

# Spin excitations and mechanisms of superconductivity in cuprates

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A microscopic theory of spin excitations in strongly-correlated electronic systems within the  $t$ - $J$  model is discussed. An exact representation for the dynamic spin susceptibility is derived. In the normal state, the excitation spectrum reveals a crossover from spin-wave-like excitations at low doping to overdamped paramagnons above the optimal doping. At low temperatures, the resonance mode at the antiferromagnetic wave vector  $\mathbf{Q} = \pi(1, 1)$  emerges which is explained by a strong suppression of the spin excitation damping caused by a spin gap at  $\mathbf{Q}$  rather than by opening of a superconducting gap. A major role of spin excitations in the  $d$ -wave superconducting pairing in cuprates is stressed in discussing mechanisms of high- $T_c$  superconductivity within the Hubbard model in the limit of strong correlations, while electron-phonon interaction and a well-screened weak Coulomb interaction are not essential.

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## I. INTRODUCTION

Recent studies of electron and spin-excitation spectra using angle-resolved photoemission (ARPES) and inelastic neutron scattering (INS) have revealed an important role of antiferromagnetic (AF) spin excitations in the “kink” phenomenon and the  $d$ -wave pairing in cuprates. In particular, in Ref. [1] quantitative analysis of the AF spin-excitation spectrum measured by INS and of ARPES data for the spin-fermion coupling of the same  $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$  ( $\text{YBCO}_{6.6}$ ) crystal were used for numerical solution of the Eliashberg-type equations. The superconducting transition temperature was found to exceed  $T_c = 150$  K.

The main argument against the spin-fluctuation pairing mechanism, a weak intensity of spin fluctuations at the optimal doping seen in INS experiments [2], was dismissed in recent resonant inelastic x-ray scattering [3]. In a large family of cuprates paramagnon AF excitations with dispersions and spectral weights similar to those of magnons in undoped cuprates were found. A numerical solution of the Eliashberg equations for the magnetic spectrum found in  $\text{YBCO}_7$  and for the electron-spin interaction described by the  $t$ - $J$  model results in  $T_c = 100 - 200$  K. These calculations based on experimental data demonstrate that spin fluctuations have sufficient strength to mediate high-temperature superconductivity in cuprates and, therefore, alternative mechanism based on electron-phonon interaction (EPI) (see, e.g., [4]) seems to play a secondary role in cuprate superconductivity. Strong EPI observed in polaronic effects in cuprates may be irrelevant for the  $d$ -wave pairing mediated by  $l = 2$  component of EPI as pointed out in Ref. [5].

In this report we briefly consider a microscopic theory of spin-excitation spectrum in strongly correlated electronic systems (SCES) [6, 7]. Using a model for the spin-

excitation spectrum, we consider spin-fluctuation pairing within the Hubbard model in the limit of strong correlations,  $U \gg t$  [8, 9]. To compare various mechanisms of superconducting  $d$ -wave pairing, we take into account also EPI and a well-screened weak Coulomb interaction considered in Ref. [10]. We show that the latter gives a small contribution for the  $d$ -wave pairing and cannot suppress the superconductivity.

## II. SPIN-EXCITATION SPECTRUM

To describe the low-energy spin excitations in SCES the one-subband  $t$ - $J$  model can be used:

$$H = \sum_{i \neq j, \sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \frac{1}{2} \sum_{i \neq j} J_{ij} (\mathbf{S}_i \mathbf{S}_j - \frac{n_i n_j}{4}), \quad (1)$$

where  $t_{ij}$  is the hopping integral and  $J_{ij}$  is the exchange interaction. Here  $\hat{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - n_{i,-\sigma})$  are the projected Fermi operators acting in the the singly occupied subband and  $n_i = \sum_\sigma n_{i,\sigma}$ ,  $n_{i,\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ .  $S_i^\alpha = (1/2) \sum_{\sigma\sigma'} \hat{c}_{i\sigma}^\dagger \tau_{\sigma\sigma'}^\alpha \hat{c}_{i\sigma'}$  are the spin-1/2 operators where  $\tau_{\sigma\sigma'}^\alpha$  are the Pauli matrices,  $\sigma = \pm 1$ .

