Electronic spectrum and superconductivity in the extended t–J model

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Abstract

A consistent microscopic theory of superconductivity for strongly correlated electronic systems is presented within the extended t–J–V where the intersite Coulomb interaction (CI) and the electron-phonon interaction (EPI) are taken into account. The exact Dyson equation for the normal and anomalous (pair) Green functions (GFs) is derived for the projected (Hubbard) electronic operators. The equation is solved in the self-consistent Born approximation for the self-energy. We obtain the d-wave pairing with high-T_c induced by the strong kinematical interaction of the order of the kinetic energy $\sim t$ of electrons with spin fluctuations. The Coulomb repulsion and EPI are suppressed for the d-wave pairing. These results support the spin-fluctuation mechanism of high-temperature superconductivity in cuprates previously proposed in phenomenological models.

Extended $t - J - V$ model

we consider electronic spectrum and superconducting pairing in the extended $t - J - V$ model on a square lattice. To study strong electron correlations in the singly occupied subband of the t–J model one has to use the projected electron operators, as $\widetilde{a}^{\dagger}_{i\sigma} = a^{\dagger}_{i\sigma}(1 - N_{i\bar{\sigma}})$. Here $a^{\dagger}_{i\sigma}$ is a creation electron operator on the lattice site i with spin $\sigma/2$, $\sigma = \pm 1$ $(\bar{\sigma} = -\sigma)$ and $N_{i\bar{\sigma}} = \widetilde{a}^{\dagger}_{i\bar{\sigma}}\widetilde{a}_{i\bar{\sigma}}$ is the number operator. The t–J model in the conventional notation reads:

$$H = -\sum_{i\neq j,\sigma} t_{ij}\widetilde{a}^{+}_{i\sigma}\widetilde{a}_{j\sigma} + \frac{1}{2}\sum_{i\neq j} J_{ij}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}N_iN_j\right) + H_{c,ep}, \tag{1}$$

where $S^{\alpha}_{i} = (1/2)\sum_{s,s'}\widetilde{a}^{+}_{is}\sigma^{\alpha}_{s,s'}\widetilde{a}_{is'}$ are spin-$1/2$ operators, $\sigma^{\alpha}_{s,s'}$ is the Pauli matrix. Here t_{ij} is the hopping parameter between i and j lattice sites and J_{ij} is the antiferromagnetic (AFM) exchange interaction. The intersite CI V_{ij} for electrons and EPI g_{ij} are taken into account by the Hamiltonian:

$$H_{c,ep} = \frac{1}{2}\sum_{i\neq j} V_{ij}N_iN_j + \sum_{i,j} g_{ij}N_i u_j, \tag{2}$$

where u_j describe atomic displacements on the lattice site j for phonon modes.

The unconventional commutation relations for the projected electron operators result in the kinematical interaction. For instance, if we consider commutation relation for the projected electron creation $\widetilde{a}^{\dagger}_{j\sigma}$ and annihilation $\widetilde{a}_{i\sigma}$ operators,

$$\widetilde{a}_{i\sigma}\widetilde{a}^{\dagger}_{j\sigma} + \widetilde{a}^{\dagger}_{j\sigma}\widetilde{a}_{i\sigma} = \delta_{ij}(1 - N_{i\sigma}/2 + \sigma S^{z}_{i}), \tag{3}$$

we observe that they are Fermi operators on different lattice sites but on the same lattice site they describe the **kinematical interaction** of electrons with charge $N_{i\sigma}$ and spin S^{α}_{i} fluctuations.

It is convenient to describe the projected electron operators by the Hubbard operators (HOs), as, e.g., $\widetilde{a}^{+}_{i\sigma} = X^{\sigma 0}_{i}$. Using the HOs, we write the Hamiltonian (1) in the form

$$\begin{aligned} H = &-\sum_{i\neq j,\sigma} t_{ij}X^{\sigma 0}_{i}X^{0\sigma}_{j} - \mu\sum_{i\sigma} X^{\sigma\sigma}_{i} \\ &+ \frac{1}{4}\sum_{i\neq j,\sigma} J_{ij}\left(X^{\sigma\bar{\sigma}}_{i}X^{\bar{\sigma}\sigma}_{j} - X^{\sigma\sigma}_{i}X^{\bar{\sigma}\bar{\sigma}}_{j}\right) + H_{c,ep}, \end{aligned} \tag{4}$$

