Stripes, Carriers, and High-$T_c$ in the Cuprates

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Abstract. Considering both “large-$U$” and “small-$U$” orbitals it is found that the high-$T_c$ cuprates are characterized by a striped structure, and three types of carriers: polaron-like “stripons” carrying charge, “quasielectrons” carrying charge and spin, and “svivons” carrying spin and lattice distortion. It is shown that this electronic structure leads to the anomalous physical properties of the cuprates, and specifically the systematic behavior of the resistivity, Hall constant, and thermoelectric power. High-$T_c$ pairing results from transitions between pair states of quasielectrons and stripons through the exchange of svivons. A pseudogap phase occurs when pairing takes place above the temperature where stripons become coherent, and this temperature determines the Uemura limit.

INTRODUCTION

The existence of static stripes in the CuO$_2$ planes has been observed in some superconducting cuprates [1,2], and there is growing evidence on the existence of dynamic stripes in others [3]. Many experimental observations have been pointing to the presence of both itinerant and almost localized (or polaron-like) carriers in these materials.

Though one-band theoretical models have been quite popular, and easier to treat, first-principles calculations [4] indicate that such models are probably oversimplified. Here an approach is proposed to the cuprates, taking into account the existence of both “large-$U$” and “small-$U$” orbitals in the vicinity of the Fermi level ($E_F$).

AUXILIARY PARTICLES

The large-$U$ orbitals are treated using the “slave-fermion” method [5]. An electron of these orbitals at site $i$ and of spin $\sigma$ is then created by $d_{i\sigma}^\dagger = e_{i\sigma}^\dagger s_{i,-\sigma}$, if it is in the “upper-Hubbard-band”, and by $d_{i\sigma}^\dagger = \sigma s_{i\sigma}^\dagger h_i$, if it is in a Zhang-Rice-type
“lower-Hubbard-band”. Here \( e_i \) and \( h_i \) are “excession” and “holon” fermion operators, and \( s_{i\sigma} \) are “spinon” boson operators. These auxiliary particle operators should satisfy in each site the constraint \( e_i^\dagger e_i + h_i^\dagger h_i + \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} = 1 \).

The constraint can be imposed on the average by introducing a chemical-potential-like Lagrange multiplier. But the Hilbert space (referred to as the auxiliary space) then contains many non-physical states. However, since the time evolution of Green’s functions is determined by the Hamiltonian which obeys the constraint rigorously, expressing Physical observables in term of Green’s functions results in a correct treatment of the physical subspace. This can be violated by applying inappropriate approximations to the Green’s functions.

Within the “spin-charge separation” approximation two-particle spinon-holon Green’s functions are decoupled into products of one-(auxiliary)-particle Green’s functions. Such an approximation has been shown to be appropriate in one dimension.

The Bogoliubov transformation \( s_{\sigma}(k) = \cosh(\xi_{\sigma}k)\zeta_{\sigma}(k) + \sinh(\xi_{\sigma}k)\zeta_{-\sigma}^\dagger(-k) \) is applied to diagonalize the spinon states. The diagonalized operators \( \zeta_{\sigma}^\dagger(k) \) create spinons of “bare” energies \( \epsilon^\zeta(k) \). These energies have a V-shape zero minimum at \( k = k_0 \), where \( k_0 \) is either \( (\pi/2a, \pi/2a) \) or \( (\pi/2a, -\pi/2a) \). Bose condensation results in antiferromagnetism (AF), and the spinon reciprocal lattice is extended over the basic reciprocal lattice by adding the vector \( Q = 2k_0 \).

**STRIPES AND CARRIERS**

It has been shown [6,7] that a lightly doped AF plane tends to phase-separate into “charged” and AF regions (gaining both hopping and exchange energies). A preferred structure under long-range Coulomb repulsion is of stripes of these phases, at least on the short range. Such a scenario is supported by experiment [1–3]. A structure of narrow charged stripes forming antiphase domain walls between wider AF stripes, has been confirmed for at least some cuprates, and there exists growing evidence indicating that such a structure probably exists, at least dynamically on the short range, in all the superconducting cuprates.