Using the projection technique for the Kubo-Mori relaxation functions, an exact representation for the dynamical spin susceptibility (DSS), the retarded Green function (GF) of the transverse spin-density operators  $S_{\mathbf{q}}^\pm = S_{\mathbf{q}}^x \pm iS_{\mathbf{q}}^y$ , can be derived [6] (see also [11]):

$$\chi(\mathbf{q}, \omega) = -\langle\langle S_{\mathbf{q}}^+ | S_{-\mathbf{q}}^- \rangle\rangle_\omega = \frac{m(\mathbf{q})}{\omega_{\mathbf{q}}^2 + \omega \Sigma(\mathbf{q}, \omega) - \omega^2}, \quad (2)$$

where  $m(\mathbf{q}) = \langle\langle [i\dot{S}_{\mathbf{q}}^+, S_{-\mathbf{q}}^-] \rangle\rangle = \langle\langle [S_{\mathbf{q}}^+, H], S_{-\mathbf{q}}^- \rangle\rangle$ . The static spin-excitation spectrum  $\omega_{\mathbf{q}}$  is calculated from the equality for Kubo-Mori correlation function  $m(\mathbf{q}) = \langle\langle -\dot{S}_{\mathbf{q}}^+, S_{-\mathbf{q}}^- \rangle\rangle = \omega_{\mathbf{q}}^2 \langle\langle S_{\mathbf{q}}^+, S_{-\mathbf{q}}^- \rangle\rangle$ , where  $(-\dot{S}_{\mathbf{q}}^+, S_{-\mathbf{q}}^-)$  is evaluated in a generalized mean-field approximation [6]. The self-energy is given by the retarded GF,

$$\Sigma(\mathbf{q}, \omega) = [1/m(\mathbf{q})\omega] \langle\langle -\dot{S}_{\mathbf{q}}^+ | -\dot{S}_{-\mathbf{q}}^- \rangle\rangle_\omega^{(\text{pp})}. \quad (3)$$

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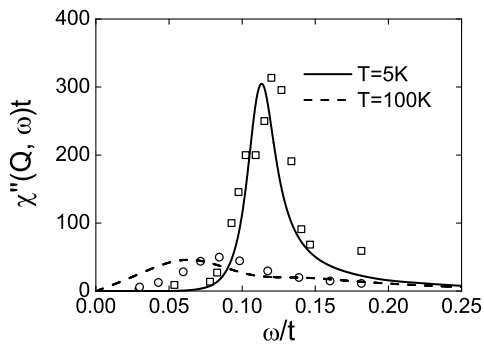


FIG. 1: Spectral function at  $\delta = 0.2$  compared with experimental data [2] at  $T = 5K$  (squares) and  $T = 100K$  (circles).

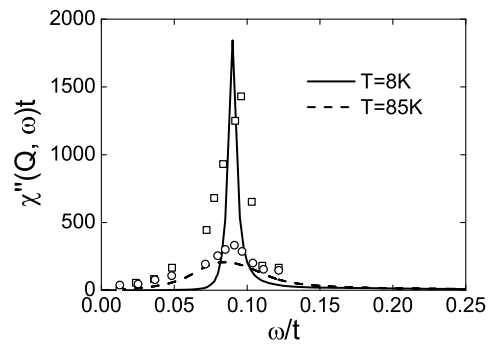


FIG. 2: Spectral function at  $\delta = 0.09$  compared with experimental data [12] at  $T = 8K$  (squares) and  $T = 85K$  (circles).

The “proper part” (pp) of the GF(3) describes the projected time evolution as in the original Mori projection technique. The self-energy (3) is defined in terms of the force operators  $-\hat{S}_i^\pm = [[S_i^\pm, (H_t + H_J)], (H_t + H_J)] \equiv \sum_\alpha F_i^\alpha$  ( $\alpha = tt, tJ, Jt, JJ$ ), where  $H_t$  and  $H_J$  are the hopping and the exchange parts of the Hamiltonian (1).

