Gauge field theory of transport and magnetic relaxation in underdoped cuprates

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Based on recently proposed $U(1) \times SU(2)$ Chern-Simons gauge field theory, an interpretation of the transport and magnetic relaxation properties of underdoped cuprates is proposed, taking into account the short range antiferromagnetic order. The interplay of the doping-dependent spin gap (explicitly derived by us) effect and dissipation due to gauge fluctuations gives rise to a crossover from metallic to insulating behavior of conductivity as temperature decreases, in semi-quantitative agreement with experimental data. For the same reason the magnetic relaxation rate shows a maximum nearby. Various crossover temperatures related to spin gap effects are shown to be different manifestations of the same energy scale.

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The understanding of the anomalous normal state properties of oxide superconductors has been a challenge for theorists since their discovery. Recently great attention has been focused on underdoped superconductors, where the pseudogap (spin gap) effects are essential. We will concentrate on the doping range where the short range antiferromagnetic order (SRAFO) exists, and propose an interpretation of the transport and magnetic relaxation properties in this region, based on the recently proposed $U(1) \times SU(2)$ gauge field theory.

The linear temperature dependence of resistivity in most of oxide superconductors over a wide range of temperature is well established, and a number of explanations have been proposed, including the $U(1)$ gauge field theory. On the other hand, in underdoped samples, a resistivity minimum and a crossover from metallic to insulating behavior has been observed. A similar divergence of resistivity at low temperatures has been found in superconducting samples in strong magnetic fields, suppressing superconductivity. An apparently "obvious" explanation of these two related phenomena would be localization of charge carriers in two dimensions. However, a more careful comparison of theory with experiments shows that the localization effects including carrier interactions cannot correctly interpret the data. Several other explanations have been proposed based on non-Fermi liquid (FL) behavior of charge carriers, but the zero field experiments have not been addressed, except for where a gauge field approach has been used. We, instead, will concentrate on the latter case. We will show that the presence of SRAFO, leading to a finite mass of spinons (bosons) is the correct starting point in this doping range. The self-generated $U(1)$ holon-spinon $(h/s)$ gauge field becomes singular due to coupling with holons (fermions), which, in turn, renormalizes the massive spinons in a nontrivial way. At low temperatures, effects due to finite spinon mass prevail leading to insulating behavior, while at higher temperatures the dissipation caused by the gauge field dominates and gives rise to metallic behavior. For similar reasons, the spin relaxation rate is low at both low and high temperatures, reaching a maximum near the resistivity crossover point which is also consistent with experiment.

Following a strategy previously applied to the 1D $t–J$ model which has reproduced there the known exact Bethe Ansatz results, the Chern-Simons bosonization with $U(1) \times SU(2)$ gauge field was applied to the 2-D $t–J$ model in the limit $t \gg J$, allowing us to rewrite the partition function and (the correlation functions) in terms of a spin-$1/2$ fermion field $\psi_{\alpha}$, $\alpha = 1, 2$, minimally coupled to a $U(1)$ field $B$ (gauging global charge), and an $SU(2)$ field $V$ (gauging global spin) whose dynamics is given by a Chern–Simons (C.S.) action. We decomposed the fermion field $\psi_{\alpha}$ into product of a spinless fermion field $H$ (holon) and a spin-$1/2$ boson field $\Sigma_{\alpha}$ (spinon), satisfying the constraint $\Sigma_{\alpha} \Sigma_{\alpha} = 1$, thus introducing a local $U(1)$ gauge invariance called $h/s$. We proved the existence of an upper bound of the partition function for holons in a spinon background, and we found the optimal spinon configuration ($s+id$-like RVB state) saturating the upper bound on average. After neglecting the feedback of holon fluctuations on field $B$ and spinon fluctuations on field $V$, the holon field is a fermion and the spinon field is a hard–core boson. Within this approximation the “mean field” (MF) $B$ produces a $\pi$ flux phase for holons, converting them into Dirac–like fermions, while the $V$ field, taking into account the feedback of holons produces a gap for spinons vanishing in the zero doping limit.

