Kinematic Spin-Fluctuation Mechanism of High-Temperature Superconductivity

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1. INTRODUCTION

One of crucial issues in the superconductivity theory is to disclose the mechanism of high-temperature superconductivity (HTSC) in cuprates (see, e.g., [1, 2]). In early studies of the problem, a model of strongly correlated electrons was proposed by Anderson [3], where superconductivity occurs at finite doping in the resonating valence bond state due to the antiferromagnetic (AF) superexchange interaction \( J \). However, the intersite Coulomb interaction \( V \) that in cuprates is of the order of \( J \) may destroy the resonating valence bond state and superconducting pairing. Recently, a competition of the intersite CI \( V \) and pairing induced by the on-site CI \( U \) in the Hubbard model has been actively discussed. In particular, it was stressed in [5] that a contribution from the repulsive well-screened weak CI in the first order strongly suppresses the pairing induced by contributions of higher orders, and a possibility of superconductivity “from repulsion” was questioned. Using the renormalization group method, the extended Hubbard model with CI \( V \) was studied in [6], where superconducting pairing of various symmetries, extended \( s - p \), and \( d \)-wave types was found depending on the electron concentration and \( V \). Following the original idea of Kohn–Luttinger [7], it was shown in [8] that the \( p \)-wave superconductivity exists in the electronic gas at low density with a strong repulsion \( U \) and a relatively strong intersite CI \( V \) (also see [9] and the references therein). Studies of the phase diagram within the extended Hubbard model in the weak correlation limit have shown that superconducting pairing of different types of symmetry, \( s - p - d_{x^2 - y^2} \), can occur depending on the CI between the nearest \( V_1 \) and the next \( V_2 \) neighbor sites and electron hopping parameters between distant sites in a broad region of electron concentration [10].

However, the Fermi-liquid model was considered in the weak correlation limit \( U \ll W \) in these investigations, while cuprates are Mott–Hubbard (more accurately, charge-transfer) doped insulators, where a theory of strongly correlated electronic systems should be applied for \( U \gg W \). Here, \( W \sim 4t \) is the electronic kinetic energy for the two-dimensional Hubbard model with the nearest-neighbor hopping parameter \( t \). In the limit of strong correlations, various numerical methods for finite clusters are commonly used. There are many investigations of the conventional Hubbard model (see, e.g., [11–14]), but only a few studies of the extended Hubbard model in which the intersite CI \( V \) is taken into account. In particular, in [15–17], the extended Hubbard model was considered in a broad region of \( U \) and \( V \). The results in [15, 16] show that a strong on-site repulsion \( U \) effectively enhances the \( d \)-wave pairing, which is preserved for large values of \( V \gg J \). In [17], using the slave-boson representation, it was found that superconductivity is destroyed at a small value of \( V = J \). We discuss these results in more detail in Sec. 4.3 by comparing them with our findings.

In our recent paper [18], we studied the extended Hubbard model in the limit of strong correlations by taking the CI \( V \) and electron–phonon coupling into account. It was found that the high-\( T_c \) \( d \)-wave pairing is mediated by the strong kinematic interaction of...
electrons with spin fluctuations. Contributions coming from a weak CI $V$ and phonons turned out to be small since only $l = 2$ harmonics of the interactions make a contribution to the $d$-wave pairing.

In this paper, we consider superconductivity in the two-dimensional extended Hubbard model with a large intersite Coulomb repulsion $V$ in the limit of strong correlations to elucidate the spin-fluctuation mechanism of high-temperature superconductivity. We argue that in the two-subband regime for the Hubbard model with $U \geq 6t$, a spin-electron kinematic interaction results from complicated commutation relations for the Hubbard operators (HOs) [19]. This interaction leads to the weak exchange interaction $J = 4t^2/U$ due to interband hopping, and at the same time intraband hopping results in a much stronger kinematic interaction $g_{sd} \sim W$ of electrons with spin excitations. Therefore, the exchange interaction $J$ is not so important for the spin-fluctuation pairing driven by the strong kinematic interaction $g_{sd}$. We calculate the doping dependence of the superconducting transition temperature for various values of $U$ and $V$ and show that as long as $V$ does not exceed the kinematic interaction, $V \lesssim W$, the $d$-wave pairing is preserved. In calculations, we use the Mori-type projection technique [20] in the equation-of-motion method for thermodynamic Green’s functions (GFs) [21] expressed in terms of the HOs. The self-energy in the Dyson equation is calculated in the self-consistent Born approximation (SCBA) as in our previous publications [18, 22].