In the Heisenberg limit at zero doping,  $\delta = 0$ , the self-energy is determined by the force  $F_i^{JJ}$ . At a finite hole doping,  $\delta > 0.05$ , the largest contribution to the self-energy (3) is given by the hopping term  $F_i^{tt} = \sum_{j,n} t_{ij} \{ t_{jn} [H_{ijn}^- + H_{nji}^+] - (i \iff j) \}$ , where  $H_{ijn}^- = \hat{c}_{i\sigma}^\dagger S_j^- \hat{c}_{n\sigma} + \hat{c}_{i\downarrow}^\dagger (1 - n_{j,-\sigma}) \hat{c}_{n\uparrow}$ . We calculate the self-energy in the mode-coupling approximation (MCA),  $\langle \hat{c}_{i\sigma}^\dagger S_j^- \hat{c}_{n\sigma} | \hat{c}_{n'\sigma}^\dagger(t) S_{j'}^+(t) \hat{c}_{i'\sigma}(t) \rangle = \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i'\sigma}(t) \rangle \langle S_j^- S_{j'}^+(t) \rangle \langle \hat{c}_{n\sigma} \hat{c}_{n'\sigma}^\dagger(t) \rangle$ . In the superconducting state, the anomalous correlation functions  $\langle \hat{c}_{i,-\sigma}^\dagger \hat{c}_{i'\sigma}(t) \rangle$ ,  $\langle S_j^- S_{j'}^+(t) \rangle$ ,  $\langle \hat{c}_{n\sigma} \hat{c}_{i',-\sigma}(t) \rangle$  are also taken into account. Using the spectral representation for these two-time correlation functions both the real,  $\Sigma'(\mathbf{q}, \omega)$ , and the imaginary,  $\Sigma''(\mathbf{q}, \omega)$ , parts of the self-energy (3) are calculated [7].

The spectrum of spin excitations  $\omega_{\mathbf{q}}$  and the damping  $\Gamma_{\mathbf{q}} = -(1/2)\Sigma''(\mathbf{q}, \omega_{\mathbf{q}})$  are calculated in a broad region of temperature and doping. In the Heisenberg limit at  $\delta = 0$  the spectrum of spin excitations reveals well-defined quasiparticles with  $\Gamma_{\mathbf{q}} \ll \omega_{\mathbf{q}}$  characteristic to the Heisenberg model. However, for non-zero doping the spin-electron scattering contribution  $\Sigma_t''(\mathbf{q}, \omega)$  increases rapidly with doping and temperature and already at moderate hole concentration far exceeds the spin-spin scattering contribution  $\Sigma_j''(\mathbf{q}, \omega)$ . We conclude, that at low enough doping and low temperatures well-defined spin-wave-like excitations propagating on the AF short-range order background are observed, while for higher doping and temperatures a crossover to AF paramagnon-like spin excitations occurs as found in INS experiments.

In the superconducting state the spectral function  $\chi''(\mathbf{Q}, \omega) = \text{Im} \chi(\mathbf{Q}, \omega)$  were calculated assuming the  $d$ -wave gap function  $\Delta_{\mathbf{q}} = (\Delta/2)(\cos q_x - \cos q_y)$  [7]. The DSS (2) reveals a pronounced resonance mode (RM) at low temperatures due to a strong suppression of the

damping of spin excitations. This is explained by an involvement of a spin excitation in the decay process described by creation of three excitations: particle-hole pair with energies  $\omega_1 + \omega_2$  and a spin excitation with energy  $\omega_3$  which is controlled by the energy and momentum conservation laws,  $\omega = \omega_1 + \omega_2 + \omega_3$  and  $\mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3$ . Due to the spin gap in the spin-excitation spectrum at  $\mathbf{Q}$  the spin excitation with the energy  $\omega_3 \simeq \omega_{\mathbf{Q}}$  in this process plays a dominant role in limiting the decay of the RM in comparison with the superconducting gap in the particle-hole excitation. Since  $\omega_{\mathbf{Q}}$  shows a weak temperature dependence at  $T \lesssim T_c$  the RM does not reveal an appreciable temperature dependence and can be observed even above  $T_c$  in the underdoped region (see, e.g., [12, 13]).

Figure 1 shows the temperature dependence of the spectral functions in the overdoped case at  $\delta = 0.2$  and experimental data (symbols) for YBCO<sub>6.92</sub> [2]. The RM having a high intensity at low temperatures strongly decreases with temperature and becomes very broad at  $T \sim T_c$ . The spectral function for the underdoped case  $\delta = 0.09$  is plotted Fig. 2. The RM shows a weak temperature dependence and is still visible even at  $T = 85 \text{ K} = 1.4 T_c$  as found in YBCO<sub>6.5</sub> crystal [12].

Thus, as compared with the spin-exciton scenario for the RM based on the random-phase approximation where only electron-hole bubble diagrams are taken into account (see, e.g., [11]), we propose an alternative explanation of the RM which is driven by the spin gap at  $\mathbf{Q}$  rather than by opening of the superconducting gap.

