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PAULI SPIN SUSCEPTIBILITY IN THE $t-J$ MODEL

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Using a self-consistent theory for the Green function of Hubbard operators, the spin susceptibility is calculated as a function of the carrier concentration.

Вычислена зависимость спиновой восприимчивости от концентрации носителей на основе самосогласованной теории для функций Грина в технике операторов Хаббарда.

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INTRODUCTION

The problem of CuO_2 ground state in high temperature superconducting cuprate compounds or how to introduce the quasiparticles in such a way that the calculated physical quantities behave as the ones obtained in the experimental measurements is still open. A classification of cuprate unusual physical properties leads to a generic (T, p) phase diagram, in terms of temperature T and the hole concentration p in the CuO_2 planes [1].

Present investigation is devoted to finding the answer about the nature of quasiparticles investigating the magnetic susceptibility χ. Many different techniques have been proposed to investigate spin response of strongly correlated electron systems, one of those is CuO_2 plane [1, 2].

One of the main questions in constructing the theory of HTSC is about the correct form for the dynamical spin susceptibility $\chi(\mathbf{q}, \omega)$. For $\omega = 0$, i.e., static $\mathbf{q}$-dependent spin susceptibility has two limits: spatially uniform with $\mathbf{q} \to 0$ and the staggered one with $\mathbf{q} \to (\pi, \pi)$, which is the antiferromagnetic (AF) wave vector [1].

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A special interest presents the investigation of the static and uniform susceptibility $\chi = \chi(0,0)$. It could be measured as macroscopic susceptibility χ_m [3–9] or indirectly through Knight shift nuclear magnetic resonance (NMR) technique [10, 11] or through specific heat measurements [13–16]. Also, the measuring of the temperature T^* of the maximum value of static spin susceptibility is very important [8, 10, 11, 17, 18].

Concerning the experimental results of the hole doped $La_{2-x}Sr_xCuO_{4-y}$ (LSCO)- and $YBa_2C_3O_{6+x}$ (YBCO)-family parent compounds, one meets with difficulties due to the different procedure of sample preparing. Since the value of the correlation length ξ of the AF fluctuation is of the range of the interatomic distance, therefore considered strongly correlated many-particle system is very sensitive to some short-range structural disorder, i.e., structural defects such as impurities and vacancies [1]. In order to obtain intrinsic spin susceptibility of hole doped CuO_2 planes, one has to subtract hole-doping independent part in LSCO [4] and Curie-like (C_g/T) paramagnetic contribution, which characterizes isolated impurities and defects in YBCO compounds [2–5].

The static uniform spin susceptibility was calculated in the framework of the Hubbard [19–24], Heisenberg [25] and $t-J$ [26–28] models. Qualitative agreement between theoretical and experimental results for temperature and doping dependencies was found. The self-consistent renormalization theory of spin fluctuations [21] describes well experimental results for the staggered part of the uniform spin susceptibility.

Among the theoretical investigations aimed at obtaining full form of $\chi(\mathbf{q},\omega)$, one should notice the semi-phenomenological Millis–Monien–Pines (MMP) theory [29–33], which was successfully applied for description of many experimental findings. Also, there are a lot of attempts to obtain $\chi(\mathbf{q},\omega)$ microscopically. Very often microscopical findings use either the method of equations of motion for Green's functions (GF) [34–38] or Mori's memory function method [39–43]. Early theoretical efforts were directed to find some universal form or scaling function which connect χ, $\chi_{\max}$, T^* and vacancy or impurity concentration x [2, 4, 44–46] and in the high-temperature limit [47]. Using the Van Hove scenario, some theories were able to qualitatively explain dependencies χ on x and T [23, 49–52]. Numerical cluster calculations in the framework of $t-J$ or two-band Hubbard model [53–55] had success in obtaining form of the dependencies of the chemical potential μ on hole concentration and T similar to the ones obtained in [56–61].

In the CuO_2 planes of LSCO compounds for low Sr content, carriers are holes, while for large x they are electrons [7]. It was confirmed by corresponding change of Hall coefficient sign from positive to the negative one and by the doping evolution of the Fermi surface form [1, 62], as also was obtained from ARPES experiments [58–61] and ED calculations [53–55].

In the proposition that the chemical potential is close to the Van Hove singularity in the quasiparticle DOS, a lot of different DOS models were considered [23, 48–52]. There was obtained satisfactory description of the experimental results of the temperature dependence macroscopic spin susceptibility [23, 48] or Knight shift [26, 49, 51].

