurity scattering rate is sufficiently small compared to the electronic bandwidth, $\Gamma_0 \ll W$, so that finite bandwidth effects can be neglected. It should be noted, however, that in the presence of electronic correlation a new electronic energy scale appears, namely the coherent quasiparticle bandwidth $W^{\text{eff}} = ZW$, in addition to the energy scales W and U which still characterize the Hubbard subbands. Close to the metal-insulator transition the shrinking of the coherent bandwidth can be so operative that $\Gamma \sim W^{\text{eff}}/2 = ZW/2$. As we are going to see, in order to preserve physical results, it is thus important that the large bandwidth limit $\Gamma_0 \ll W$ is not confused with $\Gamma/W^{\text{eff}} \ll 1$.

The impurity self-energy can now be analytically computed by using the constant DOS model. Generally speaking, both the coherent and incoherent parts of the one-particle Green’s function will contribute to the impurity self-energy (see the Appendix for an explicit expression of each contribution). As we are going to show, however, the total impurity self-energy is mainly dominated by the only coherent part. From the self-consistent evaluation of Eqs. (11) and (12) we can also determine the corresponding quasiparticle lifetime τ through the relation $\tau = \hbar/2\Gamma$, while the effective impurity potential Δ is usually disregarded since it gives just a shift of the chemical potential.

In Fig. 1 we plot the behavior of the impurity scattering rate Γ/Γ_0 (solid line, left side scale) as well as the quasiparticle scattering time τ/τ_0 (dashed line, right side scale) as a function of the amount of electronic correlation parametrized by the quasiparticle spectral weight Z . As the most represen-

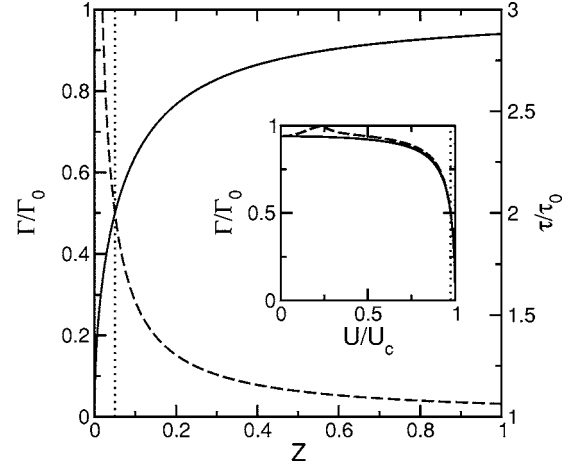


FIG. 1. Impurity scattering rate Γ/Γ_0 (solid line, left side scale) and quasiparticle lifetime τ/τ_0 (dashed line, right side scale) as a function of the quasiparticle spectral weight Z for $\mu=0$, $\Gamma_0/W=0.05$, and $\pi N(0)V_{\text{imp}}=\Gamma_0/W$. Inset: same quantity Γ/Γ_0 (solid line) plotted as a function of the reduced Hubbard repulsion U/U_c and compared to the scattering rate where the incoherent terms are fully included (dashed line) as discussed in the text. The vertical dotted lines mark the condition $\Gamma = W^{\text{eff}}/2$.

tative case of the strongly correlated regime we consider a half-filling case $\mu=0$ where $Z(U)$ is univocally determined by the Hubbard repulsion U : $Z=1$ corresponds thus to the uncorrelated limit $U=0$ while $Z \rightarrow 0$ describes the Brinkmann-Rice metal-insulator transition for $U \rightarrow U_c^-$.¹⁶ Other microscopic impurity parameters are set $\Gamma_0/W=0.05$ and $\pi N(0)V_{\text{imp}}=0.1\Gamma_0/W$. Since scattering processes are mainly determined by the coherent propagating electrons, in the evaluation of the quasiparticle scattering rate Γ we have neglected the incoherent contributions of the local Green’s function [Eqs. (A4) and (A6)]. The behavior of Γ/Γ_0 as a function of U/U_c is also shown in the inset where we compare the Γ evaluated by taking into account only the coherent part (solid line curve) with the total scattering rate including the incoherent terms (dotted line curve). The small discrepancy between the two curves points out that the scattering rate is mainly determined by the coherent part of the one-particle Green’s function. The small hump of Γ (dashed line) in the inset is due to the only incoherent part. It signals the range where the incoherent Green’s function has its highest spectral weight at the Fermi level, and it roughly corresponds to $U \approx W/2$ where a metal-insulator transition is expected in the simple Hubbard I model.

Figure 1 points out two main regimes: a low correlation regime, ruled by the parameter $2\Gamma/W^{\text{eff}} \leq 1$, where the scattering rate Γ depends very weakly on the degree of the electronic correlation; and a strong correlation regime, characterized by $2\Gamma/W^{\text{eff}} \geq 1$, where the scattering rate Γ is strongly reduced as $Z \rightarrow 0$. In this latter regime both the effective bandwidth W^{eff} of the coherent states and the scattering rate Γ vanish for $Z \rightarrow 0$, but with a different behavior, $W^{\text{eff}} \propto Z$ and $\Gamma \propto \sqrt{Z}[\Gamma(Z) \approx \sqrt{\Gamma_0 Z W / \pi}]$. In this regime the imaginary part of the one-particle self-energy is thus larger than the coherent bandwidth itself, the electronic momentum \mathbf{p} is no more a good quantum number, and the concept of quasiparticles breaks down.