### III. SPIN-FLUCTUATION $d$ -WAVE PAIRING

Despite of intensive search for the mechanism of high-temperature superconductivity in cuprates, there is still no commonly accepted theory (for a review see [14]). A microscopic theory of superconducting  $d$ -wave pairing mediated by AF exchange interaction and spin-fluctuations induced by kinematic interaction has been developed within the  $t$ - $J$  model in Ref. [15] and the Hubbard model in Ref. [8].

Recently, the problem of superconductivity in the repulsive Hubbard model in the weak correlation limit was discussed. In Ref. [16] an asymptotically exact solution for the  $d$ -wave pairing was found, while consideration of a well-screened weak Coulomb interaction (CI) has not shown a possibility for superconducting pairing [10]. To resolve this controversy, we have considered superconductivity in the Hubbard model in the limit of strong correlations,  $U \gg t$ , taking into account also a well-screened weak CI and EPI:

$$H = \varepsilon_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + \varepsilon_2 \sum_i X_i^{22} + \sum_{i \neq j, \sigma} t_{ij} \{ X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma (X_i^{2\bar{\sigma}} X_j^{0\sigma} + \text{H.c.}) \} + H_{c,ep}. \quad (4)$$

We introduced here the Hubbard operators (HOs)  $X_i^{\alpha\beta} = |i\alpha\rangle\langle i\beta|$  for the four states on the lattice site  $i$ : an empty state  $\alpha = |0\rangle$ , a one-hole state  $\alpha = |\sigma\rangle$  with the spin  $\sigma = \pm 1/2 = (\uparrow, \downarrow)$ ,  $\bar{\sigma} = -\sigma$ , and a two-hole state  $|2\rangle = |\uparrow\downarrow\rangle$ . To apply the model for cuprate superconductors, we introduce the single-particle energy  $\varepsilon_1 = \varepsilon_d - \mu$  as an energy of the one-hole  $d$ -state. The two-hole energy  $\varepsilon_2 = 2\varepsilon_1 + U$  is an energy of the  $p$ - $d$  singlet state where  $U = \varepsilon_p - \varepsilon_d$  is the charge-transfer energy between the oxygen  $p$  and copper  $d$  states.

The last term in (4) denotes a weak screened CI  $V(ij)$  between charge carriers in the plane and EPI  $g(ij)$  for charge carriers

$$H_{c,ep} = \frac{1}{2} \sum_{i \neq j} V(ij) N_i N_j + \sum_{i,j} g(i,j) N_i u_j, \quad (5)$$

where  $u_j$  is a displacement for a particular phonon mode.  $N_i = \sum_{\sigma} X_i^{\sigma\sigma} + 2X_i^{22}$  is the number operator. The chemical potential  $\mu$  depends on the average hole occupation number  $n = 1 + \delta = \langle N_i \rangle$ .

Using the projection technique in the equation of motion method for the GF in terms of the HOs as described in [8, 9] we can derive an exact Dyson equations for the two-subband matrix GFs. The normal GF can be written as,

$$\begin{aligned} \hat{G}(\mathbf{k}, \omega) &= \left\langle \left\langle \begin{pmatrix} X_{\mathbf{k}}^{\sigma 2} \\ X_{\mathbf{k}}^{0\bar{\sigma}} \end{pmatrix} \middle| \begin{pmatrix} X_{\mathbf{k}}^{2\sigma} & X_{\mathbf{k}}^{\bar{\sigma} 0} \end{pmatrix} \right\rangle \right\rangle_{\omega} \\ &= \left( \hat{G}_N^{-1}(\mathbf{k}, \omega) + \hat{\varphi}_{\sigma}(\mathbf{k}, \omega) \hat{G}_N(\mathbf{k}, -\omega) \hat{\varphi}_{\sigma}^*(\mathbf{k}, \omega) \right)^{-1} \hat{Q}, \\ \hat{G}_N(\mathbf{k}, \omega) &= \left( \omega \hat{\tau}_0 - \hat{\varepsilon}(\mathbf{k}) - \hat{\Sigma}(\mathbf{k}, \omega) \right)^{-1}, \end{aligned} \quad (6)$$

where  $\hat{\varepsilon}(\mathbf{k})$  is the hole energy in the mean-field approximation (MFA) and  $\hat{\Sigma}(\mathbf{k}, \omega)$  is the normal self-energy. The anomalous (pair) GF reads,