where we introduced the chemical potential μ. To discuss the electronic spectrum and superconducting pairing within the model we consider the retarded two-time GF:

$$\begin{aligned} \widehat{G}_{ij,\sigma}(t - t') &= -i\theta(t - t')\langle\{\Psi_{i\sigma}(t), \Psi^{+}_{j\sigma}(t')\}\rangle \\ &\equiv \langle\langle\Psi_{i\sigma}(t) \,|\, \Psi^{+}_{j\sigma}(t')\rangle\rangle, \end{aligned} \tag{5}$$

where $\{A, B\} = AB + BA$ and we introduced HOs in the Nambu notation:

$$\Psi_{i\sigma} = \begin{pmatrix} X^{0\sigma}_{i} \\ X^{\bar{\sigma}0}_{i} \end{pmatrix}, \qquad \Psi^{+}_{i\sigma} = \begin{pmatrix} X^{\sigma 0}_{i} & X^{0\bar{\sigma}}_{i} \end{pmatrix}. \tag{6}$$

Introducing the Fourier representation in $(\mathbf{k}, \omega)$-space for the GF (5)

$$\widehat{G}_{ij\sigma}(t - t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{-i\omega(t-t')}\widehat{G}_{ij\sigma}(\omega), \tag{7}$$

$$\widehat{G}_{ij\sigma}(\omega) = \frac{1}{N}\sum_{\mathbf{k}} \exp[\mathbf{k}(\mathbf{r_i} - \mathbf{r_j}]\,\widehat{G}_{\sigma}(\mathbf{k}, \omega), \tag{8}$$

we represent it as the matrix

$$\widehat{G}_{\sigma}(\mathbf{k}, \omega) = \begin{pmatrix} G_{\sigma}(\mathbf{k}, \omega) & F_{\sigma}(\mathbf{k}, \omega) \\ F^{\dagger}_{\sigma}(\mathbf{k}, \omega) & -G_{\bar{\sigma}}(-\mathbf{k}, -\omega) \end{pmatrix}, \tag{9}$$

where $G_{\sigma}(\mathbf{k}, \omega)$ and $F_{\sigma}(\mathbf{k}, \omega)$ are the normal and anomalous parts of the GF (5).

By differentiating the GF 5 over the time t and t' we can obtain the Dyson equation in the form

$$\widehat{G}_{ij\sigma}(\omega) = \widehat{G}^{0}_{ij\sigma}(\omega) + \sum_{kl}\widehat{G}^{0}_{ik\sigma}(\omega)\, Q^{-1}\,\widehat{\Sigma}_{kl\sigma}(\omega)\,\widehat{G}_{lj\sigma}(\omega), \tag{10}$$

where $Q = 1 - n/2$. Here the zero–order GF in generalized MFA (GMFA) has the form:

$$\widehat{G}^{0}_{\sigma}(\mathbf{k}, \omega) = Q\frac{\omega\hat{\tau}_0 + \varepsilon(\mathbf{k})\hat{\tau}_3 + \Delta_{\sigma}(\mathbf{k})\hat{\tau}_1}{\omega^2 - E^2(\mathbf{k})}, \tag{11}$$

where $\hat{\tau}_0,\ \hat{\tau}_1,\ \hat{\tau}_3$ are the Pauli matrices and $E^2(\mathbf{k}) = \varepsilon^2(\mathbf{k}) + \Delta^2_{\sigma}(\mathbf{k})$ is the energy of quasiparticle (QP) excitations in the superconducting state. The self–energy operator $\widehat{\Sigma}_{kl\sigma}(\omega)$ is given by the *proper* part of the scattering matrix that has no parts connected by the single zero-order GF:

$$\widehat{\Sigma}_{ij\sigma}(\omega) = \langle\langle\widehat{Z}^{(irr)}_{i\sigma} \mid \widehat{Z}^{(irr)^{+}}_{j\sigma}\rangle\rangle^{\text{proper}}_{\omega} Q^{-1} = \begin{pmatrix} M_{ij\sigma}(\omega) & \Phi_{ij\sigma}(\omega) \\ \Phi^{\dagger}_{ij\sigma}(\omega) & -M_{ij\bar{\sigma}}(\omega) \end{pmatrix}. \tag{12}$$