Spin-charge separation applies along the charged stripes (being one dimensional). Holons (excessions) within these stripes are referred to as “stripons”. They carry charge, but not spin. Their fermion creation operators are denoted by \( p_{\mu}^\dagger(k) \), and their bare energies by \( \epsilon_{\mu}^p(k) \). Note that \( k \) here corresponds to an approximate periodicity determined by the stripes structure.

It has been observed [3] that the stripes in the cuprates are quite “frustrated”, and consist of disconnected segments. Since itinerancy in one-dimension requires perfect order, it is assumed here that an appropriate starting point is of localized stripon states.

The effect of the small-\( U \) orbitals is the existence of other carriers (of both charge and spin) whose states are hybridized small-\( U \) states and those coupled holon-spinon and excession-spinon states which are orthogonal to the stripon states.
These carriers as referred to as “Quasi-electrons” (QE’s). Their fermion creation operators are denoted by $q_{i\sigma}^\dagger(k)$. Their bare energies $\epsilon_{i\sigma}^*(k)$ form quasi-continuous ranges of bands crossing $E_F$ over ranges of the Brillouin zone (BZ).

**COUPLING VERTEX**

The auxiliary space fields are coupled to each other due to hopping and hybridization terms of the original Hamiltonian. This coupling can be expressed in terms of the following effective Hamiltonian term whose parameters could be, in principle, derived self-consistently:

$$H' = \frac{1}{\sqrt{N}} \sum_{ij\lambda\sigma} \sum_{k,k'} \left\{ \sigma \epsilon_{ij\lambda\sigma}^q(k',k)q_{i\sigma}^\dagger(k)p_{j\sigma}(k') \right. $$

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

Let us denote the QE, stripon, and spinon Green’s functions by $G^q$, $G^p$, and $G^\zeta$, respectively. The propagators corresponding to them are presented diagrammatically in Fig. 1. $H'$ introduces a coupling vertex between these propagators, as shown in Fig. 1 too. As will be discussed below, the stripon bandwidth turns out to be at least an order of magnitude smaller than the QE and spinon bandwidths. Consequently one gets using a generalized Migdal theorem that “vertex corrections” are negligible.

In Fig. 2 are presented diagrammatically the self-energy corrections $\Sigma^q$, $\Sigma^p$, and $\Sigma^\zeta$, obtained for the QE’s, stripons, and spinons, respectively.

**FIGURE 1.** Diagrams for the auxiliary space propagators and the coupling vertex between them.
The auxiliary space spectral functions $A(k, \omega) \equiv \Im G(k, \omega - i0^+)/\pi$, and scattering rates $\Gamma(k, \omega) \equiv 2\Im \Sigma(k, \omega - i0^+)$ are denoted by $A_q$, $A_p$, and $A_\zeta$, and by $\Gamma_q$, $\Gamma_p$, and $\Gamma_\zeta$, for the QE’s, stripons, and spinons, respectively.

**QUASIPARTICLES**

For sufficiently doped cuprates the self-consistent self-energy corrections determine quasiparticles of the following features:

**Spinons**

One gets spinon spectral functions behaving as: $A_\zeta(k, \omega) \propto \omega$ for small $\omega$. Consequently $A_\zeta(k, \omega)b_T(\omega) \propto \omega$ for $\omega \ll T$, where $b_T(\omega)$ is the Bose distribution function (at temperature $T$). Thus there is no long-range AF order (associated with the divergence in the number of spinons at $k = k_0$).