On the right side scale of Fig. 1 (dashed line) we show also the corresponding quasiparticle lifetime τ , which is simply given by $\tau = \hbar/2\Gamma$. The vanishing of Γ for $Z \rightarrow 0$ corresponds thus to an infinite lifetime $\tau \rightarrow \infty$. This is understandable considering that for $Z \rightarrow 0$ the electronic system is completely localized and impurity scattering cannot trigger any decay processes. This seems in apparent contradiction with the previous scenario where we have described this regime as a nonquasiparticle one where scattering rate is larger than the bandwidth itself. We remind, however, the quasiparticle properties are ruled by the *ratio* $2\Gamma/W^{\text{eff}}$. As we have seen above, this parameter can be significantly larger, $2\Gamma/W^{\text{eff}} \gg 1$, pointing out the failure of the quasiparticle concept, even if $\Gamma \rightarrow 0$ since the effective bandwidth W^{eff} vanishes quicker than Γ for $Z \rightarrow 0$. Note that, in this perspective, the self-consistent evaluation of the impurity scattering rate Γ is fundamental to recover the correct physical limits for $Z \rightarrow 0$. If we would evaluate the impurity self-energy from Eq. (9) by using Eqs. (4) and (5) instead of Eqs. (7) and (8) we would predict indeed a finite Γ for $Z \rightarrow 0$, since the limit $\Gamma \ll W^{\text{eff}}/2$ is in this case implicitly enforced.

IV. TRANSPORT PROPERTIES

In the previous section we have found how the electronic correlation influences quasiparticle properties like the self-energy and the quasiparticle scattering time. Now we focus on transport properties of correlated systems. In particular we are interested in the resistivity ρ , or, equivalently, on the electrical conductivity $\sigma = 1/\rho$ which is evaluated as

$$\sigma = - \lim_{\omega \rightarrow 0} \frac{\text{Im } \Pi(\omega)}{\omega}, \quad (13)$$

where $\text{Im } \Pi(\omega)$ is the retarded part of the current-current correlation function,

$$\Pi(\omega) = - \frac{i\hbar}{3V_{\text{cell}}} \int_{-\infty}^{\infty} dt e^{i\omega t} \theta(t) \langle [\mathbf{j}^\dagger(t), \mathbf{j}(0)] \rangle, \quad (14)$$

and where \mathbf{j} is the current operator $\mathbf{j} = (e/N_s) \sum_{\mathbf{p}, \sigma} \mathbf{v}_{\mathbf{p}} c_{\mathbf{p}, \sigma}^\dagger c_{\mathbf{p}, \sigma}$ and V_{cell} the volume of the unit cell.

The evaluation of the conductivity requires thus the evaluation of $\Pi(\omega)$, which is in principle a two-particle function of the system. A standard way to relate $\Pi(\omega)$ to the one-particle Green's function is through a skeleton diagram expansion which can be obtained by expanding Eq. (14) as a function of the impurity scattering term. From a diagrammatic point of view, this expansion corresponds to the infinite sequence of bubble diagrams in which there are one or more impurity scatterings which link the Green's functions on both sides of the bubble (Fig. 2). In a Drude-like theory the current-current response function $\Pi(\omega)$ is approximated with the only first term of Fig. 2, in the so-called simple bubble approximation. In this scheme the dc electrical conductivity simply reads²¹

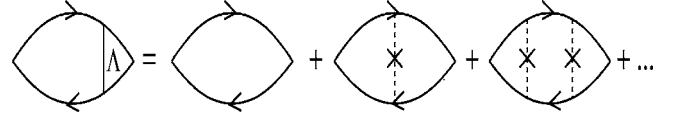


FIG. 2. Diagrammatic representation of the current-current correlation function. Solid lines represent the one-particle Green's function in the presence of impurity as given by Eqs. (7) and (8), the dashed line the interaction between electrons and impurities (crosses). We neglect here interference of scattering between two or more impurities, which is unimportant in the limit of small impurities concentration $n_{\text{imp}} \ll 1$.

$$\sigma = \frac{2\pi\hbar e^2}{3N_s V_{\text{cell}}} \sum_{\mathbf{p}} |v_{\mathbf{p}}|^2 \int d\omega A^2(\mathbf{p}, \omega) \left[- \frac{dn_{\text{F}}(\omega)}{d\omega} \right], \quad (15)$$

where $n_{\text{F}}(\omega)$ is the Fermi-Dirac distribution and $A(\mathbf{p}, \omega)$ is the electron spectral function $A(\mathbf{p}, \omega) = -(1/\pi)G''(\mathbf{p}, \omega)$. In our model for correlated systems the electronic spectral function is composed by a coherent and an incoherent term:

$$A(\mathbf{p}, \omega) = A_{\text{coh}}(\mathbf{p}, \omega) + A_{\text{inc}}(\omega), \quad (16)$$

so that the resulting conductivity contains three contributions:

$$\sigma = \sigma_{\text{coh}} + \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}. \quad (17)$$

The term σ_{coh} is associated to coherent scattering events between states with a well-defined momentum. The other two contributions are related to the incoherent part of the electronic Green's function; in particular, $\sigma_{\text{coh-inc}}$ takes into account the interference between coherent and incoherent states, while in σ_{inc} scattering processes associated to the excitations between the two Hubbard bands are considered.