The functions $M_{ij\sigma}(\omega)$ and $\Phi_{ij\sigma}(\omega)$ denote the respective normal and anomalous (pair) components of the self-energy operator. Therefore, for the single–electron GF (9) we obtain an exact representation:

$$\widehat{G}_{\sigma}(\mathbf{k}, \omega) = Q\{\omega\hat{\tau}_0 - \widehat{E}_{\sigma}(\mathbf{k}) - \widehat{\Sigma}_{\sigma}(\mathbf{k}, \omega)\}^{-1}. \tag{13}$$

Results and discussion

The normal state GF in the generalized mean-field approximation (GMFA) is given by the GF (13)

$$G^{0}(\mathbf{k}, \omega) = \langle\langle X^{0\sigma}_{\mathbf{k}}|X^{\sigma 0}_{\mathbf{k}}\rangle\rangle_{\omega} = \frac{Q}{\omega - \varepsilon(\mathbf{k})}. \tag{14}$$

Here the electronic energy is determined by the relation:

$$\varepsilon(\mathbf{k}) = -4t\,\alpha\gamma(\mathbf{k}) - 4t'\,\beta\gamma'(\mathbf{k}) - 4t''\,\beta\gamma''(\mathbf{k}) + \omega^{(c)}(\mathbf{k}) - \mu, \tag{15}$$

$$\omega^{(c)}(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{q}} V(\mathbf{k} - \mathbf{q})N(\mathbf{q}), \tag{16}$$

where $\gamma(\mathbf{k}) = (1/2)(\cos k_x + \cos k_y)$, $\gamma'(\mathbf{k}) = \cos k_x \cos k_y$, $\gamma''(\mathbf{k}) = (1/2)(\cos 2k_x + \cos 2k_y)$ and the hopping parameters are given by $t' = 0.1t$, $t'' = 0.2t$. We take $t = 0.4$ eV as the energy unit. α, β are renormalization parameters.

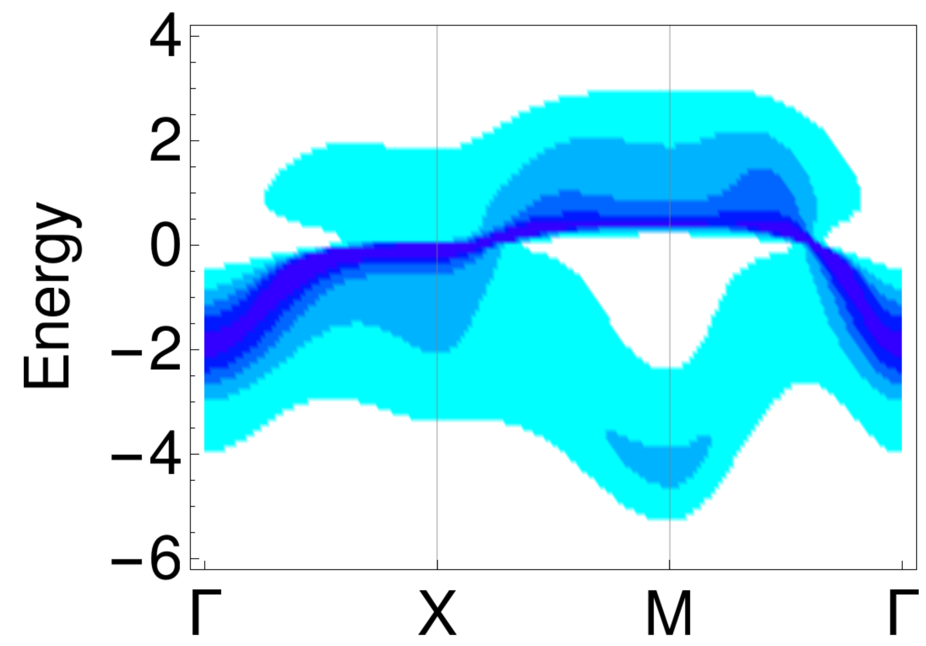

Figure 1: Energy dispersion for $\delta = 0.1$.