The continuum action for AF fluctuations around the “MF”, described by a spin-$1/2$ boson field $z_{\alpha}, \alpha = 1, 2$ (still “spinons”) is given by:

$$g^{-1} \int dx_0 d^2 x [v_s^2(|\partial_0 - A_0|)^2 - |(\partial_\mu - A_\mu)|^2 + m_s^2 z_{\alpha}^* z_{\alpha}],$$

(1)
where $A$ is the $h/s$ gauge field, $g = 8/J$, $v_s = \sqrt{2} J a$, with $a$ the lattice constant. The spinon “mass” term $m_A^2 \sim \langle \hat{V}^2 \rangle \sim -\delta \ln \delta$ (the main novelty) is due to averaged perturbation caused by holons of concentration $\delta$ via $\hat{V}$. This explicit doping dependence was derived, rather than assumed in the theory. It produces a SRAFO, with correlation length $\xi_{AF} \sim (\delta \ln \delta)^{-\frac{1}{2}}$, fully consistent with the neutron scattering data. 

Neglecting the gauge fluctuations, holons are described by FL theory with a Fermi surface (FS) consisting of 4 “half-pockets” centered at $(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$. The MF $\hat{B}$ turns the spinless fermion $\hat{H}$ into two species of 2–component Dirac fermions $\psi(r), r = 1, 2$, each of them being supported on one Néel sublattice. The continuum action for these fermions is given by:

$$
\int d^2x \sum_r \bar{\psi}(r)[\gamma^0(\partial_0 - e_r A_0 - \delta) + t(\partial - e_r A)]\psi(r),
$$

where $A = \gamma_\mu A^\mu$, $\partial = \gamma_\mu \partial_\mu$, $\gamma_0 = \sigma_z$, $\gamma_\mu = (\sigma_y, \sigma_z)$, the charges $e_r = \pm 1$, depending on sublattice. After integrating out the gapful Dirac modes, we end up with FL-like system of holons with Fermi energy $\epsilon_F \sim t \delta$, interacting through gauge field $A$. 

As shown in [22], for the gauge field model the in–plane resistivity is approximately given by:

$$
R = \lim_{\omega \to 0} \frac{\omega}{[\text{Im} \Pi^\perp_{\mu}(\omega)]^{-1} + [\text{Im} \Pi^\parallel_{\mu}(\omega)]^{-1}},
$$

where $\Pi^\perp_{\mu}$ and $\Pi^\parallel_{\mu}$ denote the transverse polarization bubbles (at $\vec{q} = 0$) due to the $h/s$ currents of holons and spinons, renormalized by gauge fluctuations. The $A$ propagator for small $|\vec{q}|$, $\omega, \omega/|\vec{q}|$ in the Coulomb gauge is given by:

$$
\left\langle P^A_{\mu} P^A_{\nu}\right\rangle(q, \omega) = (i \omega \lambda_h(\vec{q}) + \chi(\vec{q})^2)^{-1},
$$

$$
\left\langle A_0 A_0\right\rangle(q, \omega) = (\nu_h + \omega_p)^{-1},
$$

where $\lambda_h \sim \kappa/|\vec{q}|, \kappa \sim 0(\delta)$ is the Landau damping due to a finite FS for holons, $\chi = \chi_h + \chi_s, \chi_h \sim m_h^{-1} \sim O(\delta^{-1}), \chi_s = e_s m_s^{-1} \sim O((-\delta \ln \delta)^{-\frac{1}{2}})$ is the diamagnetic susceptibility, $\nu_h$ is the holon density at the FS and $\omega_p$ is the plasmon gap. 

An estimate of the holon contribution to resistivity can be derived as in [22],

$$
R_h \sim (\epsilon_F \tau_{imp})^{-1} + \frac{T}{\chi} \frac{1}{3} / \epsilon_F,
$$

where $\tau_{imp}$ is the transport relaxation time due to impurities. 

