Strips, Non-Fermi-Liquid Behavior, and High-$T_c$ Superconductivity

J. Ashkenazi

Received 19 February 1997

The electronic structure of the high-$T_c$ cuprates is studied in terms of “large-$U$” and “small-$U$” orbitals. A striped structure and three types of quasiparticles are obtained, polaron-like “stripons” carrying charge, “svivons” carrying spin, and “quasielectrons” carrying both. The anomalous properties are explained, and specifically the behavior of the resistivity, Hall constant, and thermoelectric power. High-temperature superconductivity results from transitions between pair states of quasielectrons and stripons.

KEY WORDS: High-$T_c$ superconductivity, stripes, transport properties, mechanism.

1. INTRODUCTION

The validity of the Fermi-liquid scenario for the high-$T_c$ cuprates has been doubted, and scenarios such as of a marginal Fermi liquid (MFL) [1], anomalously-screened Fermi liquid [2], and others have been suggested. Evidence is growing [3,4] that the CuO$_2$ planes are characterized by a static or dynamic striped structure. A theoretical study of the cuprates requires the consideration of both “large-$U$” and “small-$U$” orbitals [5].

A small-$U$ electron in band $\nu$, spin $\sigma$, and wave vector $k$ is created by the fermion operators $c_{\nu\sigma}(k)$. The large-$U$ states are treated by the “slave-fermion” method [6], where an electron in site $i$ and spin $\sigma$ is created by $d_{i\sigma} = \epsilon_i s_{i\sigma}$, if it is in the “upper-Hubbard-band”, and by $d_{i\sigma}^\dagger = \sigma s_{i\sigma} h_i$, if it is in a Zhang-Rice-type “lower-Hubbard-band”. Here $\epsilon_i$ and $h_i$ are (“excession” and “holon”) fermion operators, and $s_{i\sigma}$ are (“spinon”) boson operators. The constraint $\sum_{\sigma} s_{i\sigma} s_{i\sigma} = 1$ should be satisfied in every site.

An auxiliary Hilbert space is introduced where the constraint is imposed only on the average by introducing a chemical-potential-like Lagrange multiplier. Physical observables are projected into the physical Hilbert space by taking appropriate combinations of Green’s functions of the auxiliary space.

Since the time evolution of Green’s functions is determined by the Hamiltonian which obeys the constraint rigorously, effects of constraint violation may result only from approximations introduced. Within the “spin-charge separation” approximation two-particle spinon-holon Green’s functions are decoupled.

2. QUASIPARTICLES

The spinons are diagonalized by the Bogoliubov transformation, yielding creation operators $\zeta_{i\sigma}(k)$, and “bare” spinon energies $\epsilon_{\zeta}(k)$ with a V-shape zero minimum at $k = k_0$, where $k_0$ is either $(\frac{\pi}{2a}, \frac{\pi}{2a})$ or $(\frac{\pi}{2a}, -\frac{\pi}{2a})$. Bose condensation results in antiferromagnetism (AF), and the spinon reciprocal lattice is extended by adding the wave vector $Q = 2k_0$.

The decoupling of two-particle spinon-spinon Green’s functions, relevant for spin processes, is more reasonable within the slave-fermion method, where the Bose condensation of spinons does not require pair correlation, than within the “slave-boson” [6] method, where BCS condensation of spinons does require pair correlation.

A lightly doped AF plane tends to separate into a “charged” phase and an AF phase. Under long-range Coulomb interactions one expects [7] a frustrated striped structure of these phases. Experiment [4] confirms such a scenario and indicates at least in certain cases a structure where narrow charged stripes form antiphase domain walls separating wider AF stripes. Various experiments [8] support the assumption that such a structure exists, at least dynamically, in all the superconducting cuprates.
The validity of the spin-charge separation approximation has been established in one-dimension. Thus it should apply for holons (excessions) within the charged stripes, and they are referred to as “stripions”. Their fermion creation operators are denoted by $p^\dagger_j(k)$, and their bare energies by $\epsilon^p_j(k)$. Since one expects finite stripe segments, frustrations, and defects, which are fatal for itinerancy in one-dimension, it is likely that the starting point for the stripion states is of localized states.

The small-$U$ electrons hybridize with coupled holon-spinons (excessions-spinons) within the AF stripes forming, within the auxiliary space, “Quasi-electrons” (QE’s), created by $q^\dagger_{ij}(k)$. Their bare energies $\epsilon^p_j(k)$ form quasi-continuous ranges of bands crossing the Fermi level ($E_F$) over ranges of the Brillouin zone (BZ).