By using the constant DOS model introduced above and using also a constant electron velocity $|v_{\mathbf{p}}|^2 \approx |v_{\text{F}}|^2$, we obtain

$$\sigma_{\text{coh}} = \sigma_0 \frac{\Gamma_0}{\Gamma} \frac{Z}{\pi} [I_{\text{coh}}(Z) + A(Z)], \quad (18)$$

$$\sigma_{\text{coh-inc}} = \sigma_0 \frac{4N(0)\Gamma_0(1-Z)}{\pi} I_{\text{coh}}(Z) I_{\text{inc}}(Z, U), \quad (19)$$

$$\sigma_{\text{inc}} = \sigma_0 \frac{2N(0)\Gamma_0(1-Z)^2}{\pi} I_{\text{inc}}^2(Z, U), \quad (20)$$

where

$$\sigma_0 = \frac{e^2 \hbar v_{\text{F}}^2 N(0)}{3V_{\text{cell}} \Gamma_0} \quad (21)$$

is the weak scattering ($\Gamma_0 \ll W/2$) uncorrelated electrical conductivity and where the explicit expressions of the functions I_{coh} , I_{inc} , and A are reported in the Appendix. The functions I_{coh} , I_{inc} are defined to be regular ($\sim \text{const}$) for $2\Gamma/W^{\text{eff}} \ll 1$ and $A \rightarrow 0$ in the same limit, so that the leading term in the weak scattering $\Gamma_0 \rightarrow 0$ or dilute impurity $n_{\text{imp}} \rightarrow 0$ limits is the coherent one, $\sigma_{\text{coh}} \propto \sigma_0$, while the other contributions involving incoherent spectral weight are negligible [$\sigma_{\text{coh-inc}}, \sigma_{\text{inc}} \propto \sigma_0 N(0) \Gamma_0$]. The relevance of each con-

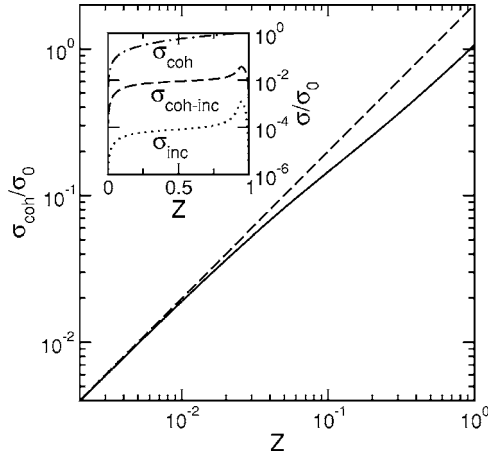


FIG. 3. Coherent contribution to the electrical conductivity σ/σ_0 from the simple bubble approximation (solid line) and asymptotic value of the coherent term in the limit $ZW/2\Gamma \ll 1$ (dashed line) as a function of the spectral weight parameter Z . Inset: comparison between the coherent and incoherent conductivity components. Microscopic parameters and details as in Fig. 1.

tribution of σ in the whole range of correlation is shown in the inset of Fig. 3 which points out that the electrical conductivity is mainly dominated by the coherent terms of the spectral function.

The dependence of only the coherent contribution to σ is also shown in the main panel of Fig. 3 on a double-logarithmic scale in order to point out the asymptotic behavior of σ in both weakly and strongly correlated regimes, respectively, $Z \rightarrow 1$ and $Z \rightarrow 0$. We find a linear behavior of the electrical conductivity with Z in both of these regimes. The weak correlation regime, characterized by $2\Gamma/W^{\text{eff}} \ll 1$, is essentially identical to the dilute impurity limit, $\Gamma \sim \Gamma_0$ (see Fig. 1) and a linear behavior $\sigma_{\text{coh}} = Z\sigma_0$ is essentially enforced by the spectral factor Z weighting the coherent processes. More delicate is the opposite case of strong correlation $Z \rightarrow 0$. In this limit, as discussed in Sec. III, the impurity scattering rate is no more than the smallest energy scale of the system since $W^{\text{eff}}/2 = ZW/2 \ll \Gamma$, and a $ZW/2\Gamma \ll 1$ expansion should be employed. Different energy scales, Γ , W^{eff} go to zero as $Z \rightarrow 0$, as the total effect of the electronic correlation of the electrical conductivity has to be determined by the asymptotic behaviors. In particular, using the asymptotic expressions $W^{\text{eff}} \sim ZW$ and $\Gamma \sim \sqrt{\Gamma_0 ZW}/\pi$ valid for $Z \rightarrow 0$, we can check in an analytical way that in the dilute limit $n_{\text{imp}} \propto 2\Gamma_0/W \ll 1$ $\sigma_{\text{coh-inc}}/\sigma_{\text{coh}} \sim \Gamma_0$ and $\sigma_{\text{inc}}/\sigma_{\text{coh}} \sim \Gamma_0^2$ (we use here also the property $U \rightarrow U_c^- \geq W/2$) so that the coherent contribution to the electrical conductivity σ_{coh} is dominant even in this regime. The asymptotic behavior of σ_{coh} as a function of Z can be determined by the same expansion, $\sigma_{\text{coh}} = 2Z\sigma_0$, resulting in a linear dependence even in this regime, although with a different prefactor. The crossover between these two opposite regimes is shown in the main panel of Fig. 3 (solid line) where the asymptotic behavior of σ_{coh} for $Z \rightarrow 0$ (dashed line) has been also superimposed.