**Stripons**

The energies of the localized stripon states are renormalized to a very narrow range around zero, thus getting polaron-like states. Some hopping via QE-spinon states results is the onset of coherent itineracy at low temperatures, with a bandwidth of $\sim 0.02$ eV. The stripon scattering rates can be expressed as:

$$\Gamma_p(k, \omega) \propto A\omega^2 + B\omega T + CT^2.$$  \hfill (2)

**FIGURE 2.** Diagrams for the self-energy corrections of the auxiliary space fields
Quasi-electrons

The QE scattering rates, can be approximately expressed as:

$$\Gamma_q(k, \omega) \propto \omega \left[ b_T(\omega) + \frac{1}{2} \right],$$

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 $$T \ll |\omega|$$, in agreement with “marginal Fermi liquid” phenomenology [8].

Phonon-dressed spinons (svivons)

It was found [1] that the charged stripes are characterized by LTT structure, while the AF stripes are characterized by LTO structure. The result would be that in any physical process induced by the $$\mathcal{H}'$$ vertex [see Eq. (1) and Fig. 1], the transformation of a stripon into a QE, or vice versa, through the emission/absorption of a spinon, is followed also by the emission/absorption of phonons. Thus the stripons have also lattice features of polarons, and the spinons are “dressed” by phonons in processes induced by the $$\mathcal{H}'$$ vertex. We refer to such a phonon-dressed spinon as a “svivon”, and its propagator can be expressed as a spinon propagator multiplied by a power series of phonon propagators, as shown diagrammatically in Fig. 3. The svivons carry spin, but not charge, however they also “carry” lattice distortion.

SOME ANOMALOUS PHYSICAL PROPERTIES

Optical conductivity

The optical conductivity of the doped cuprates can be expressed [9] as a combination of a Drude term and mid-IR peaks. Within the present approach the Drude term results from transitions between low energy QE states, while excitations of stripon states result in the mid-IR peaks. Such excitations can either leave a stripon in the same stripe segment, exciting spinon and phonon states, or transform it through $$\mathcal{H}'$$ into a QE and a svivon.

Phonon propagator:  

Svivon propagator:

\[ ... \equiv \ldots \left( 1 + \ldots + \ldots + \ldots + \ldots \right) \]

FIGURE 3. Diagrams for a phonon propagator and a svivon propagator (expressed in terms of spinon and phonon propagators).
Spectroscopic anomalies

Experiments like photoemission give information about the electronic spectral function, which is expressed as a combination of QE and stripon-svivon contributions. Thus it has a “coherent” part, due to the contributions of few QE bands, and an “incoherent” part of a comparable weight, due to the contributions of other quasi-continuous QE bands, and stripon-svivon states.

The frequently observed $\sim|E - E_F|$ bandwidth is consistent with Eq. (3). The spectroscopic ”signature” of stripons is smeared over few tenths of an eV around $E_F$ due to the accompanying svivon excitations. The observed “Shadow bands” and “extended” van Hove singularities result from the effect of the striped superstructure on the QE bands [10].

Transport properties

Within the present approach the electric current is expressed as a sum: $j = j^q + j^p$, where the QE and stripon contributions $j^q$ and $j^p$ are presented diagrammatically in Fig. 4. Since stripons transport occurs through transitions to intermediate QE-spinon states, one gets $j^p \cong \alpha j^q$, where $\alpha$ is approximately $T$-independent. In order for this condition to be satisfied gradients $\nabla \mu^q$ and $\nabla \mu^p$ of the QE and stripon chemical potentials must be formed in the presence of an electric field or a temperature gradient, where $N^q \nabla \mu^q + N^p \nabla \mu^p = 0$ ($N^q$ and $N^p$ are the contributions of QE’s and stripons to the electrons density of states at $E_F$).

Expressions for the dc conductivity and Hall constant are derived using the Kubo formalism. Within the present approach they are expressed in term if diagonal and non-diagonal conductivity QE terms $\sigma_{qq}^{xx}$ and $\sigma_{qq}^{yy}$, stripon terms $\sigma_{pp}^{xx}$ and $\sigma_{pp}^{yy}$, and mixed terms $\sigma_{ppq}^{xy}$. The diagrams for these terms are shown in Fig. 5.