### 3. SPECTRAL FUNCTIONS

The electron spectral function $A(p, \omega)$ is expressed in terms of spectral functions $A^i_j(k, \omega)$, $A^{\dagger}_j(k, \omega)$, and $A^p_j(k, \omega)$, of the QE’s, spinons, and stripions, respectively. $A(p, \omega)$ has a “coherent” contribution from a few QE bands, while the quasi-continuum of the other QE bands and the stripion-spinon spectral functions contribute an “incoherent” background of a comparable integrated weight.

The quasiparticles are coupled by a Hamiltonian term, derived from hopping and hybridization terms of the original Hamiltonian, and expressed as:

$$\mathcal{H}' = \frac{1}{\sqrt{N}} \sum_{ij}\sum_{k,k' \neq k} \left\{ \sigma^\dagger_{ij\lambda\sigma}(k', k) q_{ij\sigma}(k) p_{ij\sigma}(k') \right\}$$

$$\times \left[ \cosh (\xi_{\lambda\sigma}(k-k')) \zeta_{\lambda\sigma}(k-k') + \sinh (\xi_{\lambda\sigma}(k-k')) \zeta_{\lambda\sigma}(k-k') \right] + h.c. \right\}$$  

where the cosh and sinh terms are those appearing in the Bogoliubov transformation. $\mathcal{H}'$ introduces a vertex connecting QE, stripion and spinon propagators. Since the stripion bandwidth turns out to be much smaller than the QE and spinon bandwidths, “vertex corrections” are negligible by a generalized Migdal theorem, and a second-order perturbation expansion in $\mathcal{H}'$ is applicable. The scattering rates $\Gamma^i_j(k, \omega)$, $\Gamma^\dagger_j(k, \omega)$, and $\Gamma^p_j(k, \omega)$, of the quasiparticles are then calculated, and for sufficiently doped cuprates one gets a self-consistent solution of the following features:

- **Spinons**: One gets $A^i_j(k, \omega) \propto \omega$ for small $\omega$, and thus $A^i_j(k, \omega) b_{ij}(\omega) \propto T$ for $\omega \ll T$, where $b_{ij}(\omega)$ is the Bose distribution function.

- **Stripions**: The localized stripion states are renormalized to polaron-like states very close to $E_F$, with some hopping through QE-spinon states. One gets $\Gamma^p_j(k, \omega) \propto A \omega^2 + B \omega T + CT^2$, 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 $\Gamma^i_j(k, \omega) \propto \omega [ b_j(\omega) + \frac{1}{2} ]$, becoming $\Gamma^\dagger_j(k, \omega) \propto T$ in the limit $T \gg \omega$, and $\Gamma^p_j(k, \omega) \propto \frac{1}{2} |\omega|$ in the limit $T \ll |\omega|$, in agreement with MFL phenomenology [1].

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

### 4. TRANSPORT PROPERTIES

The dc current is expressed as a sum $j = j^p + j^p$ of QE and stripion contributions. Since stripions do not hop directly, but via QE states, one gets that $j^p \approx \alpha j^p$, where $\alpha$ is approximately T-independent. Consequently, an electric field is accompanied by gradients $\nabla \mu^p$ and $\nabla \mu^p$ of the QE and stripion chemical potentials, such that $N^q \nabla \mu^q + N^p \nabla \mu^p = 0$, where $N^q$ and $N^p$ are the contributions of QE’s and stripions to the electron density of states at $E_F$.

Expressions for the dc conductivity and Hall constant, in terms of Green’s functions, are derived using the Kubo formalism. They are expressed through diagonal and non-diagonal conductivity QE and stripion terms $\sigma_{xx^p}^{qq}$, $\sigma_{xx^p}^{qq}$, $\sigma_{x^p x}^{qq}$, and $\sigma_{pp}^{pp}$, and mixed terms $\sigma_{pq}^{pp}$. The currents in an electric field $E$ can then be expressed as:

$$j^p = \sigma_{xx^p}^{qq} E^x_j$$

where $E^x_j = E_x + \nabla \mu^p / e$. By expressing $E = (N^q E^x + N^p E^p)/(N^q + N^p)$, and $j^p = j^p + j^p = E_x / \rho_x$, one gets that the resistivity can be expressed as:
Stripes, non-Fermi-liquid behavior

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

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

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

\[\begin{align*}
\text{FIG. 1.} \text{ The resistivity (a), inverse Hall constant (b), and } \\
\text{cot } \theta_H \text{ (c), in arbitrary unit, for parameter values: } A=1,7,13,19,25; B=.001; C=1; D=0.50,100,150,200; \\
N=1,9,8,7,6; Z=2. \text{ The first value corresponds to the} \\
\text{thickest lines.}
\end{align*}\]

