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# Spin fluctuations and high-temperature superconductivity in cuprates

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ABSTRACT

To describe the cuprate superconductors, models of strongly correlated electronic systems, such as the Hubbard or $t-J$ models, are commonly employed. To study these models, projected (Hubbard) operators have to be used. Due to the unconventional commutation relations for the Hubbard operators, a specific kinematical interaction of electrons with spin and charge fluctuations emerges. The interaction is induced by the intraband hopping with a coupling parameter of the order of the kinetic energy of electrons $W$ which is much larger than the antiferromagnetic exchange interaction $J$ induced by the interband hopping. This review presents a consistent microscopic theory of spin excitations and superconductivity for cuprates where these interactions are taken into account within the Hubbard operator technique. The low-energy spin excitations are considered for the $t$–$J$ model, while the electronic properties are studied using the two-subband extended Hubbard model where the intersite Coulomb repulsion $V$ and electron-phonon interaction are taken into account.



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## 1. Introduction

Discovery of high-temperature superconductivity (HTSC) in cuprates by Bednorz and Müller [1] caused an unprecedented scientific activity in study of this extraordinary phenomenon (see, e.g., Refs. [2,3]). In recent years intensive experimental investigations have presented detailed information concerning unconventional physical properties of cuprates. However, theoretical studies of various microscopical models have not yet brought about a commonly accepted theory of superconductivity in cuprates. Two most frequently discussed mechanisms of HTSC are the conventional electron-phonon pairing (see, e.g., Refs. [4,5]) and the spin-fluctuation mediated pairing [6,7] in the framework of phenomenological spin-fermion models (see, e.g., Refs. [8–11]). A weak intensity of spin fluctuations at optimal doping found in the magnetic inelastic neutron scattering experiments [12] is the main argument against the spin-fluctuation pairing mechanism. However, recent magnetic resonant inelastic x-ray scattering (RIXS) experiments have revealed that paramagnon antiferromagnetic (AF) excitations persist with a similar dispersion and comparable intensity in a large family of cuprate superconductors, even in the overdoped region (see, e.g., Refs. [13–17]). These experiments prove that spin fluctuations have sufficient strength to mediate HTSC in cuprates and to explain various physical properties of cuprate materials such as, the "kink" phenomenon observed in the electronic spectrum by the angle-resolved photoemission spectroscopy [18], the optical and dc conductivity [19], etc. Therefore, we can assume that the spin-fluctuation mediated pairing plays the major role while the electron-phonon pairing is less important. This assumption is supported by observation of the weak isotope effect in optimally doped samples (see reviews [20–22]).

The main problem in a theoretical study of the cuprate superconductors is that strong electron correlations there precludes from application of the conventional Fermi-liquid approach in description of their electronic structure [23]. They are Mott–Hubbard (more accurately, charge-transfer) insulators where the conduction band splits into two Hubbard subbands where the projected (Hubbard) electronic operators should be used. Recently we have developed a microscopic theory of spin excitations and superconductivity for cuprates within the Hubbard operator (HO) technique [3,24–29]. We demonstrate an important role of the kinematical interaction for the HOs induced by the non-Fermy commutation relations for electronic operators, both for studying the spin excitations and electron spectrum. In this review we present the results of these investigations.

First, in Section 2, we explain how the kinematical interaction appears in the Hubbard model in the limit of strong electron correlations. Then in Section 3 we formulate a theory of spin excitations within the relaxation-function approach for calculation of the dynamical spin susceptibility (DSS) in the normal and superconducting states [24,25]. The spin dynamics at arbitrary frequencies and wave vectors is studied for various temperatures and hole doping. In the superconducting state, the DSS reveals the magnetic resonance mode at the AF wave vector $\mathbf{Q} = \pi(1,1)$ at low doping. We show that it can be observed even above superconducting $T_c$ due to its weak damping. This is explained by an involvement of spin excitations in the decay process besides the particle-hole continuum usually considered in the random-phase-type approximation where the resonance mode can appear only below $T_c$.

In the second part of the paper, in Sections 4 and 5, a theory of the electronic spectrum and superconductivity is presented within the Mori-type projection technique for the single-particle electronic Green functions (GFs) [27–29]. We consider the extended Hubbard model where the intersite Coulomb repulsion and the electron-phonon interaction are taken into account. An exact Dyson equation for the normal and anomalous (pair) GFs is derived which is solved in the self-consistent Born approximation (SCBA) for the self-energy. We found the *d*-wave pairing with high-$T_c$ mediated by the kinematical spin-fluctuation interaction which can be suppressed only for a large intersite Coulomb repulsion $V > W$. Isotope effect on $T_c$ induced by electron-phonon interaction is weak at optimal doping and increases at low doping. We emphasize that the kinematical interaction is absent in the spin-fermion models and is lost in the slave-boson (-fermion) models treated in the mean-field approximation (MFA). In conclusion we summarize our results.