Figure 3 shows that in both weakly and strongly correlated regimes the conductivity, which is substantially given by the coherent term, scales with the spectral weight param-

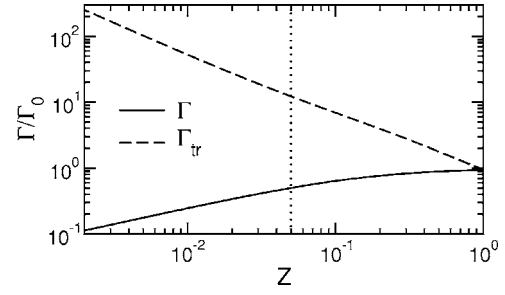


FIG. 4. Quasiparticle scattering rate (solid line) and transport scattering rate (dashed line) as a function of the spectral weight parameter Z in the half-filling case. Microscopic parameters and details as in Figs. 1 and 3.

eter Z , so that the resistivity, $\rho = 1/\sigma$, scales with the inverse of the quasiparticle spectral weight Z . In physical terms this means that as the degree of the electronic correlation is increased, the electronic states become localized, the conductivity vanishes, and the resistivity diverges.

Let us now discuss in which way the present results affect the analysis of the experimental resistivity measurements. From the experimental point of view, a common way to analyze transport properties is by means of a so-called phenomenological Drude-like model, where the electrical conductivity is expressed as²²

$$\sigma = \frac{e^2 \hbar v_F^2 N(0)}{3V_{\text{cell}} \Gamma_{\text{tr}}}, \quad (22)$$

where v_F and $N(0)$ are one-particle properties estimated by band structure calculations in the absence of electronic correlation and where Γ_{tr} represents an “effective” transport scattering rate. The same Drude-like model predicts a quasiparticle scattering rate Γ which is usually assumed to be of the same order of Γ_{tr} .

If we apply this phenomenological model to our correlated case we find an *effective* Drude-like transport scattering rate Γ_{tr} :

$$\Gamma_{\text{tr}} = \frac{\pi \Gamma}{Z[I_{\text{coh}}(Z) + A(Z)]}, \quad (23)$$

where Γ is the quasiparticle scattering rate defined in a self-consistent way by Eq. (12). Equation (23) suggests that the transport and quasiparticle scattering rates, extracted in a phenomenological way from the experimental data within a simple Drude-like model, can significantly differ from each other.

In Fig. 4 we compare the behavior of the quasiparticle Γ and of the transport scattering rate Γ_{tr} as a function of the spectral weight parameter Z . As mentioned above, Γ_{tr} differs significantly from the quasiparticle scattering rate Γ for any finite degree of electronic correlation and they approach the same value only in the uncorrelated limit $Z \rightarrow 1$.

V. RESISTIVITY SATURATION AND CORRELATION EFFECTS

So far our analysis has focused on the effects of the electronic correlation on the quasiparticle and transport proper-

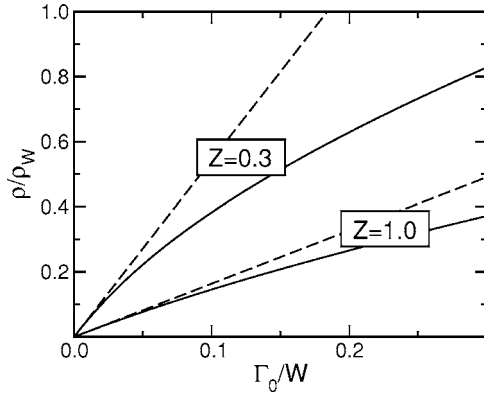


FIG. 5. Dependence of the dc resistivity as a function of the bare impurity scattering rate for two values of the amount of electronic correlation (solid lines). The dc resistivity is plotted in units of $\rho_W = 3V_{\text{cell}}W/e^2\hbar v_F^2 N(0)$ and Γ_0 in units of W . The dashed lines represent the linear asymptotic behavior in the weak $\Gamma_0 \rightarrow 0$ limit.

ties in a regime where the coherent part of the Green's function is found to dominate (zero temperature, low impurity concentration). The resistivity saturation phenomenon on the other hand is expected to appear in the opposite regime where quasiparticle properties are poorly defined. In anelastic scattering mechanism (phonons, electron-electron Coulomb interaction, ...) this regime is usually achieved at large temperature. A similar role is played in our approach by the bare impurity scattering rate Γ_0 which rules the broadening of the quasiparticle peak and the balance between coherent and incoherent contributions. The resistivity as a function of Γ_0 is shown in Fig. 5 at half-filling for the uncorrelated case ($U=0$, $Z=1$) and for an intermediate-highly correlated case ($U/U_c=0.84$, $Z=0.3$). In low impurity scattering regime, where quasiparticle properties are well-defined and the conductivity is mainly related to the coherent part, the resistivity increases linearly with Γ_0 according to Eqs. (18) and (21). In this framework the appearing of resistivity saturation is signalized by the sublinear behavior pointed out in Fig. 5. In the presence of electronic correlation the magnitude of the resistivity is enhanced, the sublinear behavior is more pronounced, and it appears for smaller values of Γ_0 .