$$\begin{aligned} \hat{F}_{\sigma}(\mathbf{k}, \omega) &= \left\langle \left\langle \begin{pmatrix} X_{\mathbf{k}}^{\sigma 2} \\ X_{\mathbf{k}}^{0\bar{\sigma}} \end{pmatrix} \middle| \begin{pmatrix} X_{-\mathbf{k}}^{\bar{\sigma} 2} & X_{-\mathbf{k}}^{0\sigma} \end{pmatrix} \right\rangle \right\rangle_{\omega} \\ &= -\hat{G}_N(\mathbf{k}, -\omega) \hat{\varphi}_{\sigma}(\mathbf{k}, \omega) \hat{G}_{\sigma}(\mathbf{k}, \omega). \end{aligned} \quad (7)$$

The superconducting gap function  $\hat{\varphi}_{\sigma}(\mathbf{k}, \omega) = \hat{\Delta}_{\sigma}(\mathbf{k}) + \hat{\Phi}_{\sigma}(\mathbf{k}, \omega)$  has a nonretarded contribution  $\hat{\Delta}_{\sigma}(\mathbf{k})$  deter-

mined by the AF exchange interaction and CI in MFA and the anomalous self-energy  $\hat{\Phi}_{\sigma}(\mathbf{k}, \omega)$ .

The self-energies  $\hat{\Sigma}(\mathbf{k}, \omega)$ ,  $\hat{\Phi}_{\sigma}(\mathbf{k}, \omega)$  are calculated in the MCA by assuming an independent propagation of Fermi-like and Bose-like excitations in multiparticle GFs. Below we consider the hole-doped case,  $n = 1 + \delta > 1$ . The diagonal components of the self-energies for the two-hole subband can be written as

$$\begin{aligned} \Sigma^{22}(\mathbf{k}, \omega) &= \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{+\infty} dz K^{(+)}(\omega, z | \mathbf{q}, \mathbf{k} - \mathbf{q}) \\ &\times [-(1/\pi Q_2) \text{Im} G^{22}(\mathbf{q}, z)], \end{aligned} \quad (8)$$

$$\begin{aligned} \Phi_{\sigma}^{22}(\mathbf{k}, \omega) &= \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{+\infty} dz K^{(-)}(\omega, z | \mathbf{q}, \mathbf{k} - \mathbf{q}) \\ &\times [-(1/\pi Q_2) \text{Im} F_{\sigma}^{22}(\mathbf{q}, z)]. \end{aligned} \quad (9)$$

where  $Q_2 = n/2$  is the weight of the second subband. The kernel of these integral equations has a form, similar to the strong-coupling Eliashberg theory [17]:

$$\begin{aligned} K^{(\pm)}(\omega, z | \mathbf{q}, \mathbf{k} - \mathbf{q}) &= \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{\tanh \frac{z}{2T} + \coth \frac{\omega'}{2T}}{\omega - z - \omega'} \\ &\left\{ |t(\mathbf{q})|^2 \text{Im} \chi_{sf}(\mathbf{k} - \mathbf{q}, \omega') \pm |g_{\mathbf{k}-\mathbf{q}}|^2 \text{Im} \chi_{ph}(\mathbf{k} - \mathbf{q}, \omega') \right. \\ &\left. \pm [V_{\mathbf{k}-\mathbf{q}}|^2 + |t(\mathbf{q})|^2/4] \text{Im} \chi_{cf}(\mathbf{k} - \mathbf{q}, \omega') \right\}, \end{aligned} \quad (10)$$

where the spectral density of bosonic excitations are determined by the dynamic susceptibility for spin fluctuations,  $\chi_{sf}(\mathbf{q}, \omega) = -\langle\langle \mathbf{S}_{\mathbf{q}} | \mathbf{S}_{-\mathbf{q}} \rangle\rangle_{\omega}$ , charge fluctuations  $\chi_{cf}(\mathbf{q}, \omega) = -\langle\langle N_{\mathbf{q}} | N_{-\mathbf{q}} \rangle\rangle_{\omega}$ , and phonon GF  $\chi_{ph}(\mathbf{q}, \omega) = -\langle\langle u_{\mathbf{q}} | u_{-\mathbf{q}} \rangle\rangle_{\omega}$ . The gap equation takes the form:

$$\begin{aligned} \varphi_{2,\sigma}(\mathbf{k}, \omega) &= \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{+\infty} dz \left\{ [J_{\mathbf{k}-\mathbf{q}} - V_{\mathbf{k}-\mathbf{q}}] \frac{1}{2} \tanh \frac{z}{2T} \right. \\ &\left. + K^{(-)}(\omega, z | \mathbf{q}, \mathbf{k} - \mathbf{q}) \right\} [-(1/\pi Q_2) \text{Im} F_{\sigma}^{22}(\mathbf{q}, z)]. \end{aligned} \quad (11)$$