To estimate the spinon contribution, we derive the large scale behavior of the spinon current $j^\mu = z^\ast D_A^\mu z$ correlation function, where $D_A^\mu = \partial_\mu - A_\mu$, by eikonal approximation, [22] strictly preserving gauge invariance. We use spinon Green functions at zero temperature, as partially justified by the spinon gap, but we retain the temperature dependence of gauge fluctuations. 

We apply the Fradkin representation [22] to the spinon propagator $\langle z(x) z^\ast(y) \rangle = G(x, y| A)$. It can be derived using a first–quantized path integral form of the propagator, with metric ($-++$), replacing integration over trajectories $q_\mu (t)$ by integration over 3–velocities $\phi_\mu = \dot{q}_\mu (t), \mu = 0, 1, 2$. Rescaling $x_0$ to $v x_0$ one obtains:

$$
G(x, y|A) = \int_0^\infty dse^{-is^2 \sum \epsilon [s(\partial_0 - A_{\mu})^2]}(x, y)
$$

$$
\sim i \int_0^\infty dse^{-is^2 \sum \int D\phi(t) e^{iS}} \int_0^\infty \int d^3p \epsilon_i (x^\mu - y^\mu - \sum_i \phi^i (t)) dt.
$$

Using an identity (Eq. (41) in the second paper of [24]), the integral $\int_0^\infty \int D\phi(t) e^{iS} \int_0^\infty \sum_i \phi^i (t) dt$ can be decomposed into a sum of an integral along a straight line (denoted by $f_{\mu} A^\mu$ and a gauge invariant part depending on the field strength $F_{\mu\nu}$. Thus $G(x, y|A) = \exp[-i \int_0^\infty \sum_i \phi^i (t) A^\mu(x, y|A)]$, the spinon current density correlation $\langle j^\mu(x) j^\nu(y) \rangle, \mu = 1, 2$, is approximately given by:

$$
\langle j^\mu(x) j^\nu(y) \rangle \sim \langle \sum_i \phi^i (t) \rangle = \langle \sum_i \phi^i (t) \rangle A(x, y|A)
$$

where $\langle \cdot \rangle$ denotes average w.r.t. $A$. The gauge–dependence terms of the two spinon propagators exactly cancel each other, yielding a strictly gauge–invariant result, at large scale given approximately by $\langle \frac{d}{d\phi} G(x, y|F) \frac{d}{d\phi} G(x, y|F) \rangle$. The $A^{\perp}$ average involves contributions weighted by “magnetic field” correlations $\langle F_{\mu
u}(z) F_{\nu\sigma}(w) \rangle, \mu, \nu, \rho, \sigma = 1, 2$, approximately evaluated for $|z^0 - w^0| < T^{-1}$ as in [23], obtaining $(\delta_{\mu\rho}\delta_{\sigma\rho} - \delta_{\mu\sigma}\delta_{\rho\nu}) \frac{2T}{(2\pi)^2} e^{-|z-w|^2/2}\delta_0^2$, where $q_0 = (\frac{e}{c})^{\perp}$. It is a momentum cutoff related to the anomalous skin effect due to the Reizer singularity in the $A^\perp$ propagator. The $A_0$ average involves contributions weighted by “electric–field” correlations $\langle F_{0\nu}(z) F_{0\nu}(w) \rangle, \nu, \nu = 1, 2$. Since they vanish in the limit $q_\nu \sim 0$ (see [3]), their contributions will be neglected. 

integrals in (7) can be approximately calculated for relatively low temperatures ($T < \chi m_s^2$) and the current-current correlation becomes:

$$
\langle j^\mu(x) j^\mu(0) \rangle \sim \left[ \frac{\partial}{\partial x_\mu} e^{-i(x^0 - |\vec{q}|^2)} \frac{m^2 - \frac{1}{2} f(1/2|x_0|)}{m^2} \right] (x^0 - |\vec{q}|^2)^{-1/2}
$$

where, for a real argument, $f$ is monotonically increasing, vanishing at zero argument and $q$ is monotonically decreasing, vanishing at large arguments. Their explicit expressions are lengthy and will be given elsewhere. [22] 

