

LOCAL SPIN MAGNETIZATION AROUND Zn ION WHICH IS DOPED IN THE CuO₂ PLANE

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The local static spin susceptibility at neighbour sites from vacant Cu in the CuO₂ plane was obtained. Calculations were performed using one of the variants of the memory function method. Charge-transfer and spin-flip correlation functions were expressed in the framework of the T-matrix formalism in terms of the corresponding Green functions for the ideal $t - J$ model on the square lattice.

Получена локальная статическая спиновая восприимчивость для ближайших соседей от вакантного Cu-узла в CuO₂-плоскости. Вычисление проведено с использованием одного из вариантов метода функции памяти. С помощью T-матричного формализма корреляционные функции с переносом заряда и с переворотом спина выражены через функции Грина для идеальной $t - J$ -модели на квадратной решетке.

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INTRODUCTION

Recently, much attention has been attracted by investigations of the electronic excitation spectrum induced by the Zn doped high-temperature superconductive cuprates (Zn:CuO₂) [1, 2]. In addition to the unexpected sharp detrimental effect on superconductivity (in the hole underdoped phase about 20 K per % of Zn substitutions) and strong suppression of the spin gap in the spin-fluctuation spectrum, the local magnetic moments appear in the close vicinity of the nonmagnetic impurity which substitutes a Cu atom in the strong electron correlated CuO₂ plane [3].

Recent results of nuclear magnetic resonance experiments on Zn:CuO₂ systems can be explained if one supposes that these magnetic moments and the corresponding site-localized spin susceptibilities χ_{ii} on the nearest neighbour ($i = \text{n.n.}$) and on the next to nearest neighbour ($i = \text{n.n.n.}$) sites to Zn ion are of the opposite sign and on the n.n.n. sites are about three times smaller than on the n.n. ones [4, 5].

One should like to obtain some additional theoretical support of these prepositions of impurity induced ordered magnetic moments on the nearly cluster sites. This motivates one to calculate the local spin susceptibility χ_{ii} on the n.n. and n.n.n. sites i , which is occupied with Cu atom in the host lattice of the CuO₂ plane, with respect to the site occupied by impure Zn atom.

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The corresponding microscopic model for Zn:CuO₂ system was derived and considered in [1], where, in accordance with the T-matrix method [6], the additional symmetrized density of states in the normal phase is calculated.

To calculate χ_{ii} , one can use the method of memory function [7], and especially its variants, which are developed for the $t - J$ model in the Hubbard operator representation [8].

Application of this method in the present case leads to some integral expression for χ_{ii} with charge-transfer $\langle X_i^{\sigma 0} X_j^{0\sigma} \rangle$ and spin-spin $\langle S_i^+ S_j^- \rangle$ correlation functions. To calculate $\langle X_i^{\sigma 0} X_j^{0\sigma} \rangle$, one uses the Green function (GF) method [9–11] and the T-matrix method [1, 6]. For $\langle S_i^+ S_j^- \rangle$ one also uses the T-matrix method, and the corresponding host lattice GF $\langle\langle S_q^+ | S_{-q}^- \rangle\rangle_\omega^0$ can be calculated numerically.

In Sec. 1, one firstly describes the corresponding microscopic model and the calculation methods. After it, in the Subsec. 1.1 some definition and identity from the memory function method [8] are given, which are necessary for the present analytical calculations. In the Subsec. 1.2, one writes some main formulae of the GF method [10]. In the Subsec. 1.3, one presents main formulae of the T-matrix method applied to the investigated system [1], and in the last Subsec. 1.4 of the first chapter, one gives some useful formulae needed to calculate spin susceptibility χ_{ii} .

In the Sec. 2, the theoretical expression is derived for the difference between n.n. and n.n.n. χ_{ii} . Then follows the Conclusions.