Here the exchange interaction  $J_{\mathbf{q}} = 2J(\cos q_x + \cos q_y)$  induces pairing in MFA, while the Coulomb repulsion  $V_{\mathbf{k}-\mathbf{q}}$  suppresses the pairing. The pairing induced by retarded interactions is described by the kernel (10).

To estimate contributions from various interactions in the gap equation (11) we consider a weak coupling approximation for the kernel (10),  $K^{(-)}(\omega, z | \mathbf{q}, \mathbf{q}') \simeq K^{(-)}(\omega = 0, z = 0 | \mathbf{q}, \mathbf{q}')$ . In this approximation the gap equation reduces to the BCS-type form where the interactions are determined by the static susceptibility,  $\chi_{\mathbf{q}} = (1/\pi) \int_{-\infty}^{+\infty} (d\omega/\omega) \text{Im} \chi(\mathbf{q}, \omega)$ :

$$\begin{aligned} \varphi(\mathbf{k}) &= \frac{1}{N} \sum_{\mathbf{q}} \left\{ J_{\mathbf{k}-\mathbf{q}} - V_{\mathbf{k}-\mathbf{q}} - |t(\mathbf{q})|^2 \chi_{sf}(\mathbf{k} - \mathbf{q}) \right. \\ &\left. + |g_{\mathbf{k}-\mathbf{q}}|^2 \chi_{ph}(\mathbf{k} - \mathbf{q}) \right\} \frac{\varphi(\mathbf{q})}{2E_{\mathbf{q}}} \tanh \frac{E_{\mathbf{q}}}{2T}, \end{aligned} \quad (12)$$

where  $E_{\mathbf{q}} = [\varepsilon_{\mathbf{q}}^2 + |\varphi(\mathbf{q})|^2]^{1/2}$  and  $\varphi(\mathbf{k}) = \varphi_{2,\sigma}(\mathbf{k}, 0)$ . The unimportant contribution from charge fluctuations  $\chi_{cf}(\mathbf{k} - \mathbf{q})$  is omitted here (see later). To obtain an equation for superconducting  $T_c$  it is sufficient to consider a linearized gap equation (12). Using a model  $d$ -wave gap function,  $\varphi(\mathbf{k}) = \Delta \eta_{\mathbf{k}}$ ,  $\eta_{\mathbf{k}} = (\cos k_x - \cos k_y)$ , a linearized gap equation (12) for  $T_c$  can be written as:

$$1 = \frac{1}{N} \sum_{\mathbf{q}} [J - \widehat{V}_c - |t(\mathbf{q})|^2 \widehat{\chi}_{sf} + \widehat{V}_{ep}] \frac{\eta_{\mathbf{q}}^2}{2\varepsilon_{\mathbf{q}}} \tanh \frac{\varepsilon_{\mathbf{q}}}{2T_c}. \quad (13)$$

The coupling constants are given by the expressions:

$$\begin{aligned} \widehat{V}_c &= \frac{1}{N} \sum_{\mathbf{k}} V(\mathbf{k}) \cos k_x, \quad \widehat{\chi}_{sf} = \frac{1}{N} \sum_{\mathbf{k}} \chi_{sf}(\mathbf{k}) \cos k_x, \\ \widehat{V}_{ep} &= \frac{1}{N} \sum_{\mathbf{k}} |g(\mathbf{k})|^2 \chi_{ph}(\mathbf{k}) \cos k_x. \end{aligned} \quad (14)$$