In the NMR Knight shift experiments [10, 11], one comes to conclusion that there is no evidence for Van Hove singularity in DOS. There were established linear relations between spin susceptibility χ_m and respectively ^{89}Y Knight shift in YBCO [10] and ^{6}3Cu Knight shift in LSCO [11] compounds. Monotonic behaviour of $\chi(x)$ on doping x was also found. However, one should note that the samples were not in the overdoped phase and

also that during the NMR measurements they were influenced by high magnetic fields (well above 10 T).

Recently, in [62] band-structure of the $t-J$ model in the normal and superconducting states of the paramagnetic phase was profoundly investigated. We extent the research in this paper taking the external magnetic field into consideration. Main goal of the present investigation is to derive the corresponding expression for $\chi = \chi(0,0)$ in the $t-J$ model with the correct band-dispersion energy spectrum [62]. To get which interaction between quasiparticles is included through the renormalization of their energies caused by AF spin fluctuations. Renormalization of quasiparticle energy also changes the uniform and static spin susceptibility.

Our paper is organized as follows. In the next section, we write the $t-J$ model using the Hubbard operators formalism and obtain the corresponding Green's function (GF). In Sec. 2 we calculate the energy-dispersion relations, similar as it was done in [62]. Section 3 is devoted to calculation of the static and uniform spin susceptibility. Section 4 contains numerical results and discussions. Our conclusions can be found at the end of the paper.

1. MODEL HAMILTONIAN AND GREEN'S FUNCTION

We intend to calculate the spin response of a strongly correlated electron system to a uniform magnetic field. So, we consider an effective $t-J$ model for the CuO_2 plane perturbated with the Zeeman interaction

$$H^h_{t-J} = H_{t-J} + H_h, \tag{1}$$

with the $t-J$ Hamiltonian written in the standard notation [1, 62]

$$H_{t-J} = \sum_{\langle i,j\rangle,\sigma} t_{ij}(1-n_{i\bar{\sigma}})c^+_{i\sigma}c_{j\sigma}(1-n_{j\bar{\sigma}}) + \sum_{\langle i,j\rangle} J_{ij}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_in_j\right), \tag{2}$$

where $\bar{\sigma} = -\sigma$ and the Zeeman's Hamiltonian in the external magnetic field $\mathbf{h} = (0,0,h)$ is

$$H_h = -h\sum_i \mu^z_i, \tag{3}$$

where $\mu^z_i = -g\mu_{_B}S^z_i$ is the z-component of magnetic moment with gyromagnetic (Landé) factor g and Bohr magneton $\mu_{_B}$. In the Hubbard operator representation $X^{\alpha\beta}_i = |i\alpha\rangle\langle i\beta|$ which preserves site no double occupancy constraint, i.e., $X^{00}_i + \sum_\sigma X^{\sigma\sigma}_i = 1$, one has

$$n_i = \sum_\sigma X^{\sigma\sigma}_i, \quad S^z_i = \frac{1}{2}\sigma(n_{i\sigma} - n_{i\bar{\sigma}}) = \frac{1}{2}\sum_\sigma \sigma X^{\sigma\sigma}_i, \quad X^{\sigma 0}_i = c^+_{i\sigma}(1-n_{i\bar{\sigma}}). \tag{4}$$

Considered Hamiltonian (1) takes the following form [62]:

$$H^h_{t-J} = \sum_{i\sigma}\xi^h_{i\sigma}X^{\sigma\sigma}_i + \sum_{i\neq j,\sigma} t_{ij}\,X^{\sigma 0}_i X^{0\sigma}_j + \frac{1}{4}\sum_{i\neq j,\,\sigma} J_{ij}(X^{\sigma\bar{\sigma}}_i X^{\bar{\sigma}\sigma}_j - X^{\sigma\sigma}_i X^{\bar{\sigma}\bar{\sigma}}_j), \tag{5}$$

where $\xi^h_{i\sigma} = \varepsilon^h_{d\sigma} - \mu$ and $\varepsilon^h_{d\sigma} = \varepsilon_d + \mu_{_B}h\sigma$ is the energy of the hole with spin σ in the magnetic field h. The exchange integral for the nearest neighbors (n.n.) is $J_{ij} = J$ and

zero in other cases, $t_{ij} = t$ and $t_{ij} = t'$ are respectively the hopping parameters for the next neighbors (n.n.) and the next to the nearest neighbors (n.n.n.) sites i, j on a two-dimensional (2D) square lattice and μ is the chemical potential.

The main goal of the present investigation is calculation of the static spin susceptibility χ for strongly correlated electronic system in a uniform static magnetic field $\mathbf{h} = (0, 0, h)$. Using the definition of the average magnetic moment or magnetization as $M_z^h = \mathcal{N}\langle\mu_z^h\rangle$, or equivalently $M_z^h = -\partial\langle H_{t-J}^h\rangle/\partial h$, where $\mathcal{N}$ is number of the 2D lattice site, one has the spin susceptibility as the zero field limit of derivation $\chi = (\partial M_z^h/\partial h)_{h\to 0}$.