As briefly mentioned in the Introduction, a simple criterion for determining the value of the resistivity saturation ρ_{sat} in a noncorrelated system was presented in Ref. 10. In this analysis the resistivity saturation is achieved when the spread of the Drude peak is of the same order of the bandwidth W and the optical conductivity is described by a featureless structure up to the energy scale W . A simple sum rule gives thus $\rho_{\text{sat}}^{\text{SR}} \propto W/T_K$, where T_K is the electronic kinetic energy. This model was also applied to strongly correlated systems, as the cuprates.¹¹ In this case, assuming a bandwidth independent of the degree of correlation, the scaling of the kinetic energy with the number of the hole doping $T_K \propto \delta$ would predict an increase of the resistivity saturation value as $\delta \rightarrow 0$, in agreement with the experiments. However, the assumption of a constant bandwidth W independent of the electronic correlation is somehow questionable since the same coherent excitations which are involved in the Drude-like peak are expected to probe a renormalized dispersion

with the effective bandwidth $W^{\text{eff}}=ZW$. Two different arguments can be invoked for justifying both the employing of W and of $W^{\text{eff}}=ZW$ in this simple model. They depends, respectively, upon two different pictures of the underlying physics. In the first case we assume that the coherent processes are dominant, and the loss of the Drude peak is due to the broadening of the peak itself. In this case the bandwidth parameter is consistently given by $W^{\text{eff}}=ZW$ and resistivity saturation is expected to be achieved when $\Gamma \sim W^{\text{eff}}/2$. In an alternative scenario we can imagine that a narrow Drude-like peak is still present in the saturation regime, but with a vanishing spectral weight so that the dominant contribution to the optical conductivity is given by the incoherent scattering. A reasonable choice of the appropriate bandwidth parameter is thus W . The consequences of the different choices are evident by considering that in the first case the scaling of the effective bandwidth itself with δ (or Z) would cancel the similar dependence of T_K giving a value of ρ_{sat} independent of the electronic correlation, whereas only in the second case the scaling $\rho_{\text{sat}} \sim 1/\delta$ proposed in Ref. 11 would be operative.

Our model permits us to check on an analytic ground both pictures. In particular, as representative of the saturation conditions, we calculate the value of the resistivity as a function of the correlation parameter Z by using Eqs. (18)–(20): in the first case for $\Gamma = W^{\text{eff}}/2$, which expresses the condition that the broadness of the Drude peak extends over the entire effective bandwidth, in the second case for $\sigma_{\text{coh}} = \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$, which determines the crossover at which the incoherent contributions to the electrical conductivity become of the same order of the coherent one. We compare these results with the ones obtained by employing the SR model of Ref. 10,

$$\rho_{\text{sat}}^{\text{SR}} = \frac{3V_{\text{cell}}}{8\pi e^2 \hbar v_F^2 N^2(0)} \frac{\tilde{W}}{T_K}, \quad (24)$$

with a proper choice of the appropriate bandwidth. In particular we evaluate the electron kinetic energy as

$$T_K = \frac{1}{N_s} \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \int d\omega n_{\mathbf{F}}(\omega) \left[-\frac{1}{\pi} \text{Im} G(\mathbf{p}, \omega) \right], \quad (25)$$

where the quasiparticle impurity scattering rate Γ in the Green's function $\text{Im} G(\mathbf{p}, \omega)$ has been assumed to be frequency-independent, $\Gamma(\omega) = \Gamma(\omega=0)$, in agreement with the previous approximation. It is easy to see that only coherent excitations contribute to T_K , so that $T_K \approx ZT_K^0$, where T_K^0 is the kinetic energy in the absence of correlation. As mentioned above, more delicate is a proper definition of bandwidth in both cases. Following Ref. 10, we relate the effective bandwidth to the lowest order momentum of the dispersion, in particular in the first case

$$\tilde{W}^{\text{eff}} = \frac{4}{N_s} \sum_{\mathbf{p}} |\epsilon_{\mathbf{p}}| \int d\omega \left[-\frac{1}{\pi} \text{Im} G_{\text{coh}}(\mathbf{p}, \omega) \right], \quad (26)$$

and in the second case

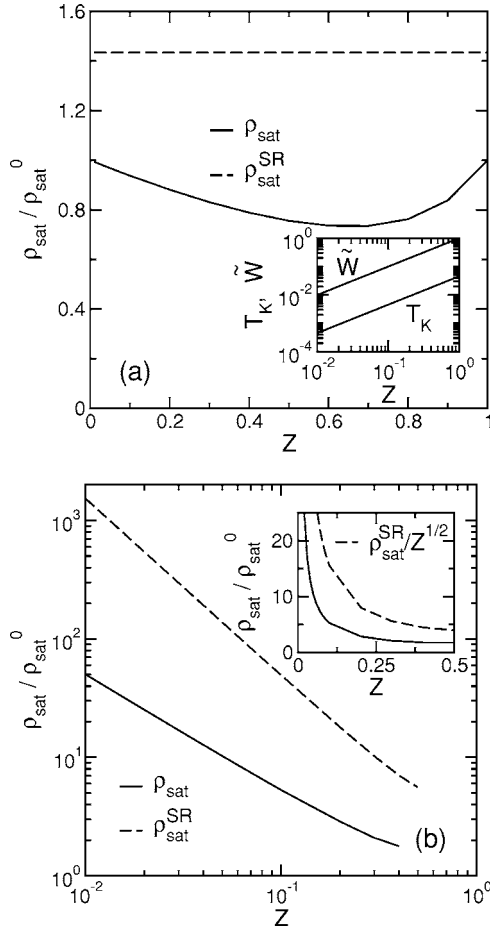


FIG. 6. (a) Value of the resistivity saturation as a function of Z evaluated in an explicit way by Eq. (15) (solid line) and by using the SR model [Eq. (24), dashed line] with the condition $\Gamma = W^{\text{eff}}/2$. Inset: linear behavior of T_K and $\tilde{W} = W^{\text{eff}}$ as a function of Z . (b) Resistivity saturation limit as a function of Z , as above, under the condition $\sigma_{\text{coh}} = \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$. Inset: as in the main picture, on a linear scale, with $\rho_{\text{sat}}^{\text{SR}}$ divided by \sqrt{Z} (see text).

