A Realistic Theory for the “Normal State” and Pairing Mechanism in the High-Tc Cuprates

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The electronic structure of the high-Tc cuprates is studied on the basis of "large-U" and "small-U" orbitals. Two types of charge carriers are predicted: (i) spinless polarons with a very small bandwidth; (ii) anomalous carriers of both charge and spin. The results are consistent with many anomalous properties of the cuprates. The spinless polarons undergo a CDW transition, and transitions between pair states of the two types of carriers provide the pairing mechanism.

KEY WORDS: High-Tc Cuprates, normal state properties, pairing mechanism, correlations.

1. INTRODUCTION

The occurrence of high-temperature superconductivity (HTS) is just one of the puzzling physical properties of the high-Tc cuprates. Recently [1], a microscopic theory has been worked out explaining many of their anomalous “normal state” properties. Here it is shown how the same approach provides a mechanism for HTS.

Within this approach, one starts from a complete set of orbitals obtained in a first-principles calculation. From such orbitals, in the vicinity of $E_F$, one then constructs orthogonal “large-U” orbitals. The orbitals remaining in the set after these orbitals have been constructed, are orthogonalized to them, and represent electron states which are treated in the “small-U” limit. They are created by fermion operators $c_{\nu\sigma}^{\dagger}(k)$, where $\nu$, $\sigma$ and $k$ are band, spin, and wave vector indices, respectively.

The large-U states are treated by the “slave fermion” method [2]. The creation operator of such a hole, corresponding mainly to hybridized Cu$(d_{x^2-y^2})$ and O$(p_x,p_y)$ orbitals around site $i$ in a CuO$_2$ plane, is expressed as $d_{\nu\sigma}^{\dagger} = s_{\nu\sigma}^{\dagger} e_i$, where $s_{\nu\sigma}^{\dagger}$ and $e_i^{\dagger}$ are boson and fermion creation operators, respectively. Similarly to the approach of Zhang and Rice [3], we introduce fermion creation operators $p_{\sigma}^\dagger$ of singlet pairs of hole orbitals. They include contributions from hybridized Cu$(d_{x^2-y^2})$ and O$(p_x,p_y)$ orbitals in a CuO$_2$ plane, and apical O$(p_z)$ orbitals, or other orbitals.

These auxiliary operators should satisfy the constraint [1,2]: $e_i^{\dagger} e_i + p_i^{\dagger} p_i + \sum_{\sigma} s_{\nu\sigma}^{\dagger} s_{\nu\sigma} = 1$. Their Fourier transforms, $e(k)$, $p(k)$, and $s_{\nu\sigma}(k)$, correspond to the periodicity of the planar Cu atoms. Within such periodicity, an antiferromagnetic (AF) state can be described by propagating, rather than standing, spin-density waves.

2. SPIN AND CHARGE CARRIERS

The $s$ spins are coupled to each other via exchange, and treated within a mean-field approach (MFA) by applying the Bogoliubov transformation for bosons [1]. The obtained “spinon” excitation energies $\varepsilon^s(k)$ have a minimum at $k = k_0$. For a rectangular lattice, $k_0$ must be chosen close to one of the four points obtained from: $(\pm \frac{\pi}{a}, \pm \frac{\pi}{a})$ by the tetragonal group operations, thus breaking tetragonal and parity (P) symmetry within a plane. If $\varepsilon^s(k_0) = 0$ one gets an AF state, and if $\varepsilon^s(k_0) > 0$ one gets a “spin-fluctuation” (SF) state, characterized by AF fluctuations. The SF state is stabilized for sufficient “doping”.

Bonding effects result in strong correlations between the $e$ and $s$ fields, and quasiparticles based on binding between them. One type of quasiparticles, referred to here as “semi-MFA carriers”, is obtained by treating the correlations between the $e$ and $p$ and $s$ fields in lowest order, and approximating the higher order bilinear products of $e$ operators...
by their expectation values. Let us introduce:

$$\delta_o(\sigma k) = \beta_k^\sigma \left\{ \exp(i\phi_k^\sigma) s_o(\sigma k) + \exp(-i\phi_k^\sigma) s_o(-\sigma k) \right\},$$

where $\sigma$ is assigned values $\pm 1$, $\phi_k^\sigma$ are chosen to minimize free energy, and $\beta_k^\sigma$ are normalization factors. Annihilation operators of semi-MFA basis states of wave vector $k$, are:

$$f_o(k', k) = c_o(k') e(k - k'),$$

$$q_o(k', k) = c_o(k') p_o(k - k'),$$

and $c_o(k)$. These operators satisfy fermion anticommutation relations if in final expressions bilinear products of $s$ operators are approximated by their expectation values [1].

In the absence of $c-f$ and $c-q$ hybridization, the $f$ and $q$ contributions to the semi-MFA excitation energies $\varepsilon_o^f(k)$ form quasi-continuous ranges of bands, corresponding to the upper and lower Hubbard bands. The $k$-dependence of each of these bands is quite flat, while bonding energy results in the width of the range of bands. When hybridization is turned on, while in an AF state $E_p$ remains in a Hubbard-type gap, in a SF state part of $\varepsilon_o^f(k)$ still resemble Hubbard bands, and part of them pass through $E_p$ and resemble LDA bands (though they are flatter) in agreement with spectroscopic results [1].