As one can see, to obtain static spin susceptibility χ, one should first calculate spin-dependent on-site occupation number $n_{i\sigma}^h$ which is

$$n_{i\sigma}^h = \langle X_i^{\sigma\sigma}\rangle^h = \langle X_i^{\sigma 0} X_i^{0\sigma}\rangle^h, \tag{6}$$

i.e., one should calculate the following anticommutator Green's function:

$$\langle\langle X_i^{0\sigma}(t); X_j^{\sigma 0}(t')\rangle\rangle = -i\Theta(t-t')\langle[X_i^{0\sigma}(t), X_j^{\sigma 0}(t')]_+\rangle, \tag{7}$$

where we have chosen Zubarev's general formulation [63].

2. QUASIPARTICLE DISPERSION

As analytical tools, we use the projection method in the GF equation of motion [62, 63]

$$\omega\langle\langle X_i^{0\sigma}|X_j^{\sigma 0}\rangle\rangle_\omega = \langle[X_i^{0\sigma}, X_j^{\sigma 0}]_+\rangle + \langle\langle Z_{i\sigma}|X_j^{\sigma 0}\rangle\rangle_\omega, \tag{8}$$

where $\langle\langle X_i^{0\sigma}|X_j^{\sigma 0}\rangle\rangle_\omega$ is the Fourier transform of GF (7), the anticommutator of the operators A and B is $[A, B]_+ = AB + BA$ and the equilibrium average value of an operator A is defined as $\langle A\rangle = \mathrm{Tr}\{\exp(-\beta H_{t-J})A\}/Z$ with canonical partition function (or «Zustandssumme») as trace (Tr) in the energy representation of the operator «$\exp(-\beta H_{t-J})$». In the projection method one extracts the main linear part after scattering in the equation of motion for transition described with $X_i^{0\sigma}$, which can be analytically described with the following procedure [62]:

$$Z_{i\sigma} = [X_i^{0\sigma}, H_{t-J}^h] = \sum_l E_{il\sigma}^h X_l^{0\sigma} + Z_{i\sigma}^{ir}. \tag{9}$$

From the projection condition $\langle[Z_{i\sigma}^{ir}, X_j^{\sigma 0}]_+\rangle = 0$, one obtains the «frequency matrix»

$$E_{ij\sigma}^h = \frac{\langle[[X_i^{0\sigma}, H_{t-J}^h], X_j^{\sigma 0}]_+\rangle}{Q}, \tag{10}$$

whose spatial and temporal Fourier transformation will give energy band dispersion $E_{\mathbf{q}}(\omega)$. In the equation of motion for the Hubbard operator $X_i^{0\sigma}$

$$\left(i\frac{d}{dt} - \xi_{i\sigma}^h\right) X_i^{0\sigma} = -\sum_{l\sigma'} t_{il} B_{i\sigma\sigma'} X_l^{0\sigma'} + \frac{1}{2}\sum_{l\sigma'} J_{il}(B_{l\sigma\sigma'} - \delta_{\sigma\sigma'}) X_i^{0\sigma'}, \tag{11}$$

appear Bose-like Hubbard operators [62]

$$B_{i\sigma\sigma'} = Q_i^\sigma \delta_{\sigma\sigma'} + X_i^{\bar{\sigma}\sigma'}, \tag{12}$$

which describe hole scattering on charge (or kinematics interactions)

$$Q_i^{\sigma} = X_i^{00} + X_i^{\sigma\sigma} = 1 - \frac{n_i}{2} + \sigma S_i^z, \tag{13}$$

and spin fluctuations (or exchange interactions) $X_i^{\bar{\sigma}\sigma} = S_i^{\bar{\sigma}}$. Like in Hubbard I approximation, we further neglect density–density charge fluctuations, but we keep spin correlations introducing spin correlation functions for the n.n. $\chi_{1s} = \langle \mathbf{S}_i \mathbf{S}_{i+\mathbf{a_1}} \rangle$ and for the n.n.n. lattice sites $\chi_{2s} = \langle \mathbf{S}_i \mathbf{S}_{i+\mathbf{a_2}} \rangle$, where n.n. describe $\mathbf{a}_1 = (\pm a_x, \pm a_y)$ and n.n.n. describe $\mathbf{a}_2 = \pm(a_x \pm a_y)$ radius vectors. For the paramagnetic phase, we have $\langle S_i^z \rangle = 0$ and also $\langle Q_i^{\sigma} \rangle = \langle Q_i^{\bar{\sigma}} \rangle \equiv Q = 1 - n/2$, where $n = \langle n_i \rangle = \mathcal{N}^{-1} \sum\limits_{i\sigma} \langle X_i^{\sigma\sigma} \rangle$ is the average hole on-site occupation number. Using the common representation for the spin products $\mathbf{S}_l \mathbf{S}_j = S_l^z S_j^z + \frac{1}{2} \sum\limits_{\sigma} S_l^{\sigma} S_j^{\bar{\sigma}}$, one has