To estimate the contribution  $\widehat{V}_c$  from the CI we consider a model for the 2D screened CI suggested in Ref. [10]:

$$V(\mathbf{k}) = u_c \frac{1}{|\mathbf{k}| + \kappa}, \quad u_c = \frac{2\pi e^2}{a \varepsilon_0}, \quad (15)$$

where  $\kappa$  is the inverse screening length ( $|\mathbf{k}|$  and  $\kappa$  are measured in units of  $1/a$ ),  $a$  is the lattice constant, and  $\varepsilon_0$  is the static dielectric constant of the lattice (in cuprates  $\varepsilon_0 \sim 30$ ). For the static spin-fluctuation susceptibility we adopt the model as in [8, 9]:

$$\chi_{sf}(\xi, \mathbf{k}) = \frac{\chi_0}{1 + \xi^2 [1 + (1/2)(\cos k_x + \cos k_y)]}. \quad (16)$$

Here  $\chi_0 = (3/4\omega_s)(1-\delta)[(1/N) \sum_{\mathbf{q}} \chi_{sf}(\mathbf{q})/\chi_0]^{-1}$  is fixed by the condition:  $\langle \mathbf{S}_i^2 \rangle = (3/4)(1-\delta)$  where  $\omega_s \sim J$  is a characteristic spin-excitation energy. The EPI coupling constant  $\widehat{V}_{ep}$  strongly depends on the  $\mathbf{k}$ -variation of the EPI matrix element  $|g(\mathbf{k})|^2$  and a phonon dispersion in  $\chi_{ph}(\mathbf{k}) = 1/M\omega_{\mathbf{k}}^2$ . In particular, for a local interaction  $g(\mathbf{k}) = g$  and a dispersionless optic phonon,  $\omega_{\mathbf{k}} = \omega_0$  the coupling constant for the  $d$ -wave pairing vanishes,  $\widehat{V}_{ep} = 0$ . A large electron-phonon coupling for the  $d$ -wave pairing can occur for a strong forward scattering,  $k \rightarrow 0$  in EPI (see, e.g., [4, 18]).

Numerical integration in (14) for the model (15) gives for the CI coupling constant:

$$\widehat{V}_c = u_c 0.05 \quad (0.11), \quad \widehat{V}_c/\widehat{V}_{c0} = 0.26 \quad (0.38), \quad (17)$$

for  $\kappa = 1$  (0.2), respectively. A small ratio  $\widehat{V}_c/\widehat{V}_{c0}$ , where  $\widehat{V}_{c0} = (1/N) \sum_{\mathbf{k}} V(\mathbf{k})$  shows that for the  $d$ -wave pairing the repulsion induced by CI is remarkably suppressed. In particular, for  $u_c \simeq 1$  eV we have still a positive, though a small contribution from the AF exchange interaction,  $J - \widehat{V}_c = 0.08$  (0.02) for  $J = 0.13$  eV. Therefore, in MFA we obtain only a weak coupling and a low  $T_c$  (cf. with [8, 15]).

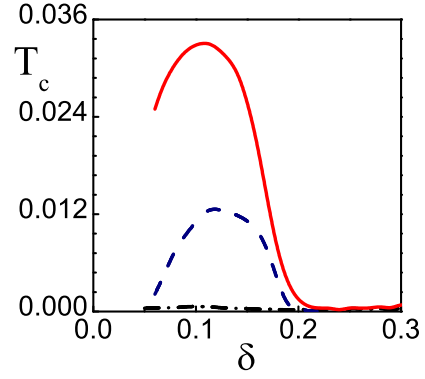


FIG. 3: (Color online)  $T_c(\delta)$  (red solid line) compared with pairing induced by spin fluctuations (blue dashed line) and AF interaction (dotted black line) (in units of  $t$ ).

The spin-fluctuation coupling constant in (14) for the model susceptibility (16) is given by,

$$\widehat{\chi}_{sf}(\xi) = -0.66, \quad (-0.26), \quad \chi_0(\xi) = 14.8 \quad (3.4), \quad (18)$$