It has been shown elsewhere [11] that the electrical resistivity can then be expressed as:

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

(4)

and the Hall constant as:

FIGURE 4. Diagrams for quasi-particles contributions to the electric current.
\[ R_H = \frac{\rho_x}{\cot \theta_H}, \quad \cot \theta_H = (1 + \alpha)\left[\frac{\sigma_{qqq} + \sigma_{qqpp}}{\sigma_{qq}^2} + \frac{\alpha(\sigma_{ppp} + \sigma_{pppp})}{\sigma_{pp}^2}\right]^{-1}. \quad (5) \]

The temperature dependencies of these transport quantities are determined by those of the scattering rates \( \Gamma^q \) and \( \Gamma^p \), given in Eqs. (2), (3), to which temperature-independent impurity scattering terms are added. Consequently one can express them in terms of parameters \( A, B, C, D, N, \) and \( Z \), as follows:

\[ \sigma_{qq} \propto \frac{1}{D + CT}, \quad \sigma_{pp} \propto \frac{1}{A + BT^2}, \]

\[ \sigma_{qqq} \propto \frac{1}{(D + CT)^2}, \quad \sigma_{ppp} \propto \frac{1}{(A + BT^2)^2}, \quad \sigma_{qqpp} \propto \frac{1}{(D + CT)(A + BT^2)}. \quad (6) \]

Resulting in the following expressions for \( \rho_x \) and \( \cot \theta_H \):

\[ \rho_x = \frac{D + CT + A + BT^2}{N}, \quad \cot \theta_H = \left(\frac{Z}{D + CT} + \frac{1}{A + BT^2}\right)^{-1}. \quad (7) \]

These expressions reproduce the systematic behavior of the transport quantities in different cuprates, as has been demonstrated elsewhere [11]. Note that one can get at the same time linear temperature dependence of \( \rho_x \) and quadratic temperature dependence of \( \cot \theta_H \), and that the temperature dependence of \( \rho_x \) can change to quadratic, and that of \( \cot \theta_H \) to linear, as has been observed [12].

Comparing the present analysis to that of Anderson [13], who first suggested that \( \rho \) and \( \cot \theta_H \) are determined by different scattering rates (attributing the \( T^2 \) term to spinons), it has been observed in ac Hall effect results [14] that the energy scale corresponding to the \( T^2 \) term is of \( \sim 120 \) K, which is in agreement with energies of stripons (suggested here) and not of spinons.

It has also been shown elsewhere [11] that the thermoelectric power (TEP) \( S \) can be expressed in terms of QE and stripon terms \( S^q \) and \( S^p \), as:

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

where \( S^q \propto T \), while the stripon term saturates at \( T \simeq 200 \) K to \( S^p = (k_B / e) \ln[\left(1 - n^p\right)/n^p] \), where \( n^p \) is the fractional occupation of the stripon band.

\[ \sigma_{\chi\chi}^{qq} = \begin{array}{c} \text{Diagram for QE conductivity terms} \end{array} \quad \sigma_{\chi\chi}^{pp} = \begin{array}{c} \text{Diagram for QE conductivity terms} \end{array} \]

\[ \sigma_{\chi\gamma}^{qq} = \begin{array}{c} \text{Diagram for stripon conductivity terms} \end{array} \quad \sigma_{\chi\gamma}^{pp} = \begin{array}{c} \text{Diagram for mixed conductivity terms} \end{array} \]

FIGURE 5. Diagrams for the QE, stripon, and mixed conductivity terms.
This result is consistent with the typical behavior of the TEP in the cuprates, and has been \[15\] parametrized as: $S = AT + BT^\alpha/(T + \Theta)^\alpha$. It was found \[16,17\] that $S^p = 0$ (namely the stripon band is half full) for slightly overdoped cuprates.

