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Impurity induced resistivity upturns in underdoped cuprates

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ABSTRACT

Impurity induced low temperature upturns in both the *ab*-plane and the *c*-axis dc-resistivities of cuprates in the pseudogap state have been observed in experiments. We provide an explanation of this phenomenon by incorporating impurity scattering of the charge carriers within a phenomenological model proposed by Yang, Rice and Zhang. The scattering between charge carriers and the impurity atom is considered within the lowest order Born approximation. Resistivity is calculated within Kubo formula using the impurity renormalized spectral functions. Using physical parameters for cuprates, we describe qualitative features of the upturn phenomena and its doping evolution that coincides with the experimental findings. We stress that this effect is largely due to the strong electronic correlations.

1. Introduction

Unlike conventional superconductors following BCS mechanism, many aspects of materials showing high temperature superconductivity are still poorly understood. Example of such materials includes hole doped cuprates which show superconductivity at higher temperature. These materials show a very rich phase diagram when carrier doping and temperature vary. These materials not only lack a proper microscopic description of superconducting transition in them, but also their normal phases above the transition temperature are poorly understood. In the over doped regime, electrons in these materials behave in a Fermi liquid manner, while a major deviation from this behavior is observed at optimal doping as well as in the underdoped regime. At low temperature, among many puzzling observations, presence of a *pseudogap* along with the superconducting gap in the electronic spectra is observed in this regime [1]. Microscopic origin of the pseudo-gap is still debatable. However there is hardly any doubt that many unconventional electronic behaviors are associated with its presence [2]. Here we focus on understanding some anomalous charge transport properties of these materials in the underdoped regime at low temperature.

The effects of pseudo-gap and impurity scattering in dc-resistivities of cuprates in the underdoped regime is of our concern here. It is well studied in the experimental literature both in presence and absence of impurities [3–5]. Universal linear in temperature behavior of dc-resistivity at optimal doping and its deviation both in the underdoped ($\rho \sim \log(1/T)$) and overdoped ($\rho \sim T^2$) regimes become hallmarks for cuprates. The upturn behavior gets enhanced when cuprates are further doped with impurities and reminds us a Kondo-like mechanism as its origin. Theoretical explanation of it is not settled yet and is highly debatable [6]. However, basic elements of theory of such upturn phenomena should contain two elements seriously. The first is the reconstruction of Fermi-surface and the presence of pseudo-gap in electronic density of states due to strong electron–electron correlations. This leads to non-Fermi liquid like behavior in the underdoped cuprates. Second is the scattering of those non-Fermi liquid quasiparticles with impurity atoms at low temperature. We incorporate these two important features within a semi-phenomenological theory in the present study.

Here we limit ourselves to the situations where cuprates are doped with non-magnetic impurities only. Experimentally, cuprates are further doped with non-magnetic Zn ions which replace few Cu ions from Cu–O plane and provide a scattering center for charge carriers. Doped Zn ions reduce superconducting correlations to certain extent. Also a magnetic field of suitable strengths (up-to $\sim$50–60T) are used to exclude the contributions due to superconducting correlations. This sets the platform for studying normal state properties of cuprates which often shows non-Fermi liquid behavior, particularly in the under-doped regime. It is also to be mentioned that, effects similar to the Zn doping can be achieved by another method such as electron irradiation with suitable fluence [6]. In the later case one creates point defects in the Cu–O plane and the gross features of the resistivity behavior in this case is almost the same as that of Zn substituted one. In such an experimental condition, depending on impurity concentrations, an impurity induced supra-linear in T ($\rho \sim T^{\nu}$, $\nu < 1$) to $\log(1/T)$ upturn in the resistivity is observed [7,8]. The later

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phenomenon hints at localization onset and is often attributed to strong electron–electron correlations, spin fluctuation effects, impurity induced electronic inhomogeneity [9–11]. Since a detailed microscopic theory for underdoped cuprates still lacking, logical direction in understanding this material is to use a phenomenological theory based on experimental inputs. Recently Yang, Rice and Zang [13,12] proposed a phenomenological model which can be used to understand properties of electronic behavior in the underdoped regime. This theory is quite successful in understanding many thermodynamic properties and ARPES findings [12] and also transport properties like optical conductivity [14,15] etc. in the recent past. We adopt it as a model non-Fermi liquid description suitable to study low temperature behavior of normal state resistivity in cuprates in presence of a pseudo-gap. For the rest of our discussion we will call it "YRZ" formalism and in the later section we present a brief review of it. In this work, we show that, without adopting additional inputs one can observe resistivity upturns within YRZ formalism. Also the present study reveals the importance of pseudo-gap to this phenomena.