in units of  $1/t = 0.4/\omega_s$  for  $\xi = 3.4$  ( $\xi = 1.4$ ) at hole doping  $\delta = 0.05$  (0.30), respectively [6]. While the spin susceptibility  $\chi_0 = \chi_{sf}(\mathbf{Q})$  at the AF wave vector  $\mathbf{Q}$  is positive and quite large, the contribution of the static susceptibility to the coupling constant  $\widehat{\chi}_{sf}(\xi)$  (18) is negative that results in attraction mediated by spin-fluctuations in the equation (13) for  $T_c$ . In the underdoped region with large AF correlation length  $\xi$  the spin-fluctuation coupling constant is quite large, while for the overdoped region with small  $\xi$  the coupling reduces resulting in lowering of  $T_c$ . Using a conventional dispersion for electrons:  $t(\mathbf{q}) = 2t(\cos q_x + \cos q_y) + 4t' \cos q_x \cos q_y$  with  $t = 0.4$  eV and  $|t'/t| \sim 0.2$ , we can estimate the spin-fluctuation coupling constant averaged over the Fermi surface,  $\langle \dots \rangle_F$  as:  $(1/t) \langle |t(\mathbf{q})|^2 \rangle_F \simeq 4t \simeq 1.6$  eV. Numerical estimation for the charge fluctuation susceptibility appears negligibly small,  $\widehat{\chi}_{cf} \sim (1/t) \times 10^{-3}$  which results in a small contribution from the CI in the kernel (10).

The gap equation (12) in strong-coupling approximation in the imaginary Matsubara frequency  $\omega_n$  representation can be written as,

$$\begin{aligned} \varphi(\mathbf{k}) &= \frac{T}{N} \sum_{\mathbf{q}} \sum_n \frac{\varphi(\mathbf{q})}{[Z_{\mathbf{k}} \omega_n]^2 + \varepsilon_{\mathbf{q}}^2} \\ &\times [J_{\mathbf{k}-\mathbf{q}} - V_{\mathbf{k}-\mathbf{q}} - |t(\mathbf{q})|^2 \chi_{sf}(\mathbf{k} - \mathbf{q})], \end{aligned} \quad (19)$$

where  $Z_{\mathbf{k}} = 1 + \lambda_{\mathbf{k}} = 1 - (d/d\omega) \text{Re}(\Sigma(\mathbf{k}, \omega))|_{\omega=0}$  is the quasiparticle weight. The latter is determined by the normal self-energy (8) which depends on contributions from all  $l$ -channels of interactions expanded in a series of the Legendre polynomials  $P_l(\cos \Theta)$ , contrary to the anomalous self-energy (9) where only the  $l = 2$  channel contributes to the  $d$ -wave pairing. Therefore, a strong EPI in the  $l = 0$  channel resulting in a large effective mass renormalization, large  $Z_{\mathbf{k}}$ , is unimportant for the  $d$ -wave

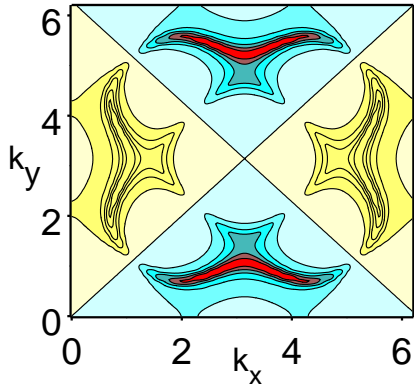


FIG. 4: (Color online) 2D projection of the superconducting gap function  $\varphi(\mathbf{k})$  for  $0 \leq k_x, k_y \leq 2\pi$ .

pairing and can only suppress the superconducting  $T_c$  (see also [18]). Figure 3 shows doping dependence  $T_c(\delta)$  in units of  $t \sim 0.4$  eV for  $Z_{\mathbf{k}} = 3$  where  $T_c(\delta)$  induced by partial contributions, AF and Coulomb interactions in MFA  $\propto (J_{\mathbf{k}-\mathbf{q}} - V_{\mathbf{k}-\mathbf{q}})$  and spin fluctuations,  $\propto |t(\mathbf{q})|^2$  are also shown. The maximal  $T_c$  is of the order of 150 K,

while for  $Z_{\mathbf{k}} = 1$  its value appears about five times higher. The gap function found for the hole concentration  $\delta = 0.12$  is shown in Fig. 4 which clearly demonstrates the  $d$ -wave symmetry.

In summary, we can conclude that the superconducting pairing mediated by the AF exchange interaction in MFA is suppressed by the screened Coulomb interaction and only charge fluctuations cannot produce superconducting pairing as found in Ref. [10]. However, spin-fluctuations induced by the kinematic interaction give a substantial contribution to the  $d$ -wave pairing and high- $T_c$  can be achieved. EPI can be important for the  $d$ -wave pairing only for particular phonon modes having a large  $l = 2$  component, while polaronic effects induced by a large  $l = 0$  component of the EPI may be detrimental for superconductivity in cuprates.

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