STRIPEs, NON-FERMI-LIQUID BEHAVIOR, AND TWO-COMPONENT TRANSPORT IN THE HIGH-$T_c$ CUPRATES

J. ASHKENAZI

Physics Department, University of Miami, P.O. Box 248046, Coral Gables, FL 33124, U.S.A.

Abstract — Non-Fermi-liquid features of the high-$T_c$ cuprates, and specifically the systematic behavior of the resistivity, Hall constant, and thermoelectric power, are shown to result from an electronic structure based on “large-$U$” and “small-$U$” orbitals, and the resulting striped structure.

The electronic structure of the cuprates is studied in terms of “large-$U$” and “small-$U$” orbitals [1]. The “slave-fermion” method is applied, where the creation operator of a large-$U$ electron in site $i$ and spin $\sigma$ is expressed as $c_i^\dagger s_i^\sigma$, if it is in the “upper-Hubbard-band”, and as $\sigma s_i^\dagger h_i$, if it is in a Zhang-Rice-type “lower-Hubbard-band”; $e_i$ and $h_i$ are (“excession” and “holon”) fermion operators, and $s_i^\sigma$ are (“spinon”) boson operators, and the constraint $e_i^\dagger e_i + h_i^\dagger h_i + \sum_\sigma s_i^\dagger s_i^\sigma = 1$ should be satisfied.

Here this constraint is imposed on the average within an auxiliary Hilbert space, and physical observables are calculated by taking appropriate combinations of Green’s functions of this space. The Green’s functions are determined by the Hamiltonian which obeys the constraint rigorously. Two-particle spinon-holon Green’s functions are decoupled only where the “spin-charge separation” approximation holds.

The Bogoliubov transformation is applied to diagonalize the spinons, yielding creation operators $\zeta^p_{\mu\lambda\sigma}(k)$, and “bare” spinon energies $\epsilon^p(k)$ with a $V$-shape zero minimum at $k = k_0$, where $2k_0 = (\pi, \pi)$. Bose condensation results in antiferromagnetism (AF).

Numerical calculations in a lightly doped AF plane, supported by neutron-scattering measurements in some cuprates [2], indicate the existence of a frustrated striped structure where narrow charged stripes form antiphase domain walls separating wider AF stripes. Growing experimental evidence supports the assumption that such a structure exists, at least dynamically, in all the superconducting cuprates.

Since the spin-charge separation approximation is valid in one-dimension, it should apply for holons within the charged stripes, and they are referred to as “stripions”, created by $p^\dagger_{\mu}(k)$, and of bare energies $\epsilon^p_{\mu}(k)$. Since one expects finite stripe segments, frustrations, and defects, which are fatal for itinerancy in one-dimension, we assume a starting point of localized stripion states.

The holon-spinon and excession-spinon pair states for which spin-charge separation does not apply hybridize with the small-$U$ electron states forming, within the auxiliary space, states of “Quasi-electrons” (QE’s), created by $q_{\mu\lambda}(k)$. Their bare energies $\epsilon^q_{\mu}(k)$ form quasi-continuous ranges of bands crossing the Fermi level ($E_F$) over ranges of the Brillouin zone (BZ).

These quasiparticles are coupled due to hopping and hybridization terms, and the coupling between them can be expressed through a Hamiltonian term:

$$\mathcal{H}' = \frac{1}{\sqrt{N}} \sum_{\mu\lambda\sigma} \sum_{k, k'} \left\{ \sigma \epsilon_{\mu\lambda\sigma}^q (k', k) d^\dagger_{\mu\sigma}(k)p_{\mu}(k') \right. $$

$$\left. \times \left[ \cosh (\xi_{\lambda\sigma}(k-k')) \zeta^q_{\lambda\sigma}(k-k') + \sinh (\xi_{\lambda\sigma}(k-k')) \zeta^q_{\lambda\sigma}(k-k') \right] + h.c. \right\}. \quad (1)$$