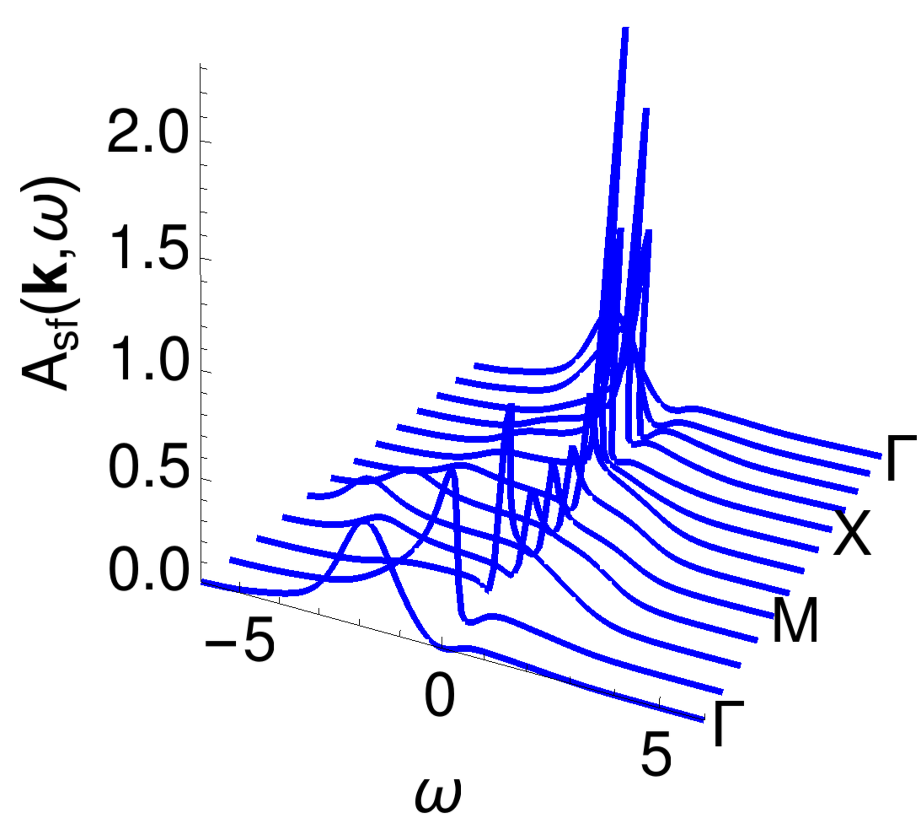

Figure 2: Spectral density $A(\mathbf{k}, \omega)$ for $\delta = 0.1$.

The self-energy 12 is determined by the many-particle GFs where the normal and anomalous (pairs) components are given by:

$$M_{ij\sigma}(\omega) = (1/Q)\,\langle\langle[X^{0\sigma}_{i}, H]|[H, X^{\sigma 0}_{j}]\rangle\rangle_{\omega}, \tag{17}$$

$$\Phi_{ij\sigma}(\omega) = (1/Q)\,\langle\langle[X^{0\sigma}_{i}, H]|[X^{0\bar{\sigma}}_{j}, H]\rangle\rangle_{\omega}. \tag{18}$$

Using the the spectral representation we represent them in terms of the time-dependent correlation functions which are calculated in the SCBA where propagation of Fermionic and Bosonic excitation on different lattice sites is assumed to be independent:

$$\langle X^{\sigma'0}_{m}B^{+}_{j\sigma\sigma'}|X^{0\sigma'}_{l}(t)B_{i\sigma\sigma'}(t)\rangle = \langle X^{\sigma'0}_{m}X^{0\sigma'}_{l}(t)\rangle\langle B^{+}_{j\sigma\sigma'}B_{i\sigma\sigma'}(t)\rangle\ , \tag{19}$$

$$\langle X^{\bar{\sigma}'0}_{m}B_{j\bar{\sigma}\bar{\sigma}'}|X^{\sigma'0}_{l}(t)B_{i\sigma\sigma'}(t)\rangle = \langle X^{\bar{\sigma}'0}_{m}X^{\sigma'0}_{l}(t)\rangle\,\langle B_{j\bar{\sigma}\bar{\sigma}'}B_{i\sigma\sigma'}(t)\rangle\ . \tag{20}$$

Calculation of the corresponding single-particle correlation functions in these equations results in the self-energy

$$M(\mathbf{k}, \omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty}\frac{dz}{\pi Q}K^{(+)}(\omega, z, \mathbf{k}, \mathbf{q})[-\mathrm{Im}]\,\mathrm{G}(\mathbf{q}, \mathrm{z}), \tag{21}$$

$$\Phi_{\sigma}(\mathbf{k}, \omega) = \frac{1}{N}\sum_{\mathbf{q}}\int_{-\infty}^{+\infty}\frac{dz}{\pi Q}K^{(-)}(\omega, z, \mathbf{k}, \mathbf{q})[-\mathrm{Im}]\mathrm{F}_{\sigma}(\mathbf{q}, \mathrm{z}). \tag{22}$$

