A Theory for the High-$T_c$ Cuprates: Anomalous Normal-State and Spectroscopic Properties, Phase Diagram, and Pairing

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Abstract A theory of highly correlated layered superconducting materials is applied for the cuprates. Differently from an independent-electron approximation, their low-energy excitations are approached in terms of auxiliary particles representing combinations of atomic-like electron configurations, where the introduction of a Lagrange Bose field enables treating them as bosons or fermions. The energy spectrum of this field accounts for the tendency of hole-doped cuprates to form stripe-like inhomogeneities. Consequently, it induces a different analytical behavior for auxiliary particles corresponding to “antinodal” and “nodal” electrons, enabling the existence of different pairing temperatures at $T^*$ and $T_c$. This theory correctly describes the observed phase diagram of the cuprates, including the non-Fermi-liquid (non-FL) to FL crossover in the normal state, the existence of Fermi arcs below $T^*$ and of a “marginal-FL” critical behavior above it. The qualitative anomalous behavior of numerous physical quantities is accounted for, including kink- and waterfall-like spectral features, the drop in the scattering rates below $T^*$ and more radically below $T_c$, and an effective increase in the density of carriers with $T$ and $\omega$, reflected in transport, optical and other properties. Also is explained the correspondence between $T_c$, the resonance-mode energy, and the “nodal gap”.

Keywords Superconductivity · Cuprates · Auxiliary particles · Anomalies · Pairing

1 Introduction

High-$T_c$ superconductivity (SC) has been in the forefront of condensed-matter physics research since its discovery in the cuprates over 23 years ago. This system is characterized by anomalous behavior of many of its physical properties [1–15] which led to the suggestion of non-Fermi-liquid (non-FL) models [16–19] for its electronic structure. The recent discovery of high-$T_c$ SC in iron-based compounds (referred to below as FeSCs), provides a new test case for high-$T_c$ theories, especially in view [20] of the striking similarity of their anomalous properties to those of the cuprates.

Recently, a unified theory for the cuprates and the FeSCs has been derived [20] on the basis of common features in their electronic structures, including quasi-two-dimensionality, and the large-$U$ nature of the electron orbitals close to the Fermi level ($E_F$). Electrons of such orbitals cannot be treated through a mean-field independent-particle approach; therefore, their behavior is studied in terms of auxiliary particles, representing combinations of atomic-like electron configurations.

Within this auxiliary-particles method [21], configurations in sites $i$ can be, approximately, treated as bosons or fermions, if each site is mathematically constrained to be occupied by one (and only one) configuration. There is a freedom in choosing configurations of an odd number of electrons as fermions, and of an even number of electrons as bosons, or vice versa [20]. The choice here is that configurations corresponding to undoped cuprates or FeSCs (thus the parent compounds) are bosons.

These auxiliary particles have been treated beyond mean-field theory [18]. A grand-canonical Hamiltonian $\mathcal{H}$ has been written down [20], where (in addition to the chemical potential $\mu$) a field of Lagrange multipliers $\lambda_i$ was introduced ($\lambda \equiv \langle \lambda_i \rangle$) to maintain the above auxiliary-particles’
constraint. This Lagrange field represents an effective fluctuating potential which enables the treatment of the above configurations as bosons or fermions; its effect on them is analogous to the effect of vibrating atoms on electrons, and similarly to lattice dynamics, this is a Bose field [20] (see discussion about it below).

These auxiliary particles are assigned the following ad hoc names [20]: (i) combinations of boson atomic-like configurations are referred to as “sivions”; their Bose condensation results in static or dynamical inhomogeneities which could be manifested in the existence of a commensurate or an incommensurate resonance mode [20]; (ii) combinations of fermion atomic-like configurations are referred to as “quasi-electrons” (QEs); they carry charge \(-e\) and are introduced through electron or hole doping (in the second case the configurations correspond to holes of QEs); (iii) the Lagrange-field bosons are referred to as “lagrons”, and their coupling to the sivions and QEs provides a dynamical enforcement of the auxiliary-particles’ constraint.

Stripe-like inhomogeneities have been observed [22–29] within the phase diagram of the cuprates. Even though such an inhomogeneous behavior is often dynamical within the SC regime, it is not treated here as a perturbation to a homogeneous state, but as a correction to a static inhomogeneous structure. The application of the constraint, approached here through the Lagrange field, must take into account the existence of these inhomogeneities. This results in a multi-component scenario.