In Section 2, the two-subband extended Hubbard model is introduced and equations for the GFs in the Nambu representation are derived. A self-consistent system of equations for GFs and the self-energy is formulated in Section 3. Results and discussion are presented in Section 4. Concluding remarks are given in Section 5.

2. GENERAL FORMULATION

2.1. Extended Hubbard Model

We consider the extended Hubbard model on a square lattice,

$$H = \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - \mu \sum_i N_i$$

$$+ \frac{U}{2} \sum_i N_{i\sigma} N_{i\bar{\sigma}} + \frac{1}{2} \sum_{i,j} V_{ij} N_i N_j,$$

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

In the strong correlation limit, the model describes the Mott--Hubbard insulating state at half-filling ($n = \langle N \rangle = 1$) when the conduction band splits into two Hubbard subbands. In this case, the Fermi operators $a_{i\sigma}^\dagger$ and $a_{i\sigma}$ in (1) fail to describe single-particle electron excitations in the system and the Fermi-liquid picture becomes inapplicable to cuprates. The projected-type operators, the HOs, referring to the two subbands, singly occupied $a_{i\sigma}^\dagger (1 - N_{i\bar{\sigma}})$ and doubly occupied $a_{i\sigma}^\dagger N_{i\bar{\sigma}}$, must be introduced. In terms of the HOs, model (1) becomes

$$H = \varepsilon_1 \sum_i X_{i}^{\sigma\sigma} + \varepsilon_2 \sum_i X_{i}^{22} + \frac{1}{2} \sum_{i,j} V_{ij} N_i N_j$$

$$+ \sum_{i,j,\sigma} t_{ij} \{ X_{i}^{\sigma0} X_{j}^{0\sigma} + X_{i}^{\sigma2} X_{j}^{2\sigma} + \sigma(X_{i}^{\sigma2} X_{j}^{2\sigma} + H.c.) \},$$

where $\varepsilon_1 = -\mu$ is the single-particle energy and $\varepsilon_2 = U - 2\mu$ is the two-particle energy. The matrix HO $X_{i}^{\alpha\beta} = |i\alpha\rangle \langle \beta i|$ describes transition from the state $|i, \alpha\rangle$ to the state $|i, \alpha\rangle$ on a lattice site $i$ taking four possible states for holes into account: an empty state ($\alpha = \beta = 0$), a singly occupied hole state ($\alpha, \beta = 1$), and a doubly occupied hole state ($\alpha, \beta = 2$). The number operator and the spin operators are defined in terms of the HOs as

$$N_i = \sum_{\sigma} X_i^{\sigma\sigma} + 2X_i^{22},$$

$$S_i^\sigma = X_i^{\sigma\sigma}, \quad S_i = (\sigma/2)\{X_i^{\sigma\sigma} - X_i^{\bar{\sigma}\bar{\sigma}}\}.$$  

The chemical potential $\mu$ is determined from the equation for the average occupation number for holes

$$n = 1 + \delta = \langle N \rangle,$$

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

The HOs obey the completeness relation $X_{i}^{00} + \sum_{\sigma} X_{i}^{\sigma\sigma} + X_{i}^{22} = 1$, which rigorously preserves the constraint that only one quantum state $\alpha$ can be occupied on any lattice site $i$. The commutation relations for the HOs

$$[X_{i}^{\alpha\beta}, X_{j}^{\delta\gamma}]_\pm = \delta_{ij}\delta_{\delta\gamma}X_{i}^{\bar{\epsilon}\delta} \pm \delta_{\alpha\delta}X_{i}^{\alpha\bar{\gamma}}),$$

with the upper sign for Fermi-type operators (such as $X_{i}^{\alpha\beta}$) and the lower sign for Bose-type operators (such as $N_i$ in (3) or the spin operators in (4)), result in the so-called kinematic interaction. To demonstrate this,