$$\langle B_{l\sigma\sigma} Q_j^{\sigma} + B_{l\sigma\bar{\sigma}} X_j^{\sigma\bar{\sigma}} \rangle = \langle \mathbf{S}_l \mathbf{S}_j \rangle + 1 - \langle n_j \rangle + \frac{\langle n_l \rangle \langle n_j \rangle}{4}. \tag{14}$$

In such a way we obtain the following elements of the «frequency matrix»:

$$E_{ij\sigma}^h = \delta_{ij} (\xi_{i\sigma}^h + \delta\mu) + (1 - \delta_{ij}) \tilde{E}_{ij\sigma}, \tag{15}$$

with diagonal and

$$\xi_{i\sigma}^h + \delta\mu = \left\{ \xi_{i\sigma}^h Q + \sum_l t_{il} \langle X_i^{\bar{\sigma}0} X_l^{0\bar{\sigma}} \rangle + \frac{1}{2} \sum_l J_{il} \left(\langle \mathbf{S}_l \mathbf{S}_i \rangle - \frac{1}{2} \langle n_j \rangle + \frac{1}{4} \langle n_l \rangle \langle n_j \rangle \right) \right\} / Q, \tag{16}$$

next to them

$$\tilde{E}_{ij\sigma} = \left\{ t_{ij} \left(\langle \mathbf{S}_i \mathbf{S}_j \rangle + 1 - \langle n_j \rangle + \frac{1}{4} \langle n_i \rangle \langle n_j \rangle \right) + \frac{1}{2} J_{ij} \langle X_j^{\bar{\sigma}0} X_i^{0\bar{\sigma}} \rangle \right\} / Q \tag{17}$$

matrix elements. Further we perform the spatial Fourier transformations of the upper correlation functions

$$\begin{gathered} \langle X_i^{\bar{\sigma}0} X_l^{0\bar{\sigma}} \rangle = \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} n_{\mathbf{k}\bar{\sigma}} \, \mathrm{e}^{i\mathbf{k}\mathbf{R}_{il}}, \quad n_{\mathbf{k}\bar{\sigma}} = \langle X_{\mathbf{k}}^{\bar{\sigma}0} X_{-\mathbf{k}}^{0\bar{\sigma}} \rangle, \\ n_{i\sigma} = \langle X_i^{\sigma\sigma} \rangle = \langle X_i^{\sigma 0} X_i^{0\sigma} \rangle = \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} n_{\mathbf{k}\sigma} \end{gathered} \tag{18}$$

and

$$\sum_l t_{il} \langle X_i^{\bar{\sigma}0} X_l^{0\bar{\sigma}} \rangle = \frac{1}{\mathcal{N}} \sum_{\mathbf{k}} t(\mathbf{k}) \, n_{\mathbf{k}\bar{\sigma}}, \quad t(\mathbf{k}) = 4t\gamma(\mathbf{k}) + 4t'\gamma'(\mathbf{k}), \tag{19}$$

with $\gamma(\mathbf{q}) = [\cos(a_x q_x) + \cos(a_y q_y)]/2$ and $\gamma'(\mathbf{q}) = \cos(a_x q_x) \cos(a_y q_y)$. As we consider only n.n. exchange interactions, one has

$$\frac{1}{2} \sum_l J_{il} \langle \mathbf{S}_l \mathbf{S}_i \rangle = \frac{1}{2} J \sum_{\mathbf{a}_1} \langle \mathbf{S}_i \mathbf{S}_{i+\mathbf{a}_1} \rangle = 2J \, \chi_{1s}. \tag{20}$$

In $\mathbf{q}$-representation one obtains the following GF:

$$\langle\langle X^{0\sigma}|X^{\sigma 0}\rangle\rangle^{h}_{\mathbf{q},\,\omega} = \frac{Q}{\omega - E^{h}_{\mathbf{q}\sigma}} = \frac{Q}{\omega - (\tilde{E}_{\mathbf{q}\sigma} + \tilde{\xi}^{h}_{i\sigma})}. \tag{21}$$