$\mathcal{H}'$ introduces a vertex between QE, stripion and spinon propagators. Vertex corrections are negligible by a generalized Migdal theorem, since the obtained stripion bandwidth is much smaller than the QE and spinon bandwidths. Thus a second-order perturbation expansion in $\mathcal{H}'$ is applicable. The QE, spinon, and stripion scattering rates $\Gamma^q_{\mu}(k, \omega)$, $\Gamma^s_{\lambda}(k, \omega)$, and $\Gamma^p_{\mu}(k, \omega)$, are then calculated, and for sufficiently doped cuprates one gets a self-consistent solution of the following features:

Spinons: Their spectral function $A^s(k, \omega) \propto \omega$ for small $\omega$, and thus $A^s(k, \omega)b_\omega(\omega) \propto T$ for $\omega \ll T$, where $b_\omega(\omega)$ is the Bose distribution function.
Stripons: Their localized states are renormalized to polaron-like states very close to $E_v$, with some hopping through QP-spinon states. One gets $\Gamma^q(k,\omega) \propto A\omega^2 + B\omega T + CT^2$, and a two-dimensional itinerant behavior at low temperatures, with a bandwidth of $\sim 0.02$ eV.

Quasi-electrons: An approximate expression for their scattering rates is given by $\Gamma^q(k,\omega) \propto \omega[b_2(\omega) + \frac{1}{2}]$, becoming $\Gamma^q(k,\omega) \propto T$ in the limit $T \gg |\omega|$, and $\Gamma^q(k,\omega) \propto \frac{1}{2|\omega|}$ in the limit $T \ll |\omega|$, as in marginal-Fermi-liquid phenomenology.

Lattice effects (“svivons”): The charged stripes are characterized by an LTT-like structure [3]. Thus, spinon excitations due to $\mathcal{H}_L$ are followed by phonon excitations, and stripions have polaron-like lattice features. A spinon propagator linked to a vertex is thus “dressed” by phonon propagators. We refer to such a phonon-dressed spinon as a svivon.

The dc current is expressed as a sum $j = j^q + j^p$ of QE and stripion currents. Since stripions hop only via QE states, one gets that $j^p \propto \alpha q^f$, where $\alpha$ is $T$-independent. Consequently, an electric field is accompanied by gradients $\nabla \mu^q$ and $\nabla \mu^p$ of the QE and stripion chemical potentials, satisfying $N^q \nabla \mu^q + N^p \nabla \mu^p = 0$, where $N^q$ and $N^p$ are the contributions of QE and stripion states to the electrons density of states at $E_v$.

By using the Kubo formula we derive expressions for the dc conductivity and Hall constant, in terms of Green’s functions. These expressions include diagonal and non-diagonal conductivity QE and stripion terms $\sigma_{xx}^{qq}$, $\sigma_{xy}^{qq}$, $\sigma_{yy}^{pp}$, $\sigma_{xx}^{pp}$, and mixed terms $\sigma_{xy}^{qp}$. The currents are expressed as: $j_x^q = \sigma_{xx}^{qq} E^q + \sigma_{xy}^{qp} E^p$, where $E^q = E + \nabla \mu^q$, $E^p = E + \nabla \mu^p$, and $E$ is the electric field. By expressing $E = (N^q E^q + N^p E^p)/(N^q + N^p)$, and $j_x^q + j_x^p = j_x = E_x/\rho_x$, one gets that the resistivity can be expressed as:

$$\rho_x = \frac{1}{(N^q + N^p)(1 + \alpha)} \left( \frac{N^q}{\sigma_{xx}^{qq}} + \frac{\alpha N^p}{\sigma_{xx}^{pp}} \right). \quad (2)$$

Similarly, the Hall constant $R_H = E_y/j_x H$ can be expressed as $R_H = \rho_x / \cot \theta_H$; where:

$$\frac{1 + \alpha}{\cot \theta_H} = \left[ \frac{\sigma_{xy}^{qq} + \alpha \sigma_{xy}^{qp}}{\sigma_{xx}^{qq}} \right] + \frac{\alpha (\sigma_{xy}^{pp} + \sigma_{xy}^{qp})}{\sigma_{xx}^{pp}}. \quad (3)$$