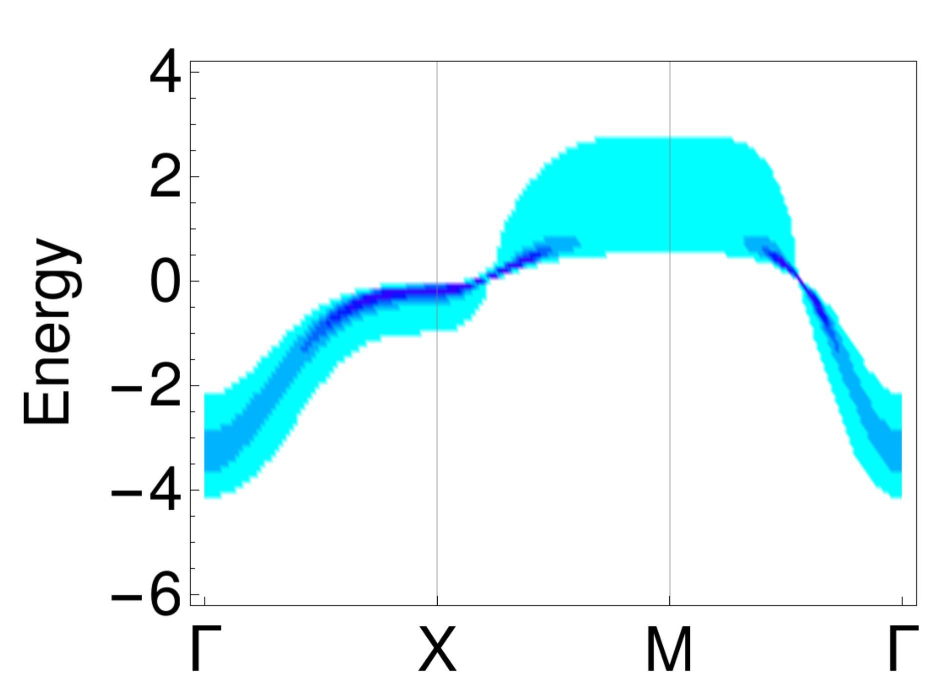

Figure 3: Energy dispersion for $\delta = 0.3$.

The kernel of the integral equations is defined as

$$\begin{aligned} K^{(\pm)}(\omega, z, \mathbf{k}, \mathbf{q}) &= \int_{-\infty}^{+\infty}\frac{d\Omega}{2\pi}\frac{\tanh(z/2T) + \coth(\Omega/2T)}{\omega - z - \Omega} \\ &\times\{|t(\mathbf{q})|^2\mathrm{Im}\chi_{sf}(\mathbf{k} - \mathbf{q}, \Omega) \pm |g_{ep}(\mathbf{k} - \mathbf{q})|^2\mathrm{Im}\chi_{ph}(\mathbf{k} - \mathbf{q}, \Omega) \\ &\pm\left[|V(\mathbf{k} - \mathbf{q})|^2 + |t(\mathbf{q})|^2/4\right]\mathrm{Im}\,\chi_{cf}(\mathbf{k} - \mathbf{q}, \Omega)\} \\ &\equiv \int_{-\infty}^{+\infty}\frac{d\Omega}{2\pi}\frac{\tanh(z/2T) + \coth(\Omega/2T)}{\omega - z - \Omega}\lambda^{(\pm)}(\mathbf{k}, \mathbf{q}, \Omega). \end{aligned} \tag{23}$$

The spectral densities of bosonic excitations are determined by the dynamic susceptibility for spin (sf), number (charge) (cf), and lattice (phonon) (ph) fluctuations

$$\chi_{sf}(\mathbf{q}, \omega) = -\langle\langle\mathbf{S}_{\mathbf{q}}|\mathbf{S}_{-\mathbf{q}}\rangle\rangle_{\omega}, \tag{24}$$

$$\chi_{cf}(\mathbf{q}, \omega) = -\langle\langle\delta N_{\mathbf{q}}|\delta N_{-\mathbf{q}}\rangle\rangle_{\omega}, \tag{25}$$

$$\chi_{ph}(\mathbf{q}, \omega) = -\langle\langle u_{\mathbf{q}}|u_{-\mathbf{q}}\rangle\rangle_{\omega}. \tag{26}$$