As in [62], the quasiparticle energy $\tilde{E}_{\mathbf{k}\sigma}$ is renormalized due to the kinematic $\epsilon(\mathbf{k}) = t(\mathbf{k})$, bonding between it and exchange $\epsilon_s(\mathbf{k}) = 4t\gamma(\mathbf{k})\chi_{1s} + 4t'\gamma'(\mathbf{k})\chi_{2s}$ and the net exchange interaction ($\propto J$) as follows:

$$\tilde{E}_{\mathbf{k}\sigma} = -Q\epsilon(\mathbf{k}) - \frac{\epsilon_s(\mathbf{k})}{Q} - \frac{2J}{\mathcal{N}}\sum_{\mathbf{q}}\frac{\gamma(\mathbf{k}-\mathbf{q})}{Q}\,n_{\mathbf{q}\bar{\sigma}}. \tag{22}$$

Within the model used in [62], the static spin correlation functions which appear in the definition of $\epsilon_s(\mathbf{k})$ are respectively

$$\chi_{1s} = \langle \mathbf{S}_i\mathbf{S}_{i+a_1}\rangle = \frac{1}{\mathcal{N}}\sum_{\mathbf{q}}\gamma(\mathbf{q})\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle, \tag{23}$$

and

$$\chi_{2s} = \langle \mathbf{S}_i\mathbf{S}_{i+a_2}\rangle = \frac{1}{\mathcal{N}}\sum_{\mathbf{q}}\gamma\,'(\mathbf{q})\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle, \tag{24}$$

where $\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle = (\pi\omega_s/2)\chi_s(q)$. Here $\mathbf{q}$-dependent part of spin-fluctuation susceptibility [62] is

$$\chi_s(q) = \frac{\chi_0}{1 + \xi^2\,[1+\gamma(q)]}, \tag{25}$$

where ξ is the characteristic AF correlation length, spin-fluctuation energy is $\omega_s \simeq J$ and χ_0 is some normalization parameter [62].

The renormalized one-particle on-site spin-dependent energies are

$$\tilde{\xi}^{h}_{i\sigma} = \xi^{h}_{i\sigma} + \delta\mu_{\sigma},$$

where the chemical potential shift is

$$\delta\mu_{\sigma} = \frac{1}{\mathcal{N}}\sum_{\mathbf{q}}\frac{t(\mathbf{q})}{Q}\,n_{\mathbf{q}\bar{\sigma}} - \frac{2J}{Q}\left(\frac{1}{2}\,\langle n_j\rangle - \chi_{1s} - \frac{1}{4}\langle n_l\rangle\langle n_j\rangle\right). \tag{26}$$

In the upper formulae we should take $n_{\mathbf{q}\bar{\sigma}} = n_{\mathbf{q}\sigma} \equiv n_{\mathbf{q}}$, which means that $\tilde{E}_{\mathbf{k}\sigma} = \tilde{E}_{\mathbf{k}\bar{\sigma}} \equiv \tilde{E}_{\mathbf{k}}$ and $\delta\mu_{\sigma} = \delta\mu_{\bar{\sigma}} \equiv \delta\mu$, since these quantities relate to the paramagnetic phase in the absence of the external magnetic field.

3. QUASIPARTICLE SPIN SUSCEPTIBILITY

As one can see in GF (21), the only dependence on magnetic field h and on the spin direction σ is contained in the on-site hole energy $\xi^{h}_{i\sigma}$. This means that in the lowest order, the effect of an external static uniform magnetic field is to shift the relative energy distributions

of the up and down spins. So, we have different on-site occupation numbers for spin up and down, but our many-particle system of holes will reach an equilibrium in such a manner that their Fermi levels (or the renormalized chemical potential $\mu - \delta\mu_\sigma$) will be the same.

For on-site spin and field-dependent occupation numbers we have

$$n_\sigma^h = \langle X_i^{\sigma\sigma}\rangle^h = \langle X_i^{\sigma 0} X_i^{0\sigma}\rangle^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\langle X^{\sigma 0} X^{0\sigma}\rangle_{\mathbf{k}}^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega \langle X^{\sigma 0} X^{0\sigma}\rangle_{\mathbf{k},\,\omega}^h, \tag{27}$$

i.e., according to the general receipt of the GF spectral representation [63] we have

$$n_\sigma^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\frac{1}{2\pi}\int\limits_{-\infty}^{+\infty} d\omega \frac{-2}{\mathrm{e}^{\beta\omega}+1}\,\mathrm{Im}\langle\langle X^{\sigma 0}|X^{0\sigma}\rangle\rangle_{\mathbf{k},\,\omega}^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\int\limits_{-\infty}^{+\infty} d\omega \frac{Q}{\mathrm{e}^{\beta\omega}+1}\,\delta(\omega - \tilde{E}_{\mathbf{k}}^h), \tag{28}$$