1. MODEL HAMILTONIAN AND CALCULATION METHODS

To investigate properties of a strongly correlated electron system with impurity such as Zn:CuO₂, one can consider an effective $t - J$ model for the CuO₂ plane with vacant Cu site $i = 0$:

$$H = H_{t-J} + V. \quad (1)$$

The hamiltonian of the $t - J$ model in the standard notation takes the form

$$H_{t-J} = \sum_{i \neq j, \sigma} t_{ij} (1 - n_{i\bar{\sigma}}) c_{i\sigma}^+ c_{j\sigma} (1 - n_{j\bar{\sigma}}) + \sum_{i \neq j} J_{ij} \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j \right). \quad (2)$$

To strongly keep the local constraint on doubly occupied sites, one is favourable to use the advantage of the Hubbard operators, whose algebra leads to that they satisfy the constraint rigorously.

In the Hubbard operator representation $X_i^{\alpha\beta} = |i, \alpha\rangle \langle i, \beta|$, one has $X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} = 1$ and

$$X_i^{\sigma 0} = c_{i\sigma}^+ (1 - n_{i\bar{\sigma}}), \quad n_i = \sum_{\sigma} X_i^{\sigma\sigma}, \quad S_i^z = \frac{1}{2} \sigma (n_{i\sigma} - n_{i\bar{\sigma}}) = \frac{1}{2} \sum_{\sigma} \sigma X_i^{\sigma\sigma}, \quad S_i^{\sigma} = X_i^{\sigma\bar{\sigma}}. \quad (3)$$

The hamiltonian of the $t - J$ model in the Hubbard operator notation takes the form

$$H_{t-J} = \epsilon \sum_{i\sigma} X_i^{\sigma\sigma} + \sum_{i \neq j, \sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} + \frac{1}{4} \sum_{i \neq j, \sigma} J_{ij} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}}), \quad (4)$$

where $t_{ij} = t$ and $J_{ij} = J$, if $i = \text{n.n.}(j)$ and $t_{ij} = t'$ and $J_{ij} = 0$, if $i = \text{n.n.n.}(j)$. The vacancy contribution is given by

$$V_{\text{vac}} = -\epsilon \sum_{\sigma} X_0^{\sigma\sigma} - t \sum_{\Delta\sigma} (X_0^{\sigma 0} X_{\Delta}^{0\sigma} + \text{h.c.}) - \frac{1}{4} J \sum_{\Delta\sigma} (X_0^{\sigma\bar{\sigma}} X_{\Delta}^{\bar{\sigma}\sigma} - X_0^{\sigma\sigma} X_{\Delta}^{\bar{\sigma}\bar{\sigma}} + \text{h.c.}) \quad (5)$$

with $\epsilon = \epsilon_d - \mu$ being on-site electron energy «measured» from the chemical potential level μ . The summation over nonequal indices $i \neq j$ is performed over the nearest neighbor (n.n.) and the next to them (n.n.n.) Cu-sites of the host square lattice, and the Zn-impurity is at the $i = 0$ site with $\Delta = 1, 2, 3, 4$ denoting its n.n. sites, as shown in Fig. 1.

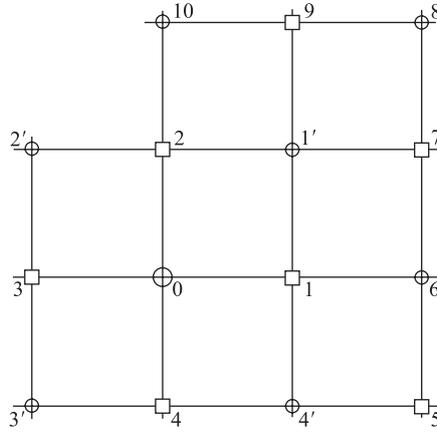


Fig. 1. Schematic presentation of the nearest neighbouring (n.n.) and the next to n.n. sites of the impurity (or, vacancy) site 0 and of the sites 1 and 1' which one needs in calculations. Different symbols: \circ and \square , also point out a different orientation of the localized magnetic moments

1.1. Using the Memory Function Method. To calculate real space static spin susceptibility [8–10]

$$\chi_{ij}^{+-}(\omega = 0) = -\langle\langle S_i^+ | S_j^- \rangle\rangle_{\omega=0} = (S_i^+, S_j^-), \quad (6)$$

one can use the identity [8]

$$m_{ij} \equiv \langle\langle [i\dot{S}_i^+, S_j^-] \rangle\rangle = (-\ddot{S}_i^+, S_j^-), \quad (7)$$

where the sought quantity (S_i^+, S_j^-) appears as a factor after developing the corresponding commutators in the equation of motion for the spin operators.