## 2. Kinematical interaction in the Hubbard model

We consider the extended Hubbard model [30] on a square lattice

$$H = \sum_{i\neq j,\sigma} t_{ij}\, a^{\dagger}_{i\sigma} a_{j\sigma} - \mu \sum_i N_i + (U/2) \sum_{i,\sigma} N_{i\sigma} N_{i\bar{\sigma}} + (1/2) \sum_{i\neq j} V_{ij} N_i N_j, \tag{1}$$

where $t_{i,j}$ is the single-electron hopping parameter, $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ are the Fermi creation and annihilation operators for electrons with spin $\sigma/2$ ($\sigma = \pm 1$), $\bar{\sigma} = -\sigma$) on the lattice site $i$, $U$ is the on-site Coulomb interaction (CI) and the $V_{ij}$ is the intersite CI. $N_i = \sum_\sigma N_{i\sigma}$, $N_{i\sigma} = a^{\dagger}_{i\sigma} a_{i\sigma}$ is the number operator and $\mu$ is the chemical potential.

In the strong correlation limit, $U \gg |t_{i,j}|$, the Fermi operators $a^{\dagger}_{i\sigma}$, $a_{i\sigma}$ in (1) fail to describe single-particle electron excitations in the system and the HOs [31], referring to the singly occupied and doubly occupied subbands, should be used: $a^{\dagger}_{i\sigma} = a^{\dagger}_{i\sigma}(1 - N_{i\bar{\sigma}}) + a^{\dagger}_{i\sigma} N_{i\bar{\sigma}} \equiv X^{\sigma 0}_i + \sigma X^{2\bar{\sigma}}_i$. In terms of the HOs the model (1) reads

$$H = \varepsilon_1 \sum_{i,\sigma} X^{\sigma\sigma}_i + \varepsilon_2 \sum_i X^{22}_i + \frac{1}{2} \sum_{i\neq j} V_{ij} N_i N_j + \sum_{i\neq j,\sigma} t_{ij} \left\{ X^{\sigma 0}_i X^{0\sigma}_j + X^{2\sigma}_i X^{\sigma 2}_j + \sigma \left( X^{2\bar{\sigma}}_i X^{0\sigma}_j + \text{H.c.} \right) \right\}, \tag{2}$$

where $\varepsilon_1 = -\mu$ is the single-particle energy and $\varepsilon_2 = U - 2\mu$ is the two-particle energy. The matrix HOs $X^{\alpha\beta}_i = |i\alpha\rangle\langle i\beta|$ describes transition from the state $|i,\ \beta\rangle$ to the state $|i,\ \alpha\rangle$ on a lattice site $i$ taking into account four possible states for holes: an empty state ($\alpha, \beta = 0$), a singly occupied hole state ($\alpha, \beta = \sigma$), and a doubly occupied hole state ($\alpha, \beta = 2$). The number operator and the spin operators in terms of the HOs are defined as

$$N_i = \sum_\sigma X^{\sigma\sigma}_i + 2X^{22}_i, \tag{3}$$

$$S^{\sigma}_i = X^{\sigma\bar{\sigma}}_i, \quad S^{z}_i = (\sigma/2)\left[X^{\sigma\sigma}_i - X^{\bar{\sigma}\bar{\sigma}}_i\right]. \tag{4}$$

To compare our results with cuprates, we consider the hole-doped case where the chemical potential $\mu$ is determined by the equation for the average hole occupation number

$$n = 1 + \delta = \langle N_i \rangle. \tag{5}$$

Here $\langle \ldots \rangle$ denotes the statistical average with the Hamiltonian (2).

From the multiplication rule for the HOs, $X^{\alpha\beta}_i X^{\gamma\delta}_i = \delta_{\beta\gamma} X^{\alpha\delta}_i$, it follows their commutation relations

$$\left[ X^{\alpha\beta}_i, X^{\gamma\delta}_j \right]_{\pm} = \delta_{ij} \left( \delta_{\beta\gamma} X^{\alpha\delta}_i \pm \delta_{\delta\alpha} X^{\gamma\beta}_i \right), \tag{6}$$

with the upper sign for the Fermi-type operators (such as $X^{0\sigma}_i$) and the lower sign for the Bose-type operators (such as the number or