In deriving the spinon current correlation at $\vec{q} = 0$ we
evaluate the $x$-integration by saddle point. For $x_0 > q_0^{-1}$ the integral is dominated by a complex saddle point at $|\vec{x}| = 2q_0^{-1} \alpha(x_0)$, with finite $\alpha(x_0)$ (in the first quadrant), having a weak dependence on $x_0$. To justify the saddle point approximation we need to assume $T > \chi m_s q_0$. It turns out that in the physical range of parameters considered in the paper, this and the above conditions are both satisfied for temperatures between tens and a few hundred degrees.

Let us define $\Pi^+(\omega) = \int_0^\infty dx_0 (j^\mu(j^\mu)^*)(\vec{q}) = 0, x_0) e^{ix_0 \omega}$. Using the Lehmann representation we find $\lim_{\omega \to 0} \text{Im} \Pi^+(\omega) \omega^{-1} = -\frac{2 \delta}{\pi} \text{Re} \Pi^+(0)$. Taking note that the main contribution comes from small $x^0$, introducing lower cut-off and performing scale renormalization, we obtain for the $\omega \to 0$ limit: $\text{Re} \Pi^+(\omega)/\omega$

$$\sim \text{Re} \left[ (\alpha(0))^{3/2}(q_0)^{3/2} Z^{1/4} (i f^\mu)^{-1/2} \left( \frac{T}{\chi} \right)^{-1/2} (\omega - Z^{1/2})^{-1} \right],$$

where

$$Z = |Z| e^{-i \theta} \equiv m^2 - \frac{T}{\chi} f(\alpha(0)), \quad f''(\alpha(0)). \quad (8)$$

(renormalization eliminates the contribution of the $q$ function, being subleading). We find that at large $x_0$ arg $\alpha(0) = \frac{\pi}{4}$ and arg $f''(\alpha(0)) = 0$. We extrapolate $\alpha(x_0)$ to $\alpha(0)$, keeping these features. This way we recover the correct behavior, $R \to \infty$, as $T \to 0$. As $x_0 \to 0$, the saddle point extrapolates to $x_s \sim q_0^{-1} e^\mp z$, and we find the “spinon contribution” to resistivity:

$$R_s = 2^{-4} \left( \frac{|f''(\infty)|}{\kappa} \right)^{1/2} |\alpha(0)|^{-3} \frac{|Z|^{1/4} \sin(\theta/4)}{\pi^4 \sin^2(z/4)}.$$  

(9)

In Fig. 1 our calculated resistivity (sum of (5) and (6)), is plotted as a function of temperature for various dopings in comparison with experimental data taken on LSCO (inset). We have taken $t/J = 3, J = 0.1$ eV. Apart from the resistivity scale, there are no other adjustable parameters (similarly for Fig. 3). We find a resistivity minimum below 100K in very good agreement with experiment. We see from (6) that the imaginary part of $Z$ is proportional to temperature $T$. At low temperatures the spin gap effect $(\sim m_s)$ dominates, $\theta \to 0$, so the system shows an insulating behavior. (The functional dependence $R \sim 1/T$, different from the “standard” exponential law due to spin gap, is a prediction of our theory.) On the contrary, at higher temperatures the imaginary and real parts of $Z$ become comparable, so the resistivity grows with temperature due to gauge fluctuations via $|Z|$. Moreover, the minimum shifts to higher temperatures, as the doping decreases, also in agreement with experiment (our theoretical prediction $m_s^2 \sim -\delta \ln \delta$, rather than $\sim \delta$ is responsible for this shift). We have also compared the calculated conductivity in the semi-log scale with data taken on a very good single crystal of La$_{1.96}$Sr$_{0.04}$CuO$_4$ (inset). We find a symmetric shape of curve around the maximum, and a reflection point as well as a linear piece on the low temperature side in both theory and experiment. So far we have not included the external magnetic field. We believe the experimentally observed crossover from metallic to insulating behavior in strong magnetic fields when superconductivity is suppressed, can be understood in a similar way, and this issue will be addressed in our future communication.