In small-\(U\) systems, where low-energy electrons are appropriate quasiparticles (QPs), the FLEX approximation [30] could be applied [31] to derive an effective pairing interaction between them, due to their own spin and charge fluctuations. The low-energy large-\(U\) electrons, discussed here, cannot be considered as appropriate QPs; but their description in terms of independent auxiliary Fermi and Bose fields provides an intrinsic pairing mechanism through QE-lagron coupling; it can be treated [20] within the Migdal–Eliashberg theory [32–34], similarly to electron–phonon coupling in the case of phonon-induced pairing, but with coupling constants which are so strong that lattice instabilities would have been driven in the electron–phonon case.

In this paper auxiliary particles which are specific for the cuprates are introduced, and their Green’s functions are applied to derive those of the electrons. The detailed QE and electron spectral functions are calculated, with further emphasis on the anomalous low-energy features. The QE, sivion and electron scattering rates are derived in the non-FL regime, and the resulting physical anomalies are discussed. \(\mathcal{H}\) is then applied to derive QE and electron pairing which is demonstrated to result in the distinct pseudo-gap (PG) and SC phases; the associated anomalous physical behavior is discussed. Further calculations on part of these aspects (specifically in the paired states) will appear in separate papers.

### 2 Hamiltonian

Electronic-structure calculations, and a variety of experimental data, indicate that the “universal” (thus not characteristic of just specific compounds) low-energy properties of the cuprates are primarily determined by \(\text{Cu}(d)\) and \(\text{O}(p)\) orbitals of the \(\text{CuO}_2\) planes. Within the LDA, these orbitals generate a multiple-band structure extending over a range of [35] about 9 eV. However, the electronic states at the vicinity of \(E_F\) dominantly reside [35–37] in one of these bands, of Wannier functions [38] which are centered at the planar \(\text{Cu}\) atoms, and correspond mainly to \(\sigma\)-antibonding states between \(\text{Cu}(d_{x^2−y^2})\) and \(\text{O}(p_x, p_y)\) orbitals (though a minor contribution of other orbitals exists as well). Due to this orbital nature of the band, its treatment requires effective transfer (hopping) integrals up to the third-nearest neighbor (see below).

The effective intra-site Coulomb parameter \(U\), for electrons in this band, corresponds to its Wannier functions which are, primarily, combinations of \(\text{Cu}(d)\) and \(\text{O}(p)\) functions. Estimates of \(U\) must take into account the fact that the \(d\) intra-atomic integral \(U_d\) is considerably larger than the \(p\) integral \(U_p\). In an early derivation of the effective one-band Hamiltonian [39] in hole-doped cuprates, the large-\(U_d\) and small-\(U_p\) limits have been assumed, resulting in approximately ionic \(\text{Cu}(d)\) and itinerant \(\text{O}(p)\) states. The resulting [39] upper Hubbard band corresponds to \(\text{Cu}^{+1}\) ions, and the lower Hubbard band to \(\text{Cu}^{+2}\) ions, part of which are forming singlet states with the doped \(\text{O}(p)\) holes (known as “Zhang–Rice singlets”).

Consequently, the value of \(U\), derived through this analysis, consists of \(U_d\) plus corrections, due to the singlet energy and the difference between the one-electron \(p\) and \(d\) energies which are considered to be substantially smaller. A more realistic evaluation of \(U\) would result in a somewhat smaller value than \(U_d\); however, since the width of the effective band, within a two-dimensional (2D) Brillouin zone (BZ), is [35–37] about 3 eV, it is appropriate to treat it using a large-\(U\) approach.

Within this one-band approach, a 2D square lattice of \(N\) sites \(i\) is considered (assuming translational symmetry between them); the \(\text{Cu}\) atoms are located at the lattice points \(\mathbf{R}_i\), generated by the unit vectors \(a\mathbf{x}\) and \(a\mathbf{y}\). An electron of spin \(\sigma\) in site \(i\) is created by \(d_{i\sigma}^\dagger\) (the two spin states are denoted as \(\sigma = \uparrow, \downarrow\), or \(\sigma = \pm 1\)). The Hamiltonian is expressed as:

\[
\mathcal{H} = \sum_{\sigma} \left[ (e_d - \mu) d_{i\sigma}^\dagger d_{i\sigma} + \sum_{j \neq i} t(\mathbf{R}_i - \mathbf{R}_j) d_{j\sigma}^\dagger d_{i\sigma} \right] + \frac{1}{2} U d_{i, -\sigma}^\dagger d_{i\sigma}^\dagger d_{i\sigma} d_{i, -\sigma},
\] 

(1)