with $\beta = 1/(k_{_B}T)$. In such a way, in the magnetic field h we obtain the following expression for the spin σ-dependent on-site occupancy

$$n_\sigma^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}} n_{\mathbf{k}\sigma}^h = \frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\frac{Q}{1+\exp\left[\beta(\tilde{E}_{\mathbf{k}} + \tilde{\xi}_{i\sigma}^h)\right]}, \tag{29}$$

and the magnetization in a uniform magnetic field h is $M^h = -g\mu_{_B}\mathcal{N}(n_\uparrow^h - n_\downarrow^h)/2$. Further one should calculate derivative on h of the M^h to obtain the uniform and static susceptibility

$$\chi_0^h = \left(\frac{\partial M^h}{\partial h}\right) = \mathcal{N} g\,\mu_{_B}\frac{\partial}{\partial h}\,\frac{(n_\downarrow^h - n_\uparrow^h)}{2}. \tag{30}$$

Making the derivative on h of the n_σ^h, one gets

$$\frac{\partial\, n_\sigma^h}{\partial h} = \frac{1}{\mathcal{N}}\frac{-\sigma g\mu_{_B}}{k_{_B}T}\,Q\sum_{\mathbf{k}}\frac{\exp\left[\beta(\tilde{E}_{\mathbf{k}} + \tilde{\xi}_{i\sigma}^h)\right]}{\{1+\exp\left[\beta(\tilde{E}_{\mathbf{k}} + \tilde{\xi}_{i\sigma}^h)\right]\}^2}, \tag{31}$$

which including (29) and (30) gives the following expression for the uniform and static spin susceptibility in the uniform magnetic field $\mathbf{h} = (0, 0, h)$ in a paramagnetic phase:

$$\chi_0^h = \frac{g\mu_{_B}^2}{k_{_B}T}\sum_{\mathbf{k}\sigma}\left[\frac{n_{\mathbf{k}\sigma}^h - (n_{\mathbf{k}\sigma}^h)^2}{Q}\right], \tag{32}$$

with

$$n_{\mathbf{k}\sigma}^h - (n_{\mathbf{k}\sigma}^h)^2/Q = \frac{\beta Q}{2[1+\cosh(\beta x)]} = \frac{\beta Q}{(1+\mathrm{e}^{\beta x})(1+\mathrm{e}^{-\beta x})}, \tag{33}$$

where $x = \tilde{E}_{\mathbf{k}} + \delta\mu - \mu + \mu_\sigma h\sigma + \varepsilon_d$ and spin σ and field h-dependent on-site hole occupancy is given in Eq. (29).

For large sample ($\mathcal{N} \to \infty$), one can pass in the upper expressions on the continual limit $\frac{1}{\mathcal{N}}\sum_{\mathbf{k}}\ldots \Longrightarrow \int\limits_{1\mathrm{st\,B.Z}}\ldots\, d\mathbf{k}/(2\pi)^2$, where one integrates over the first Brillouin zone

(1st B.Z.). In the zero-field limit, one finds the static and uniform spin susceptibility in the paramagnetic phase

$$\chi_0 = (2\mu_{_B})^2 \int\limits_{1\text{st B.Z}} \frac{d\mathbf{k}}{(2\pi)^2} \left(-\frac{dn_{\mathbf{k}}}{d\tilde{E}_{\mathbf{k}}}\right) = (2\mu_{_B})^2 \int\limits_{1\text{st B.Z}} \frac{d\mathbf{k}}{(2\pi)^2} \left(\frac{dn_{\mathbf{k}}}{d\mu}\right) = 2\mu_{_B}^2 \frac{d}{d\mu} N, \quad (34)$$

where we use $g \simeq 2$. Total number of the holes (in dependence of CuO_2 plane hole doping) which in canonical ensemble fix the Fermi-level position is given by

$$N = \int\limits_{1\text{st B.Z}} \frac{d\mathbf{k}}{(2\pi)^2}\, n_{\mathbf{k}} = \int\limits_{1\text{st B.Z}} \frac{d\mathbf{k}}{(2\pi)^2} \frac{Q}{1+\exp\left[\beta(\tilde{E}_{\mathbf{k}}+\delta\mu-\mu)\right]}, \quad (35)$$

where the quasiparticle energy $\tilde{E}_{\mathbf{k}}$ is given by (22) and the chemical potential shift is given by (26), taking into account the remark below Eq. (26).

