On the Theory of Kinetic Phenomena in 2D Doped Antiferromagnet with Strong Spin–Hole Interaction

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Abstract The problem of constructing the kinetic equation for a hole motion in systems with strong spin-hole interaction (such as HTSC) is treated in terms of the spin polaron concept for a regular 2d antiferromagnetic (AFM) s–d model. It is shown that kinetics is determined by the properties of the spin polaron bands (rather than “bare hole”) for which the hole residues Z_k can be far from 1. In both cases of low and optimal doping, the obtained electrical resistivity $\rho(T)$ and Hall coefficient $R(T)$ T -dependence demonstrates qualitative agreement with experimental data if we take into account the rearrangement of the lower polaron band spectrum and Z_k residues on doping, as well as a strong anisotropy of hole–spin scattering.

Keywords Kinetic · Antiferromagnet (AFM)

Anomalous properties of high- T_c cuprates include a complex behavior of the spectral properties and peculiar $\rho(T)$ and $R_H(T)$ T -dependence. Our study of kinetics is based on the microscopic description in terms of spin-fermion Hamiltonian. It consists of the motion of bare holes $\hat{H}_{0h} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}$, AFM spin–spin interaction $\hat{I} = 1/2 \sum_{\mathbf{R}, \mathbf{r}} I_{\mathbf{r}} S_{\mathbf{R}+\mathbf{r}}^\alpha S_{\mathbf{r}}^\alpha$ and spin–hole interaction $\hat{J} = J \sum_{\mathbf{r}} a_{\mathbf{r}, \gamma_1}^\dagger \hat{\sigma}_{\gamma_1 \gamma_2}^\alpha a_{\mathbf{r} \gamma_2} S_{\mathbf{r}}^\alpha$.

To study the charge excitations we introduce a finite set of the basic operators: $\varphi_{\mathbf{r}\sigma}^{(1)} = a_{\mathbf{r}\sigma}$, $\varphi_{\mathbf{r}\sigma}^{(2)} = S_{\mathbf{r}}^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha a_{\mathbf{r}\sigma_1}$, describing the in-site pairing of bare hole with the localized

spin and the operators

$$\varphi_{\mathbf{r}\sigma}^{(3)} = \frac{1}{N} \sum_{\rho, \mathbf{q} \in \Omega} e^{i\mathbf{q}\rho} S_{\mathbf{r}+\rho}^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha a_{\mathbf{r}\sigma_1},$$

$$\varphi_{\mathbf{r}\sigma}^{(4)} = \frac{1}{N} \sum_{\rho, \mathbf{q} \in \Omega} e^{i\mathbf{q}\rho} S_{\mathbf{r}+\rho}^\alpha \hat{\sigma}_{\sigma\sigma_1}^\alpha S_{\mathbf{r}}^\beta \hat{\sigma}_{\sigma_1\sigma_2}^\beta a_{\mathbf{r}\sigma_2},$$

corresponding to the spin polaron of the intermediate radius, which describe the pairing of local operators $\varphi_{\mathbf{r}\sigma}^{(1)}$ and $\varphi_{\mathbf{r}\sigma}^{(2)}$ with the spin wave operators $S_{\mathbf{q}}^\alpha$, $\mathbf{q}$ close to (π, π) .

The standard Mori–Zwanzig projection procedure gives the Green’s functions of a bare hole in the mean-field approximation (see [1]), $G_h(\mathbf{k}, \omega) = \langle a_{\mathbf{k}\sigma}; a_{\mathbf{k}\sigma}^\dagger \rangle = \sum_{s=1}^4 Z_{\mathbf{k}}^{(s)} / (\omega - E_{\mathbf{k}}^{(s)})$, expressed in terms of the residue function $Z_{\mathbf{k}}^{(s)}$ and spin-polaron bands $E_{\mathbf{k}}^{(s)}$ ($s = 1-4$ is the band number).

In the polaron representation, the Hamiltonian takes the form $\hat{H} = \sum_{\mathbf{k}, s} E_{\mathbf{k}}^{(s)} \alpha_{\mathbf{k}\sigma}^{(s)\dagger} \alpha_{\mathbf{k}\sigma}^{(s)} + \hat{J} + \hat{I}$, $\hat{J}_p = \hat{P} \hat{J} \hat{P}$, $\hat{P} = \sum_{\mathbf{k}, s} |\alpha_{\mathbf{k}, \gamma}^{(s)}\rangle \langle \alpha_{\mathbf{k}, \gamma}^{(s)}|$. Here, $\hat{P}$ is the projection operator on the polaron space, $\varphi_{\mathbf{k}, \sigma}^{(i)} = U_{ij}^{-1}(\mathbf{k}) \alpha_{\mathbf{k}\sigma}^{(j)}$. The matrix $U_{ij}^{-1}(\mathbf{k})$ is expressed in the explicit form in terms of the spin–spin correlation functions, which are in turn determined in terms of spin–spin susceptibility $\chi(\mathbf{q}, \omega)$ for the frustrated AFM spin subsystem [4, 5].