$$\tilde{W}^T = \frac{4}{N_s} \sum_{\mathbf{p}} |\epsilon_{\mathbf{p}}| \int d\omega \left[-\frac{1}{\pi} \text{Im} G(\mathbf{p}, \omega) \right]. \quad (27)$$

It is easy to check that the above definitions give the correct result for the constant DOS model here considered in the noninteracting uncorrelated case, while in the presence of correlation we recover $\tilde{W}^T = W$ and $\tilde{W}^{\text{eff}} = ZW$. A slight modification has been employed with respect to Ref. 10, namely to relate the bandwidth parameters to the first momentum of the electronic dispersion more than to the second one, in order to recover the correct scaling $\tilde{W}^{\text{eff}} \propto Z$.

In Fig. 6 we compare the direct calculation of the resistivity saturation value with the SR model in both cases. All the resistivity values are expressed in terms of a “bare” resistivity saturation value,

$$\rho_{\text{sat}}^0 = \frac{3V_{\text{cell}}}{\hbar e^2 v_F^2 N^2(0) [1 + 2/\pi]}, \quad (28)$$

which represents the saturation value expected for an infinite bandwidth uncorrelated system, and which depends only on

structural and band-structure properties. As discussed above, the criterion for the resistivity saturation has been determined by $\Gamma = W^{\text{eff}}/2$ in the first case (panel a) and by $\sigma_{\text{coh}} = \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$ in the second case (panel b). The agreement between the direct calculation of the electrical resistivity by means of Kubo’s formula Eqs. (15) and the SR model is quite good considering the simplicity of the SR model.

Figure 6(a) describes the case where the coherent part of the electrical conductivity is predominant and the resistivity saturation is driven by the broadening of the Drude-like peak. The disappearing of the spectral weight Z in this case is accompanied by a similar scaling of T_K , $\tilde{W}^{\text{eff}} \propto Z$ (see inset). These two similar dependences cancel each other both in the SR model and in the coherent contribution of Eq. (15), yielding a resistivity saturation value independent of the correlation degree. The weak dependence of ρ_{sat} on Z in the direct evaluation of the resistivity saturation by using Eq. (15) is indeed due to the small incoherent contributions to the transport properties and it would not be present if only the coherent part would be taken into account.

The alternative scenario for saturation is shown in Fig. 6(b) where the criterion for resistivity saturation is related to the predominance of the incoherent parts of the conductivity. In this case the vanishing amount of coherent states, evaluated by T_K ($T_K \rightarrow 0$ for $Z \rightarrow 0$), is not compensated by a corresponding reduction of the effective bandwidth \tilde{W}^T , and the resistivity saturation value ρ_{sat} is expected to diverge as the correlation effects increase $Z \rightarrow 0$. Once more, these simple physical argumentations, employed in the simple SR model, give a qualitative insight which agrees in a satisfactory way with the explicit calculation of the resistivity through Kubo’s formula, Eq. (15), although the scaling law is different. In particular the explicit calculation of ρ from Eq. (15) predicts an inversely proportional dependence of ρ_{sat} as a function of the spectral weight Z , $\rho_{\text{sat}} \propto 1/Z$, whereas $\rho_{\text{sat}}^{\text{SR}} \propto 1/Z^{3/2}$. This discrepancy is related to the somehow anomalous behavior of T_K , $T_K \propto Z^{3/2}$, which stems from the fact that, in the strongly correlated limit $Z \rightarrow 0$, $W^{\text{eff}} \ll \Gamma$ ($W^{\text{eff}} \propto Z, \Gamma \propto \sqrt{Z}$) and $T_K \propto W^{\text{eff}}\Gamma$. In the inset of Fig. 6(b) we compare thus the explicit evaluation of ρ_{sat} from Eq. (15) with $\rho_{\text{sat}}^{\text{SR}}/\sqrt{Z}$, showing indeed a good agreement between the two quantities.

Summarizing the present results, we have investigated the dependence of the resistivity saturation in two alternative scenarios. In the first case the resistivity saturation is achieved when the coherent Drude-like peak broadens over the coherent bandwidth, ruled by the condition $\Gamma \approx ZW/2$. In the second case the resistivity saturation is expected to appear when the incoherent contributions to the electrical conductivity become dominant with respect to the coherent one, and it is related to the regime $\sigma_{\text{coh}} \approx \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$. We have shown that in the first scenario the resistivity saturation value is essentially independent of the degree of electronic correlation, and it could not account for the experimental lack of saturation in the underdoped region of cuprates. On the other hand, the resistivity saturation is expected to scale in the second scenario with the reduced spectral weight Z due to the correlation effects, $\rho_{\text{sat}} \propto 1/Z$. This result is in a good agreement with recent experimental data by Takenaka *et al.*,⁷ which nicely show the $\rho_{\text{sat}} \propto 1/Z$ behavior of the dc resistiv-