4. NUMERICAL RESULTS AND DISCUSSION

In this section we present numerical results, namely, the chemical potential $\mu(p)$, uniform static quasiparticle spin susceptibility $\chi_0(p)$ (at zero and finite temperatures) and the energy dispersion and FS shape evolution with hole doping p. To perform the numerical calculations, we have chosen the following parameter values: $t' = -0.3$ and $J = 0.4$. The n.n. hoping parameter t was chosen as the energy unit. In order to get the self-consistent solution, 64×64 cluster was used. The energy mesh was less than 0.001.

In Fig. 1, we plot dependencies $\mu(p)$ and $\chi_0(p)$ at two temperatures $T = 0$ and $T = 0.3\,t > 1000$ K. The zero temperature dependencies of the chemical potential (solid lines) and the susceptibility (dot-dashed line) are linear functions on the hole doping. We obtain that μ does not depend on T in the considered doping interval. For small hole doping $p < 0.05$, one can see only weak increase of μ as T increases from 0 to $0.3\,t$. In the ED numerical studies [53, 54] in the hole over doped phase ($0.15 < p$), it was obtained that μ does not depend on T. Under assumption that the chemical potential is T-independent and that DOS peak is narrow with rectangular shape [48], one successfully describes many of the normal state properties of HTSC compounds on qualitative level. It gives some support that our result about weak temperature independence of μ is correct.

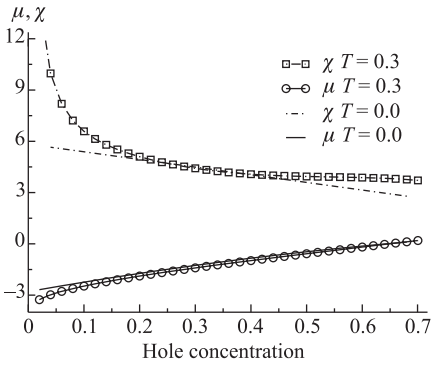

Fig. 1. Doping dependence of the chemical potential μ at temperatures $T = 0$ (solid line) and $T = 0.3$ (in units of t) (solid line with circles) is plotted in the figure. The susceptibility χ vs doping at $T = 0$ is plotted by dot-dashed line and $T = 0.3$ case is shown by dot-dashed line with squares. The susceptibility χ is in units of $2\mu_B^2$

One of the basic features which follows from the experiments is an increase of the macroscopic χ_m in the hole underdoped phase and χ_m decreases in the hole overdoped phase, which is better seen in the LSCO compounds [6, 7, 48] rather than in the YBCO compounds [3, 5], where the overdoping phase is very short. Existence of the maxima in the $\chi_m(p)$ dependence can be concluded from Sommerfeld's γ parameter dependence on p in the electronic specific heat measurements [1, 13–16], and also from the numerical results obtained in the framework of Hubbard model [55]. However, in some experiments performed in YBCO [10, 11] and LSCO [11, 12] compounds, one finds a linear scaling between NMR Knight shifts ^{89}K (or ^{63}K) in the magnetic field of about $H = 10$ T and χ_m at about $H = 1$ T and Knight shifts are monotone increasing functions on hole doping p. In other words, one does not find maxima in the $K(p)$ and $\chi(p)$ dependencies. Generally, one should be careful extracting inherent characteristics of the quasiparticles in CuO_2 without oxygen vacancy and different inhomogeneity contributions. From our numerical results it follows that χ_0 decreases with hole doping p increase which is in agreement with theoretical results [28] for $p > 0.05$ (where our approximations are available for paramagnetic phase).

Looking after the experimental results about χ_m with maxima in dependence on p, one can conclude that our numerical results for $\chi(p)$ and $\mu(p)$ have the form as one could expect for hole overdoped phase.