Let us consider the electronic spectrum in the normal state which is determined by normal state GF in Eq. (13)

$$G(\mathbf{k}, \omega) = \langle\langle X^{0\sigma}_{\mathbf{k}}|X^{\sigma 0}_{\mathbf{k}}\rangle\rangle = \frac{Q}{\omega - \varepsilon(\mathbf{k}) - M(\mathbf{k}, \omega)}. \tag{27}$$

The normal state self-energy is given by Eqs. (21), (23). The spectral density of electronic excitations is determined by

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi Q}\mathrm{Im}G(\mathbf{k}, \omega + i\epsilon) = \frac{-M''(\mathbf{k}, \omega)/\pi}{[\omega - \varepsilon(\mathbf{k}) - M'(\mathbf{k}, \omega)]^2 + [M''(\mathbf{k}, \omega)]^2} \tag{28}$$

Here we introduce the real, $M'(\mathbf{k}, \omega)$, and imaginary, $M''(\mathbf{k}, \omega)$, parts of the self-energy: $M(\mathbf{k}, \omega + i\epsilon) = M'(\mathbf{k}, \omega) + iM''(\mathbf{k}, \omega)$. The renormalization parameter for the electronic energy close to the FS, $\omega \to 0$, reads:

$$Z_{\mathbf{k}}(0) = 1 - [\partial M'(\mathbf{k}, \omega)/\partial\omega]_{\omega=0} \equiv 1 + \lambda(\mathbf{k}), \tag{29}$$

where $\lambda(\mathbf{k})$ is the coupling parameter.

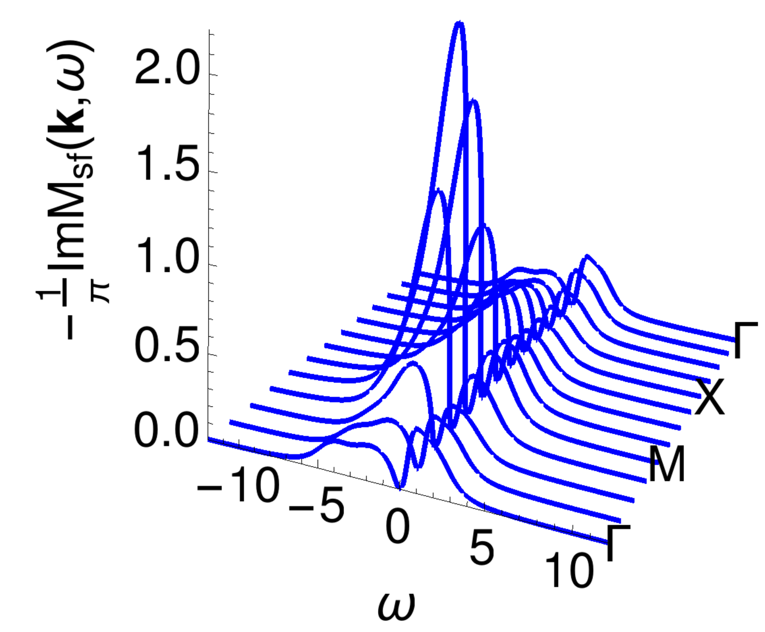

Figure 4: Imaginary part of the spin-fluctuation self-energy $-(1/\pi)\mathrm{Im}M_{sf}(\mathbf{k}, \omega)$ for $\delta = 0.1$.