Another type of fermion quasiparticles is of "spinless polarons", resulting from the trapping of $e$ ($p$) carriers by neighboring $s$ spins and a local lattice deformation [4]. The semi-MFA and polaron states must be orthogonalized to each other. Transitions between them require spinon $\tilde{e}^s(k)$ excitations. In an AF state $\tilde{e}^s(k_0)=0$, and the polaron energies are at $E_p$, within the gap in $\tilde{e}^f(k)$. The polaron then form an incoherent gas, and transport is non-metallic.

On the other hand, in a SF state, though both semi-MFA and polaron energies are found very close to $E_p$, the existence of $\tilde{e}^s(k_0)>0$ provides a gap for transitions between them. In this state the polaron form a coherent liquid [5] of a very small band-width (estimated to be $\gtrsim 10$ meV). The polaron band is restricted to a CuO$_2$ plane (including the apical O atom), while the semi-MFA bands are three-dimensional (though interplanar coherence may not be maintained above $T_c$) and include the effect of hybridization with interlayer orbitals.

Since a spin-wave excitation consists of two spinons, the 41 meV excitation peak observed [6] at $k \cong (\frac{\pi}{2}, \frac{\pi}{2})$ by neutron scattering in YBa$_2$Cu$_3$O$_7$ is interpreted as $2\tilde{e}^s(k_0)$. This peak is strongly damped above $T_c$ since the spinon operators [1] do not commute with the semi-MFA operators (2).

### 3. SPECTROSCOPIES

Let $A^f_o(k, \epsilon)$ and $A^q_o(k, \epsilon)$ be the contribution of semi-MFA states to the spectral functions for emission of electrons and holes, respectively. They depend on self-consistent parameters determined to minimize free energy. In a SF state, at a given $k$, a spectral function peak which straddles $E_p$ consists of energies $\tilde{e}^f_o(k)$ of varying degrees of bonding. If the center of the peak is below $E_p$, then free-energy minimization will introduce to it such a width that the energies of minimal bonding will be pushed above $E_p$.

This explains the linewidths observed in angle-resolved photoemission (ARPES) results [1,7]. The minimal peak width $\Delta \tilde{e}^f_o(T)$ at temperature $T$, when $\tilde{e}^f_o(k)\rightarrow E_p$, should exceed $\sim \sqrt{\frac{k_B T}{a}}$. By assuming a linear dependence of the peak's shape on $[\tilde{e}^f_o(k)]$, for $[\tilde{e}^f_o(k)] > \Delta \tilde{e}^f_o(T)$, and saturation for $[\tilde{e}^f_o(k)] < \Delta \tilde{e}^f_o(T)$, we get that $A^f_o(k, \epsilon)$ can be sealed around $E_p$ [1] in terms of a shape function $\tilde{A}^f_o$ ($\tilde{A}^f_o(T)$):

$$A^f_o(k, \epsilon) \approx \begin{cases} \tilde{A}^f_o(k) \frac{[\tilde{e}^f_o(k)]}{\Delta \tilde{e}^f_o(T)}, & \text{if } [\tilde{e}^f_o(k)] > \Delta \tilde{e}^f_o(T) \\
\tilde{A}^f_o(k) \frac{[\tilde{e}^f_o(k)]}{\Delta \tilde{e}^f_o(T)}, & \text{if } [\tilde{e}^f_o(k)] < \Delta \tilde{e}^f_o(T), \end{cases}$$

$$\Delta \tilde{e}^f_o(T) \approx \max \left\{ \Delta \tilde{e}^f_o(0), \tilde{e}^f_o k_B T \right\},$$

where $\tilde{e}^f_o \sim 1$, and $\Delta \tilde{e}^f_o(0)$ depends on stoichiometry. This accounts [1] for the observed behavior of the spin susceptibility $\chi_p$, and the imaginary part of generalized susceptibilities $\chi''(q, \omega)$. For $\tilde{e}^f_o k_B T > \Delta \tilde{e}^f_o(0)$, one expects Fermi-liquid like behavior of $\chi_p$, and marginal-Fermi-liquid like behavior of $\chi''(q, \omega)$. For $\Delta \tilde{e}^f_o(0) > \tilde{e}^f_o k_B T$ one gets a behavior reminiscent of a pseudogap.

The observation of "extended van Hove singularities" near $E_p$ in ARPES results [8] is interpreted here as the effect of renormalization of LDA saddle-point singularities due to spin and lattice effects related to the existence of the spinless polarons. It turns out that the symmetry of the polaron lattice deformation [9] corresponds to the $k$ point where the singularity is observed [8]. Thus the renormalization of the singularity is due to a dynamic Jahn-Teller effect [10] allowing free energy reduction due to coupling between the polaron and semi-MFA states. This amplifies the compatible effect of AF fluctuations on the singularity [11]. A related effect is the appearance of "shadow bands" in ARPES results [12].

The direct contribution of polaron states to the spectral functions includes also the effect of spinon