The effect of the doping is \[2\] both to change the density of the charged stripes within a CuO$_2$ plane, and to change the density of carriers (stripons) within a charged stripe. It is the second type of doping effect that changes $n^p$.

**PAIRING MECHANISM**

The $\mathcal{H}'$ vertex provides a pairing mechanism which is suggested here to drive high-$T_c$ superconductivity as well as the normal-state pseudogap in the cuprates. This mechanism involves transitions between pair states of QE’s and stripons through the exchange of svivons, as demonstrated diagrammatically in Fig. 6. It is conceptually similar to the interband pair transition mechanism proposed by Kondo \[18\]. The symmetry of the superconducting gap is affected by k-space symmetry which maximizes pairing.

A condition for superconductivity is that the narrow stripon band maintains coherence between different stripe segments. The diagram described in Fig. 6 can, however, drive pairing even when the stripons are incoherent. If this occurs, the carriers do not carry supercurrent, but a gap for pair breaking is still expected to exist. Such condensate is interpreted here as the pseudogap phase found in underdoped cuprates.

Thus a normal-state psuedogap is expected to have a similar size and symmetry to that of the superconducting gap, as has been observed \[19\]. Also the opening of the pseudogap should account for most of the pair-condensation energy, as has been observed.

If the BCS-like pairing temperature (below which the gap opens) is denoted by $T_{\text{pair}}$ and the stripon coherence temperature is denoted by $T_{\text{coh}}$, one expects superconducting transition at:

$$T_c = \min (T_{\text{pair}}, T_{\text{coh}}).$$  \hspace{1cm} (8)

Thus $T_c = T_{\text{coh}} < T_{\text{pair}}$ in underdoped cuprates, and $T_c = T_{\text{pair}} < T_{\text{coh}}$ in overdoped cuprates, in agreement with the observed behavior of the gap \[20\].

![FIGURE 6. Diagram for transitions between pair states of QE’s and stripons, leading to pairing.](image-url)
Stripon coherence is energetically favorable at temperatures where there is a clear distinction between occupied and unoccupied stripon band states. Thus, an estimate for $T_{\text{coh}}$ for an almost empty (full) stripon band is given by the distance $E_F$ of the Fermi level from the bottom (top) of the band at $T = 0$. Using a two-dimensional parabolic approximation one can express:

$$k_B T_{\text{coh}} \simeq E_F = 2\pi h^2(n^*/m^*),$$

where $m^*$ in the stripons effective mass and $n^*$ is their density per unit area of a CuO$_2$ plane (note that the stripons are spinless).

This result agrees with the “Uemura plots” [21] if the $n^*/m^*$ ratio for stripons is approximately proportional to that for the supercurrent carriers, appearing in the expression for the London penetration depth. The “boomerang-type” behavior of the Uemura plots in overdoped cuprates [22] is consistent with as a transition from a band-top $T_c = T_{\text{coh}}$ to a band-bottom $T_c = T_{\text{pair}}$ behavior, as discussed above.

**CONCLUSIONS**

The existence of high-$T_c$ superconductivity in the cuprates has been a challenge for both experimentalists and theorists over the last 13 years. These complex materials have been found to be anomalous in almost any physical property, and the traditional methods developed for simple materials may be inadequate dealing with them.

Here these materials are approached going beyond the “standard” models, and considering the effect of both large-$U$ and small-$U$ orbitals. A locally inhomogeneous striped structure is obtained, as well as a non-standard existence of three types of carriers: polaron-like stripons carrying charge, quasielectrons carrying charge and spin, and svivons carrying spin and lattice distortion.

Anomalous normal-state properties of the cuprates, and specifically transport properties, are clarified, and a pairing mechanism based on transitions between pair states of stripons and quasielectrons through the exchange of svivons is derived, leading to high-$T_c$ superconductivity and to the normal-state pseudogap.

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