In order to obtain an explicit form for $\rho(T)$ and $R_H(T)$, we take a multimoment variant of the linear-response theory where the deviation from equilibrium is characterized by a finite set of operators $\hat{F}_l^s = \sum_{\mathbf{k}} F_l^s(\mathbf{k}) \alpha_{\mathbf{k}\sigma}^{(s)\dagger} \alpha_{\mathbf{k}\sigma}^{(s)}$. The collision term is expressed in terms of moments F_l^s (we introduce up to seven moments), residues $Z_{\mathbf{k}}^{(s)}$, polaron bands $E_{\mathbf{k}}^{(s)}$ and the imaginary part of spin–spin susceptibility $\chi''(\mathbf{q}, \omega)$. For $\chi(\mathbf{q}, \omega)$ we adopt the spherical-symmetric form with damping γ : $\chi(\mathbf{q}, \omega) = -A_{\mathbf{q}} / (\omega^2 - \omega_{\mathbf{q}}^2 + i\omega\gamma)$; $\gamma = \gamma(T)$. To obtain an explicit form for $\chi(\mathbf{q}, \omega)$ we use

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Fig. 1 Residue function $Z_{\mathbf{k}}^{(1)}$ (low doping) presented by contour curves in the first quarter of the Brillouin zone. The thick line is the Fermi surface

a full self-consistent approach with spin-constraint fulfilling. To test overdamped magnons approach, we also use the $\chi_{\text{ovd}}(\mathbf{q}, \omega)$ of the form $\chi_{\text{ovd}}(\mathbf{q}, \omega) = A_{\mathbf{q}}/(i\omega\gamma(\mathbf{q}, \omega) - \omega_{\mathbf{q}}^2)$. The details are in Refs. [2, 3].

Figure 1 presents the characteristic residue spectra function $Z_{\mathbf{k}}^{(1)}$ for lower polaron band in a case of a larger spin correlation length ($\xi \simeq 10g$, g is the lattice constant) of underdoped cuprates. $Z_{\mathbf{k}}^{(1)}$ decrease from 0.24 to 0.04 when moving along the Fermi surface. This decrease qualitatively reflects the known opening of the pseudogap on the Fermi surface. For the number of holes $n_h = 0.08$, calculations lead to $\rho = 230 \mu\Omega\text{cm}$, which is close to $\rho(T = 120 \text{ K}) = 220 \mu\Omega\text{cm}$ for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ with $x \approx 0.1$ [6].

Our results for optimal doping, presented in Fig. 2, give, in accordance with the experiment [6], that $\rho(T)$ curve exhibits T dependence close to a linear one starting from low T with the value $\rho(400 \text{ K})/\rho(100 \text{ K}) \approx 5$. The overdamped $\chi_{\text{ovd}}(\mathbf{q}, \omega)$ strongly underestimates the scattering for large ω . The $\cot \Theta_H$ exhibits nearly linear behavior on T^2 in a wide T -range.

Given in Fig. 3 (optimal doping), $R_H(T)$ decreases upon heating, which corresponds to the experimentally observed behavior. In the inset we show the dependence $\tau(\mathbf{k})/\tau(\mathbf{k}_{\text{cold}})$ to demonstrate the presence of hot and cold spots.

In summary, we show that the spin polaron concept (“good” quasi-particles are polarons, not bare holes) allows to reproduce T -anomalies for two kinetic coefficients simultaneously in a wide doping range. It gives a possibility to take into account strong dependence of polaron bands and bare hole residues $Z_{\mathbf{k}}$ on spin–spin correlation length from the very beginning. It is also important to treat the kinetic equation, namely for polarons, and to introduce a multimoment approach (seven F_l^s operators give a possibility to take into account strong scattering anisotropy).

Fig. 2 $\rho(T/I)$ and cotangent of the Hall angle $\cot \Theta_H(T^2/I^2)$ at 10 T (upper inset). The solid lines correspond to $\chi(\mathbf{q}, \omega)$. The dashed lines for $\chi_{\text{ovd}}(\mathbf{q}, \omega)$. Lower inset: the spectrum $\epsilon_{\mathbf{k}} = \text{const}$; bold curve is the Fermi line for optimal doping

Fig. 3 $R_H(T)$ (optimal doping): curves a, b, c , correspond to $\chi(\mathbf{q}, \omega)$ with $\gamma/I = 0.5, 1.0$ and 1.5 , respectively; the dashed curve mf corresponds to mean-field spin spectrum. In inset, for $T/I = 0.3, 0.1$, and 0.05 , curves $a\text{---}mf, b\text{---}mf$, and $c\text{---}mf$ demonstrate strong scattering anisotropy by showing the dependence $\tau(\mathbf{k})/\tau(\mathbf{k}_{\text{cold}})$, $\tau(\mathbf{k})$ to relaxation time. Angle ϑ is formed by the radius vector $\mathbf{k}$ lying on the circle arc $k_0 = 0.83\pi$ and the axis $M(\pi, \pi) - X(0, \pi)$. The circle is centered at M and adjoins the Fermi surface

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References

1. Barabanov, A.F., Belemuk, A.M.: Sov. Phys. JETP **111**, 258 (2010)
2. Belemuk, A.M., Barabanov, A.F., Maksimov, L.A.: Sov. Phys. JETP **102**, 431 (2006)
3. Belemuk, A.M., Barabanov, A.F., Maksimov, L.A.: JETP Lett. **86**, 321 (2007)
4. Barabanov, A.F., Mikheyenkov, A.V., Belemuk, A.M.: Phys. Lett. A **365**, 469 (2007)
5. Barabanov, A.F., Mikheyenkov, A.V., Shvartsberg, A.V.: Theor. Math. Phys. **163**, 1192 (2011)
6. Ando, Y., et al.: Phys. Rev. Lett. **925**, 197001 (2004)