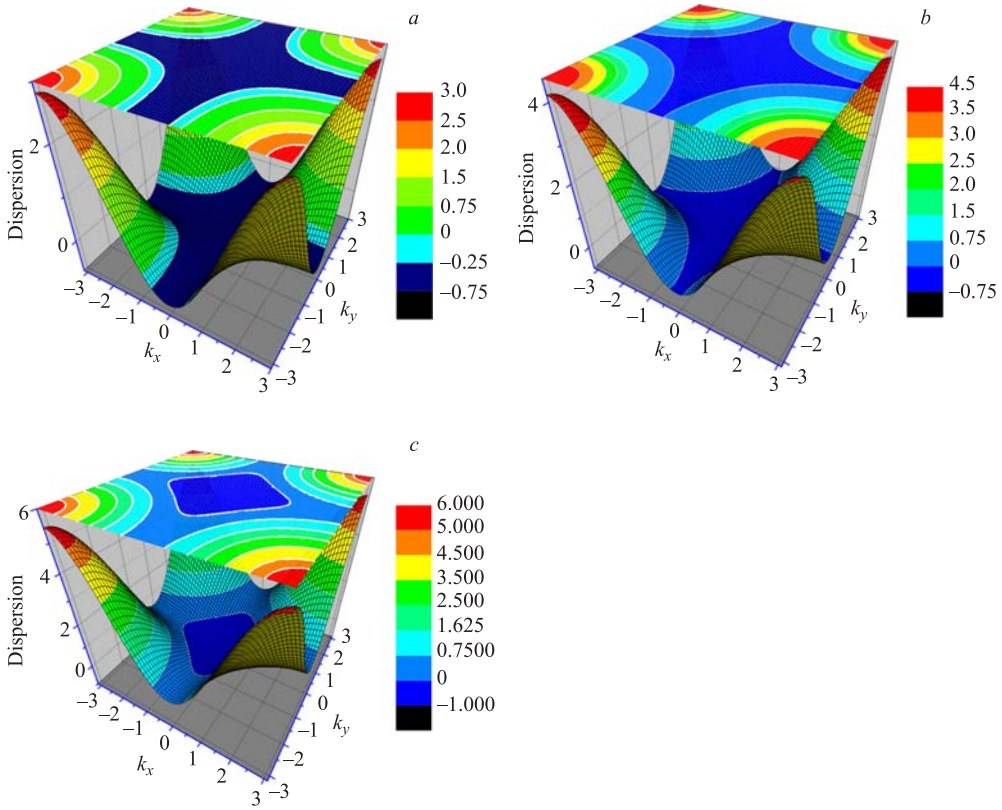

Fig. 2. 3D and contour plot of the hole dispersion is plotted for hole concentration: 0.3 (*a*), 0.5 (*b*), 0.7 (*c*)

On the other hand, the staggered part $\chi_{\mathbf{Q}}$ of the static spin susceptibility decreases and shifts to the higher energies upon hole doping, see, for example, [1, 2, 20, 26]. Uniform static quasiparticle part χ_0 even gets enhanced with Stoner exchange, and is approximately T-independent [19, 21], what is in agreement with our results presented in Fig. 1. As it follows from results of [21], the origin of the temperature dependence of χ_m is the effect of the AF spin fluctuations, which is described by $\chi_{\mathbf{Q}}$. The same conclusion also comes out from results of investigations of the relaxation of a rare-earth impurity ion, where one can explain the T dependence of the crystal field linewidth as the effect of the spin fluctuations, described with the staggered spin susceptibility $\chi_{\mathbf{Q}}$ [64–68]. Although we should notice that there is also another point of view, that $\chi_{\mathbf{Q}}$ describes charge density wave instability of the ground state [26]. In the equation for uniform spin susceptibility, influence of the AF spin fluctuations is included in the corresponding renormalization of the quasiparticle energy spectrum $\tilde{E}_{\mathbf{q}}$, so one can understand strong increase of χ_0 at low-hole doping and in the high-temperature regime, presented in Fig. 1 as effect of the AF spin fluctuations.

In Fig. 2, *a–c*, we present evolution of the Fermi surface (FS) and the quasiparticle energy dispersion on the hole doping. In the top contour plots one can see transformation of the 2D FS from four pocket-like centered at $M(\pi, \pi)$ points of the B.Z. for small doping $p < 0.5$ to the electron-like FS centered at $\Gamma(0, 0)$ point of B.Z. for large doping $p > 0.5$. However, from the experimental results [59], FS shape transforms at $p = 0.22$, similar to the numerical results (for $p < 0.3$) in the framework of the Hubbard model [55]. This point could indicate that $t - J$ model is not an adequate model for quantitative description of real materials.

CONCLUSIONS

In the framework of $t - J$ model we have investigated hole concentration dependencies of the chemical potential μ and static spatially uniform spin susceptibility χ_0 in the CuO_2 plane, the common block of the HTSC cuprate compounds. We used the projection method technique of the GF equations of motion. In the considered case Pauli-like itinerant susceptibility presents inherent quasiparticle part of the magnetic response. Antiferromagnetic fluctuations and strong correlations were included in the mean-field approximation method used to obtain corresponding renormalization of the quasiparticle energies. For small doping at high temperature, contribution of the AF fluctuations became dominant, which led to strong increase of the quasiparticle magnetic response.

Evolution of the FS shape had no essential effect on the inherent quasiparticle uniform static susceptibility. One could expect that FS transformation will lead to a strong influence on the staggered part of magnetic response, what can explain temperature and doping dependence of the static spin susceptibility. However, in order to better fit experimental results, one should repair hole concentration dependencies obtained in the framework of the $t-J$ model probably using the Hubbard model as the more adequate one for the description of high-temperature superconductors.

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