Now turn to the spin–lattice relaxation rate $T^{-1}$ which can be expressed approximately as:

$$(T_1 T)^{-1} \sim \lim_{\omega \to 0} \int d^2 q \mathcal{F}(\vec{q}) \frac{\text{Im} \chi_s(\vec{q}, \omega)}{\omega},$$

where $\chi_s$ is the spin susceptibility and $\mathcal{F}(\vec{q})$ is the form factor. To evaluate $\chi_s$ we use the representation for spin deduced at large scales $\vec{S}_z \sim e^{i \pi |\vec{z}|^2} (\mathcal{T}(\vec{x}, 0) F(x, 0) G(x, 0) - F)(\vec{x}, 0)$ which can be calculated as before. Define $\chi^+ (\vec{q}, \omega) = \int_0^\infty dx_0 (\vec{S}(\vec{q})^* x_0) e^{ix_0 \omega}$, using the Lehman representation and taking into account that $\mathcal{F}(\vec{q})$ is even in $\vec{q}$, one obtains $(T_1 T)^{-1} = -2 \int d^2 q \mathcal{F}(\vec{q}) \frac{\text{Re} \chi^+ (\vec{q}, 0)}{\omega}$. Since $\mathcal{F}(\vec{q})$ is peaked around $\vec{Q}_{AF}$ for Cu, integrating over $q$ in a small region around that point, and introducing a cutoff in the real space $\Lambda \sim \pi/|x_s|$, we find

$$(T_1 T)^{-1} \sim (1 - \delta^2)^2 | \vec{q}| (\alpha(0) \frac{\theta}{4} + b \sin(\theta/4)), \quad (10)$$

where $a = \text{Re} \int_\Lambda d^2 y J_0(2|\vec{y}| \alpha(0))$, $b = -\text{Im} \int_\Lambda d^2 y J_0(2|\vec{y}| \alpha(0))$, and $J_0$ is the zero-order Bessel function.
rate $T^{-1}$ of $^{63}$Cu as a function of temperature for various dopings in comparison with experimental data taken on underdoped samples of YBCO. We observe a maximum near the crossover temperature for conductivity, although the shape around maximum is not symmetric anymore, due to the presence of the cosine term.

In Fig. 3 we plot our calculated spin-lattice relaxation rate $(T^*)^{-1}$ for $^{63}$Cu as a function of temperature for the CuO planes of YBa$_2$Cu$_3$O$_{6.52}$ single crystals in units of s$^{-1}$K$^{-1}$, taken from [18].

To summarize, we have shown using the $U(1) \times SU(2)$ gauge field theory that the metal-insulator behavior crossover and peculiar behavior of NMR relaxation in underdoped cuprates might be due to the interplay of the spin gap (derived in our approach) effect and the gauge field fluctuations. More precisely, the crossover is taking place when the real and imaginary parts of $Z$ (Eq. (8)) become comparable. In Fig. 3 we have plotted three different crossover temperatures related to the spin gap effects, namely the metal-insulator crossover $T_{M-I}$ (minimum of the in-plane resistivity), the spin gap crossover temperatures, detected by NMR $T_0$ and by resistivity $T^*$, identified with their respective reflection points, in the low-doping region ($\delta \sim 0.02 - 0.08$). The last two temperatures, roughly speaking, limit from the above the region of significant spin gap effects and validity of our approximation. These crossover temperatures are different manifestations of the same energy scale. The fact that their relative order $T^* > T_0 > T_{M-I}$, as well as their order of magnitude agrees with experiments, provides further support for our approach.

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