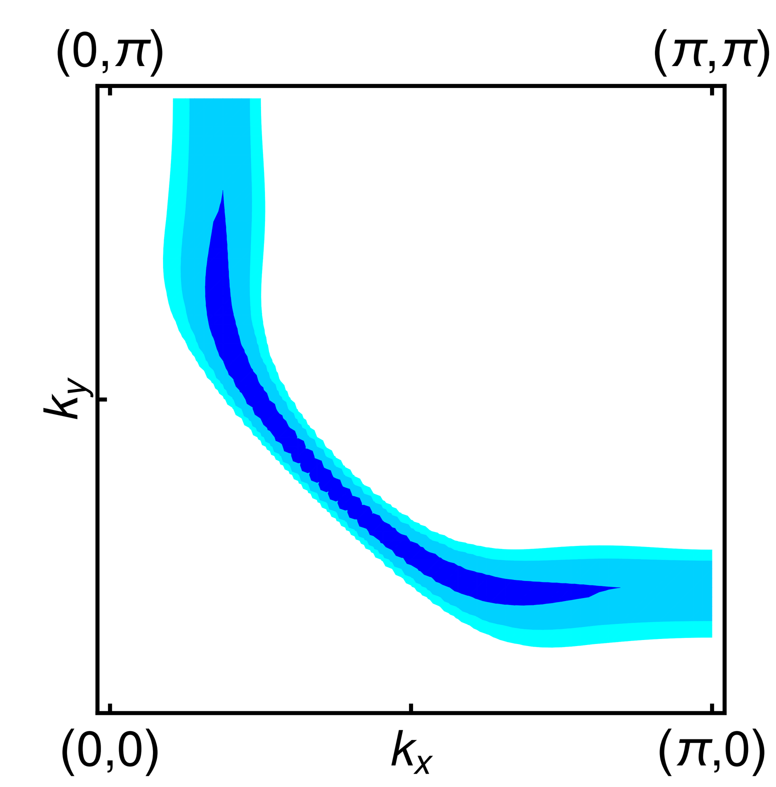

Figure 5: Spectral density $A(\mathbf{k}, 0)$ in the quarter of the BZ for $\delta = 0.05$.

The self-energy and the spectral density are calculated by iteration. The results of the 10-th order of iterations for the spectral density for the electron interaction with spin-fluctuations $A_{sf}(\mathbf{k}, \omega)$ (28) and the energy dispersion $\tilde{\varepsilon}(\mathbf{k})$ along the main directions in the Brillouin zone (BZ), $\Gamma(0,0) \to X(\pi, 0) \to M(\pi, \pi) \to \Gamma(0, 0)$, are presented in Figs. 2 – 3.

At low doping the spectral density shows a large incoherent background, in particular close to the (π, π)-point of the BZ, as shown in Figs. 2, 1 for $\delta = 0.1$. With increasing doping the spin-fluctuation interaction becomes weak and the incoherent background decreases, as shown in Fig. 3 for $\delta = 0.3$. The spectrum of excitations in Fig. 3 is close to that one in the GMFA. However, at low doping where the self-energy renormalization is strong the spectrum in the GMFA is quite different from those shown in Fig 1. In particular, a large intensity of excitations at the (π, π)-point of the BZ appears at much lower energy than in the GMFA due to a shift of the excitation energy caused by the real part of the self-energy. Therefore, we can conclude that the self-energy effects are very important in studies of the QP excitations in the t-J model.

The QP damping determined by the imaginary part of the self-energy (21) $\Gamma(\mathbf{k}, \omega) = -(1/\pi)\mathrm{Im}M_{sf}(\mathbf{k}, \omega)$ due to spin-fluctuation interaction is plotted in Fig. 4 at doping $\delta = 0.1$. For a larger doping, $\delta = 0.3$, the intensity of the QP damping decreases and the large FS emerges as in the GMFA.

The results of spectral density close to the FS $A_{sf}(\mathbf{k}, \omega = 0)$ (28) which determines the FS are presented in Figs. 5 for low doping. It reveals the arc-type form which transforms to the large FS for high doping as in the GMFA. This FS transformation from the arc-type at low doping to the large FS at high doping is observed in ARPES experiments.

Conclusion

A detailed study of the electronic spectrum and superconductivity for strongly correlated electronic systems within the microscopic theory for the extend $t - J$ model is presented. Besides the conventional AFM exchange interaction J, the EPI and the intersite Coulomb repulsion are taken into account. The projection technique was employed to obtain the exact Dyson equation for the normal and anomalous (pairs) GF's in terms of Hubbard operators. The self-energy given by many-particle GF's was calculated in the SCBA in the second order of interaction. The most important contribution is induced by the kinematical interaction for the HOs. It results in strong coupling of electrons with spin fluctuations of the order of hopping parameter $t(\mathbf{q})$ much larger than the exchange interaction $J(\mathbf{q})$. Therefore, we suggest that the spin-fluctuation pairing is the mechanism high-T_c in cuprates.

References

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