To get the temperature dependencies of $\rho$ and $\cot \theta_H$ we use those derived for $\Gamma^q$ and $\Gamma^p$ (to which temperature-independent impurity scattering terms are added). Thus one can parametrize:

$$\sigma_{xx}^{qq} \propto (D + CT)^{-1}, \quad \sigma_{xy}^{qq} \propto (A + BT^2)^{-1}, \quad \sigma_{xx}^{pp} \propto (D + CT)^{-2}, \quad \sigma_{xy}^{pp} \propto (A + BT^2)^{-2}, \quad \sigma_{xy}^{qp} \propto [(D + CT)(A + BT^2)]^{-1},$$

and express:

$$\rho \propto \frac{(D + CT + A + BT^2)}{N}, \quad \cot \theta_H \propto \left( \frac{Z}{D + CT} + \frac{1}{A + BT^2} \right)^{-1}. \quad (4)$$

These expressions reproduce the systematic behavior of $\rho$ and $\cot \theta_H$ in different cuprates, except for the effect of the pseudogap, not included in this parametrization. Results corresponding to data in YBa$_2$Cu$_{3-x}$Zn$_x$O$_7$ [4], Tl$_2$Ba$_2$CuO$_{6+\delta}$ [5], and La$_{2-x}$Sr$_x$CuO$_4$ [6], are presented in Figs. 1, 2, and 3, respectively.

![Graph](image)

FIG. 1. The transport coefficients, in arbitrary unit, for A=1,7,13,19,25; B=.001; C=1; D=50,100,150,200; N=1,...,8,7,6; Z=2. The first value corresponds to the thickest lines.

The idea of different scattering rates for $\rho$ and $\cot \theta_H$ has been first suggested by Anderson [7], where in his analysis the $T^2$ term is due to stripions. Note however that in recent ac Hall effect results [8] the energy scale corresponding to this term is found to be $\sim 120$ K, in agreement with that of our
Under a temperature gradient one gets:

\[ j^q = eT^{-1}L^{q(11)}(T^{-1}) \partial T^q + L^{q(12)}(T^{-1}) \nabla T^q \]

\[ j^p = eT^{-1}L^{p(11)}(T^{-1}) \partial T^p + L^{p(12)}(T^{-1}) \nabla T^p \]

The thermoelectric power (TEP) is given by

\[ S = \frac{E}{\nabla T} \]

Since \( j^p \sim \alpha j^q \), the condition \( j = 0 \) means \( j^q \sim j^p \sim 0 \). Thus one gets:

\[ S = \frac{(N^q S^q + N^p S^p)}{(N^q + N^p)} \]

\[ S^q = -\frac{L^{q(12)}}{eT L^{q(11)}} \]

\[ S^p = -\frac{L^{p(12)}}{eT L^{p(11)}} \]

One gets \( S^q \propto T \), as for electrons in metals, while \( S^p \) saturates at \( T \approx 200 \) K to the narrow-band result:

\[ S^p = \left( k_u / e \right) \ln \left( 1 - n_p / n^p \right) \]

where \( n_p \) is the fractional occupation of the stripon band. This is consistent with the typical behavior of the TEP in the cuprates. It was found [9] that \( S^p = 0 \) (and thus \( n_p = 0.5 \)) for slightly overdoped cuprates.

Considering large-\( U \) and small-\( U \) orbitals in the cuprates results in a striped structure, and three types of quasiparticles: polaron-like stripons carrying charge, phonon-dressed spinons (svivons) carrying spin, and quasi-electrons carrying both. Non-Fermi-liquid features of the cuprates are explained, and specifically the systematic behavior of the resistivity, Hall constant, and thermoelectric power.

FIG. 2. The transport coefficients, in arbitrary unit, for \( A=20,40,60,80,100 \); \( B=.01 \); \( C=.5,2,5,10,20 \); \( D=20,40,80,160,320 \); \( N=1,1.3,1.8,2.5,3.4 \); \( Z=.01 \). The first value corresponds to the thickest lines.

FIG. 3. The transport coefficients, in arbitrary unit, for \( A=3,2.4,2,1.7,1.5 \); \( B=.00025, .0004, .0006, .0008, .001 \); \( C=1,1.1,1.3,1.6,2 \); \( D=40 \); \( N=1.1,1.5,2,2.3,4 \); \( Z=3 \). The first value corresponds to the thickest lines.

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