The temperature dependencies are determined by those of \( \Gamma^q \) and \( \Gamma^p \), obtained above, to which we add temperature-independent impurity scattering terms. Thus one can parametrize:

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

and express:

\[
\rho_x \approx \frac{(D + CT + A + BT^2)}{N}, \quad (4)
\]

\[
cot \theta_H \approx \left( \frac{Z}{D + CT + A + BT^2} \right)^{-1}. \quad (5)
\]

\[\begin{align*}
\text{FIG. 2.} \text{ The resistivity (a), inverse Hall constant (b), and } \\
\text{cot } \theta_H \text{ (c), in arbitrary unit, for parameter values: } A=20,40,60,80,100; B=.01; C=.5,2.5,10,20; \\
D=20,40,80,160,320; N=1,1.3,1.8,2.5,3.4; Z=.01. \text{ The} \\
\text{first value corresponds to the thickest lines.}
\end{align*}\]

This parametrization reproduces the systematic behavior of the transport quantities in different cuprates, except for the effect of the pseudogap for underdoped cuprates. Results for sets of parameters corresponding to data in \( \text{YBa}_2\text{Cu}_{3-x}\text{Zn}_x\text{O}_7 \) [12], \( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta} \) [13], and \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) [14], are presented in Figs. 1, 2, and 3, respectively.

When also a temperature gradient is present, one can express:

\[
\begin{align*}
J^y &= e CT^{-1} \mathbf{L}^{(11)} \mathbf{E}^y + \mathbf{L}^{(11)} \nabla (T^{-1}), \\
J^p &= e CT^{-1} \mathbf{L}^{(11)} \mathbf{E}^p + \mathbf{L}^{(12)} \nabla (T^{-1}).
\end{align*}
\]

The thermo-
5. MECHANISM FOR HIGH-$T_c$

$\mathcal{H}'$ provides a mechanism for high-$T_c$ due to transitions between pair states of QE's and stripons through the exchange of svivons. The symmetry of the superconducting gap is determined by the symmetry of coupling through $\mathcal{H}'$, and is thus close to the symmetry of the normal-state pseudogap, as has been observed [11]. This pairing mechanism is similar to the interband pair transition mechanism proposed by Kondo [18]. An upper limit for $T_c$ is determined by the temperature where the stripon band becomes coherent, and similarly to a previous work [5], this turns out to be consistent with the Uemura limit.

6. SUMMARY

The consideration of 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 QE's carrying both. Anomalous normal-state properties of the cuprates are explained, and specifically the systematic behavior of the resistivity, Hall constant, and thermoelectric power. A mechanism for high-$T_c$ is obtained on the basis of transitions between pair states of stripons and QE's through the exchange of svivons.

REFERENCES

1. C. M. Varma et al., Phys. Rev. Lett. 63, 1996 (1989).
2. M. Weger, et al., Z. Phys. B 101, 573 (1996).
3. A. Bianconi et al., Phys. Rev. B 54, 12018, (1996); Phys. Rev. Lett. 76 3412 (1996).
4. J. M. Tranquada et al., Phys. Rev. B 54, 7489, (1996); Phys. Rev. Lett. 78, 338 (1997).
5. J. Ashkenazi, J. Supercond. 7, 719 (1994); ibid 8, 559 (1995).
6. S. E. Barnes, Adv. Phys. 30, 801 (1980).
7. V. J. Emery, and S. A. Kivelson, Physica C 209, 597 (1993).
8. Papers in this issue.
9. D. B. Tanner, and T. Timusk, Physical Properties of High Temperature Superconductors III, edited by D. M. Ginsberg (World Scientific, 1992), p. 363.
10. M. I. Salkola, et al., Phys. Rev. Lett. 77, 155 (1996).
11. D. S. Marshall, et al., Phys. Rev. Lett. 76, 4841 (1996).
12. T. R. Chien, et al., Phys. Rev. Lett. 67, 2088 (1991).
13. Y. Kubo and T. Manako, Physica C 197, 378 (1992).
14. H. Takagi, et al., Phys. Rev. Lett. 69, 2975 (1992); H. Y. Hwang, et al., ibid. 72, 2636 (1994).
15. S. Tanaka, et al., J. Phys. Soc. Japan 61, 1271 (1992).
16. B. Fisher, et al., J. Supercond. 1, 53 (1988); J. Genossar, et al., Physica C 157, 320 (1989).
17. K. Matsuura, et al., Phys. Rev. B 46, 11923 (1992); S. D. Obertelli, et al., ibid., p. 14928; C. K. Subramaniam, et al., Physica C 203, 298 (1992).
18. J. Kondo, Prog. Theor. Phys. 29, 1 (1963).