This paper is organized as follows. In Section 2 we first review the YRZ formalism as proposed by Yang, Rice and Zang [13,12]. and then derive an expression for the dc-resistivity using Kubo formalism and considering the scattering of YRZ-quasiparticles with non-magnetic impurities. Then in Section 3, we numerically evaluate the expression for the dc-resistivity and discuss the results. Finally, in Section 4 we summarize our results and conclude.

2. YRZ-quasiparticles and impurity scattering

In the presence of a pseudogap, YRZ formalism is defined with the following ansatz for the coherent part of the electronic self-energy based on a resonating valence bond (RVB) spin liquid [13, 12].

$$\Sigma^{YRZ}(\mathbf{k},\omega,x) = \frac{\Delta_{pg}^2}{\omega+\epsilon_{\mathbf{k}}^0} \tag{1}$$

Thus the quasiparticle propagator or Green's function in this formalism takes the form,

$$\mathcal{G}(\mathbf{k},\omega,x) = \frac{g_t(x)}{\omega-\epsilon_{\mathbf{k}}-\frac{\Delta_{pg}^2}{\omega+\epsilon_{\mathbf{k}}^0}}. \tag{2}$$

The interaction renormalized band–structure dispersion is given as $\epsilon_{\mathbf{k}} = -2t(x)(\cos(k_x a)+\cos(k_y a)) - 4t'\cos(k_x a)\cos(k_y a) - 2t''\times(\cos(2k_x a)+\cos(2k_y a)) - \mu_p(x)$. Here a is the unit cell dimension in the Cu–O plane. Electronic energy band is defined by the renormalized parameters, $t(x) = g_t(x)t_0 + 3g_s(x)J\chi/8$, $t'(x) = g_t(x)t_0'$ and $t''(x) = g_t(x)t_0''$. The Gutzwiller factors which constrain electronic motion in an interacting environment are given by $g_t(x) = \frac{2x}{1+x}$ and $g_s(x) = \frac{4}{(1+x)^2}$. Here, t_0, t_0', and t_0'' are the bare band hopping parameters with $t_0' = -0.3t_0$ and $t_0'' = 0.2t_0$. J is the magnetic energy of the t–J model taken to be $J = t_0/3$, $\chi = 0.338$ is the spin susceptibility. $\epsilon_{\mathbf{k}}^0 = -2t(x)(\cos(k_x a)+\cos(k_y a))$ is a second energy dispersion which gives the antiferromagnetic Brillouin zone boundary for $\epsilon_{\mathbf{k}}^0 = 0$, which is also referred to as the umklapp surface. The shift in chemical potential $\mu_p(x)$ is to be determined to get the correct hole doping x based on the Luttinger sum rule. Self-energy contains a phenomenological input for pseudo-gap energy scale and is given as, $\Delta_{pg}(x) = \Delta_{pg}^0(x)(\cos(k_x a)-\cos(k_y a))/2$, where $\Delta_{pg}^0(x) = 3t_0(0.2-x)$. In this description $x = 0.2$ is the optimal doping and we restrict to the regime $x < 0.2$. In the normal state, the quasiparticle propagator can be written in a form,

$$\mathcal{G}(\mathbf{k},\omega,x) = \sum_{\alpha=\pm1}\frac{g_t(x)W_{\mathbf{k}}^{\alpha}(x)}{\omega-E_{\mathbf{k}}^{\alpha}(x)}. \tag{3}$$

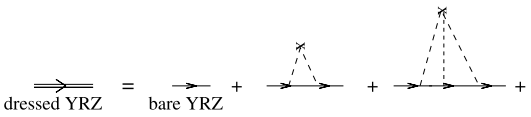

Fig. 1. Diagram representing renormalized quasiparticle propagator due to impurity scattering in the Born approximation. Second and the third diagrams in the right hand side represent impurity induced self-energy corrections. In the present work we consider the lowest order correction, i.e. up-to the second diagram in the right hand side.