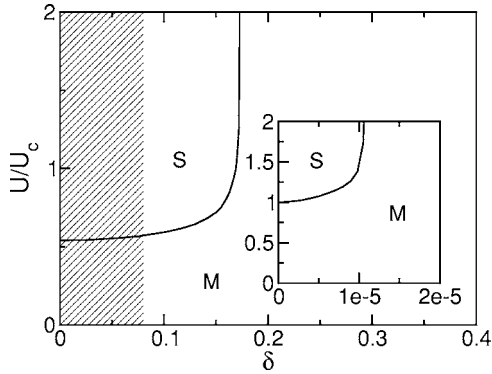


FIG. 7. Phase diagram for the saturation effects in the U vs δ space. The label S indicates regions where saturation occurs according the condition $\sigma_{\text{coh}} < \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$, while in the M region the system presents Drude-like metallic behavior. Main frame: $\Gamma_0/W=1.0$; inset: $\Gamma_0/W=0.05$. In both cases $\pi N(0)V_{\text{imp}}=0.005$.

ity in the low doping region $0 < x < 0.3$ where the spectral weight Z itself is expected to scale with x , $Z \propto x$.²³ Similar results were also found by numerical calculation based on the exact diagonalization technique.¹¹

The resulting phase diagram in the U - δ space for the relevance of the saturation effects is shown in Fig. 7. According the above discussion the criterion for saturation has been determined by the condition $\sigma_{\text{coh}} = \sigma_{\text{coh-inc}} + \sigma_{\text{inc}}$. Here the label M indicates the region where the conductivity is dominated by the coherent part and the system behaves like a strongly correlated metal but with metallic characteristics, while in the S region the incoherent contributions prevail and the saturation behavior is expected. Since the coherent and incoherent contributions to the conductivity scale in a different way with the bare impurity scattering rate $\sigma_{\text{coh}} \propto 1/\Gamma_0$, $\sigma_{\text{coh-inc}}, \sigma_{\text{inc}} \sim \text{const}$, the balance is strongly dependent on Γ_0 . In the main frame of Fig. 7 we show the phase diagram for a sizable scattering rate $\Gamma_0/W=0.1$, where saturation effects extend up to $\delta \sim 0.175$ in the correlated regime. The shadow area points out qualitatively the region where Van Hove singularity effects are expected in the two-dimensional tight-binding model appropriate for cuprates and where the constant DOS model is expected to fail. The inset shows also the very weak impurity case $\Gamma_0/W=0.05$. In this case the coherent part is almost always dominant and strong correlation effects, for $U \geq U_c$ and $\delta \sim 0$ where $Z \rightarrow 0$, are needed in order to show saturation. We remind that in the generalization of the present analysis to the electron-phonon scattering mechanism, the scattering rate Γ_0 plays the role of the temperature dependent scattering rate, which can be easily of the order of the bandwidth $\Gamma_0^{\text{el-ph}}(T)/W$ for large enough temperatures.

VI. CONCLUSION

The aim of this work has been to investigate electronic correlation effects on the quasiparticle and transport properties. A key role in this context is thought to be played by the reduction of the coherent spectral weight accompanied by the onset of localized state. For instance, the lack of resistiv-

ity saturation at the Mott-Ioffe-Regel limit in cuprates superconductors has been recently related to an effective renormalization of single-particle quantities, as the kinetic energy, due to the strong electronic correlation. Although some analytical models based on a sum rule conservation have been proposed, the effects of the electronic correlation have been mainly studied by means of numerical approaches.

In this paper we have introduced a simple phenomenological model in order to describe in an analytical way the transfer of spectral weight from coherent to incoherent states as the degree of electronic correlation is increased. We have studied the interplay between electronic correlation and impurity scattering in quasiparticle and transport properties. We identify two different regimes, a low correlated regime, where the effective bandwidth of coherent states is much greater than the impurity scattering rate, and a highly correlated regime where the renormalization effects induced by the electronic correlation yield an effective coherent bandwidth W^{eff} smaller than the impurity scattering rate itself. Contrary to what one should expect, correlation effects in this latter regime increase the quasiparticle life-time.

We have also evaluated the electrical resistivity by means of the current-current response function. Within the simple bubble approximation, we have shown that correlation effects enhance the resistivity ρ (suppress the conductivity σ) according the scaling law $\rho \propto 1/Z$ in both low and highly correlated regimes. This result suggests that the ‘‘phenomenological’’ quasiparticle and transport scattering rate, respectively, Γ and Γ_{tr} , as extracted by the experiment within a quasiparticle analysis, should scale in an opposite way upon the relevance of the electronic correlation. Our analysis permits one in addition to test in a direct way some predictions of a simple sum-rule model employed to describe the resistivity saturation limit. We found that the lack of resistivity saturation in cuprates can be interpreted as an effective enhancement of the saturation limit as correlation effects are increased approaching the half-filling case, in agreement with Ref. 11. This regime is, however, achieved when the incoherent contributions to the electrical conductivity become of the same order to the coherent one.