Above form describes YRZ quasiparticles by the energy dispersions,

$$E_{\mathbf{k}}^{\alpha}(x) = \frac{\xi_{\mathbf{k}}^-}{2} + \alpha\sqrt{\left(\frac{\xi_{\mathbf{k}}^+}{2}\right)^2 + \Delta_{pg}^2(x)}, \tag{4}$$

and the Luttinger weights are given as,

$$W_{\mathbf{k}}^{\alpha}(x) = \frac{1}{2}\left(1+\alpha\frac{1}{2}\frac{\xi_{\mathbf{k}}^+}{\sqrt{\left(\frac{\xi_{\mathbf{k}}^+}{2}\right)^2+\Delta_{pg}^2(x)}}\right). \tag{5}$$

Here $\alpha = \pm1$ and $\xi_{\mathbf{k}}^{\pm} = \epsilon_{\mathbf{k}} \pm \epsilon_{\mathbf{k}}^0$. We consider scattering of YRZ-quasiparticles with non-magnetic impurities in the first Born Approximation. They provide scattering centers for quasiparticles and changes their lifetime via impurity contribution to the self-energy. Diagrammatic representation of the self-energy correction due to impurity scattering is shown in Fig. 1. Here arrowed parallel lines in the left hand side represent impurity renormalized propagator. The first diagram in the right hand side is the bare YRZ propagator as given by Eq. (3) and the third term represents self-energy corrections to the carrier propagator due to its interaction with impurities at the lowest order. The later is given as [21],

$$\begin{aligned}\Sigma_{imp}(\mathbf{k},i\omega_n) &= N_i\sum_{\mathbf{k}'}\left|v(\mathbf{k}-\mathbf{k}')\right|^2\mathcal{G}(\mathbf{k}',i\omega_n)\\ &\approx \rho v^2\frac{1}{\mathcal{V}}\sum_{\mathbf{k}'}\mathcal{G}(\mathbf{k}',i\omega_n)\\ &= \rho v^2\frac{1}{\mathcal{V}}\sum_{\alpha=\pm}\sum_{\mathbf{k}'}\frac{g_t(x)W_{k'}^{\alpha}}{i\omega_n-E_{k'}^{\alpha}}.\end{aligned} \tag{6}$$

Here impurities potential is assumed to be highly localized i.e. given by $v(\mathbf{r}) = v\delta(r)$. This is justified when doped ions sit in the Cu–O plane and charge carriers screen the Coulomb potential. Impurity density $N_i/\mathcal{V}$ is given by ρ and $\mathcal{V}$ is the system volume. After performing an analytical continuation we get the frequency dependent impurity self-energy as,

$$\begin{aligned}\Sigma_{imp}(\omega) &= \sum_{\alpha=\pm}\sum_{\mathbf{k}'}\frac{\tilde{W}_{k'}^{\alpha}}{\omega-E_{k'}^{\alpha}+i\eta}\\ &= \sum_{\alpha=\pm}\sum_{\mathbf{k}'}\frac{\tilde{W}_{k'}^{\alpha}}{\omega-E_{k'}^{\alpha}} - i\pi\sum_{\alpha=\pm}\sum_{\mathbf{k}'}\tilde{W}_{k'}^{\alpha}\delta(\omega-E_{k'}^{\alpha}),\end{aligned} \tag{7}$$

where $\tilde{W}_k^{\alpha} = \rho v^2 g_t(x)W_k^{\alpha}/\mathcal{V}$. This will be different from that of non-interacting case. In case of normal metal, and for constant electronic density of states, the real part of the Born self-energy vanishes, while imaginary part of it becomes constant [22]. That is not necessarily the case here. We see from the above equation that,

$$\begin{aligned}Im\Sigma_{imp}(\omega) &= -\pi\sum_{\alpha=\pm}\sum_{\mathbf{q}}\tilde{W}_q^{\alpha}\delta(\omega-E_q^{\alpha})\\ &= -\rho v^2 N^{YRZ}(\omega).\end{aligned} \tag{8}$$