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APPENDIX: ANALYTICAL EXPRESSIONS FOR SOME COHERENT AND INCOHERENT ONE-PARTICLE AND TWO-PARTICLE QUANTITIES

In this appendix we summarize and provide the analytical expressions for some one- and two-particle quantities which have been employed in the previous sections. We first consider the impurity self-energy defined in Eqs. (11) and (12), which are expressed as a function of the real and imaginary part of the local electron Green’s function, respectively, $G'_{\text{loc}} \equiv \text{Re } G_{\text{loc}}(\omega=0)$ and $G''_{\text{loc}} \equiv \text{Im } G_{\text{loc}}(\omega=0)$. Both of them

are characterized by a coherent and an incoherent contribution. Simple analytical expressions for these quantities can be obtained from Eqs. (4) and (5):

$$G'_{\text{loc}} = R_{\text{coh}} + R_{\text{inc}}, \quad (\text{A1})$$

$$G''_{\text{loc}} = I_{\text{coh}} + I_{\text{inc}}, \quad (\text{A2})$$

where

$$R_{\text{coh}} = \frac{1}{2} \log \left[\frac{(ZW/2 - \mu)^2 + \Gamma^2}{(ZW/2 + \mu)^2 + \Gamma^2} \right], \quad (\text{A3})$$

$$R_{\text{inc}} = \frac{1}{2} \left\{ \log \left[\frac{[(1 - n/2)W/2 - \mu + U/2]^2 + \Gamma^2}{[(1 - n/2)W/2 + \mu - U/2]^2 + \Gamma^2} \right] + \log \left[\frac{(nW/4 - \mu - U/2)^2 + \Gamma^2}{(nW/4 + \mu + U/2)^2 + \Gamma^2} \right] \right\}, \quad (\text{A4})$$

$$I_{\text{coh}} = \arctan \left[\frac{ZW/2 - \mu}{\Gamma} \right] + \arctan \left[\frac{ZW/2 + \mu}{\Gamma} \right], \quad (\text{A5})$$

$$I_{\text{inc}} = \left\{ \arctan \left[\frac{(1 - n/2)W/2 - \mu + U/2}{\Gamma} \right] + \arctan \left[\frac{(1 - n/2)W/2 + \mu - U/2}{\Gamma} \right] + \arctan \left[\frac{nW/4 - \mu - U/2}{\Gamma} \right] + \arctan \left[\frac{nW/4 + \mu + U/2}{\Gamma} \right] \right\}. \quad (\text{A6})$$

Some of the same quantities are employed also in the definition of the electrical conductivity as well as in the transport impurity scattering rate evaluated in the simple bubble approximation, respectively, Eqs. (18)–(20) and (23), together with the quantity

$$A = \Gamma \left[\frac{ZW/2 - \mu}{(ZW/2 - \mu)^2 + \Gamma^2} + \frac{ZW/2 + \mu}{(ZW/2 + \mu)^2 + \Gamma^2} \right]. \quad (\text{A7})$$

¹A. F. Ioffe and A. R. Regel, *Prog. Semicond.* **4**, 237 (1960).

²N. F. Mott, *Metal-Insulator Transitions*, 2nd ed. (Taylor and Francis, London, 1990).

³Z. Fisk and G. W. Webb, *Phys. Rev. Lett.* **36**, 1084 (1976).

⁴Y. Ando, A. N. Lavrov, S. Komiya, K. Segawa, and X. F. Sun, *Phys. Rev. Lett.* **87**, 017001 (2001).

⁵A. F. Hebard, T. T. M. Palstra, R. C. Haddon, and R. M. Fleming, *Phys. Rev. B* **48**, 9945 (1993).

⁶H. Takagi, B. Batlogg, H. L. Kao, R. J. Cava, J. J. Krajewski, and W. F. Peck, Jr., *Phys. Rev. Lett.* **69**, 2975 (1992).

⁷K. Takenaka, J. Nohara, R. Shiozaki, and S. Sugai, *Phys. Rev. B* **68**, 134501 (2003).

⁸A. J. Millis, J. Hu, and S. Das Sarma, *Phys. Rev. Lett.* **82**, 2354 (1999).

⁹O. Gunnarsson and J. E. Han, *Nature (London)* **405**, 1027 (2000).

¹⁰M. Calandra and O. Gunnarsson, *Phys. Rev. B* **66**, 205105 (2002).

¹¹M. Calandra and O. Gunnarsson, *Europhys. Lett.* **61**, 88 (2003).

¹²O. Gunnarsson, M. Calandra, and J. E. Han, *Rev. Mod. Phys.* **75**, 1085 (2003).

¹³P. F. Maldague, *Phys. Rev. B* **16**, 2437 (1977).

¹⁴A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinsky, *Methods*

of Quantum Field Theory in Statistical Physics (Dover, New York, 1963).

¹⁵M. C. Gutzwiller, *Phys. Rev. Lett.* **10**, 159 (1963).

¹⁶W. F. Brinkmann and T. M. Rice, *Phys. Rev. B* **2**, 4302 (1970).

¹⁷J. Hubbard, *Proc. R. Soc. London, Ser. A* **276**, 238 (1963).

¹⁸A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).

¹⁹Since in this paper we mainly use only retarded Green's functions, unless explicitly stated, the frequency ω is understood to contain an infinitesimally small imaginary part $\omega \equiv \omega + i0^+$. Such an infinitesimally small imaginary part of course does not play any role when a finite imaginary self-energy is present.

²⁰L. Boeri, E. Cappelluti, C. Grimaldi, and L. Pietronero, *Phys. Rev. B* **68**, 214514 (2003).

²¹G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluwer Academic, New York, 2000).

²²T. Timusk and B. W. Statt, *Rep. Prog. Phys.* **62**, 61 (1999).

²³T. Yoshida, X. J. Zhou, T. Sasagawa, W. L. Yang, P. V. Bogdanov, A. Lanzara, Z. Hussain, T. Mizokawa, A. Fujimori, H. Eisaki, Z.-X. Shen, T. Kakeshita, and S. Uchida, *Phys. Rev. Lett.* **91**, 027001 (2003).