For the system with impurity (or, vacant) site, one can expect a different value of the on-site (local) quantity m_{ii} for $i = \text{n.n.}$ and $i = \text{n.n.n.}$ sites, because of a different contribution of quasiparticle scatterings to the equation of motion for the spin rising operators S_i^+ due to the interaction V between the impurity and host lattice.

1.2. Using the Green Function Method. After completing the corresponding algebraic calculations described in the next section, one obtains local static spin susceptibilities at the n.n. sites χ_{11} and the n.n.n. sites $\chi_{1'1'}$ in terms of the charge transfer $\langle X_0^{\sigma 0} X_i^{0\sigma} \rangle$ and spin-fluctuation correlation functions $\langle S_0^- S_i^+ \rangle$.

To calculate them, one can use the GF method as, for example, the Zubarev general formulation [9, 10]. One considers two-time temperature GF:

$$G_{ij\sigma}(t, t') = \langle \langle A(t); B(t') \rangle \rangle = -i\theta(t - t')[A(t), B(t')]_{\eta}, \quad (8)$$

where $[A(t), B(t')]_{\eta} = A(t)B(t') - \eta B(t')A(t)$ with $\eta = \pm 1$, respectively, for the commutator (anticommutator) of the operators A and B in the Heisenberg representation.

Instantaneous correlation functions can be calculated using temporary dependent correlation functions and the relation of their temporary Fourier transformation (F.T.) to the corresponding F.T. of the GF, respectively:

$$\langle AB \rangle \equiv \langle A(t)B(0) \rangle \Big|_{t=0} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} J_{AB}(\omega) e^{-i\omega t} \Big|_{t=0} d\omega = \frac{1}{2\pi} \int_{-\infty}^{+\infty} J_{AB}(\omega) d\omega \quad (9)$$

with

$$J_{BA}(\omega) = \frac{-2}{e^{\beta\omega} - \eta} \text{Im} G_{AB}(\omega + i\varepsilon) \quad (10)$$

and $\beta = 1/(k_B T)$. To find the Im part of the GF, one usually uses the identity

$$\frac{1}{x \pm i\varepsilon} = \text{PP} \frac{1}{x} \mp i\pi\delta(x) \quad (11)$$

and for the GF's real part one has

$$\text{Re} G(\omega) = -\frac{1}{\pi} \text{PP} \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} \text{Im} G(\omega') \quad (12)$$

with PP being the Cauchy principal part of the corresponding singular integral. The GF's of the operators in the direct and opposite order are connected with $\langle \langle A|B \rangle \rangle_{\omega+i\varepsilon} = \eta \langle \langle B|A \rangle \rangle_{-(\omega+i\varepsilon)}$ [10].

1.3. Using the T-Matrix Method. As the considered system is not translationally invariant (because of the vacant site $i = 0$), one should express the corresponding «scattered GF» in terms of the «zero-order GF», as was presented in [1, 6].

Using the GF equation of motion method for the given system, one obtains the «Dyson equation» for the GF in the matrix notation as

$$\hat{G} = \hat{G}^0 + \hat{G}^0 \hat{V} \hat{G} = \hat{G}^0 + \Delta \hat{G}, \quad (13)$$

where \hat{G}^0 is the site-index matrix «zero-order GF» and only nonzero elements of the perturbation matrix are, according to the model (5), n.n. sites close to the impurity (or, vacancy). The scattering addition to «zero-order GF» is $\Delta \hat{G} \equiv \hat{G}^0 \hat{M} \hat{G}^0$ with the scattering matrix

$$\hat{M} = \hat{V} \frac{1}{1 - \hat{G}^0 \hat{V}}. \quad (14)$$

After symmetrization of the scattering, i.e., performing the corresponding unitary transformation in accordance with irreducible group theory representations [6] of the symmetry

transformations of the considered system, one obtains «scattering additions to GF» $\Delta\hat{G}$ for the nonideal system expressed in terms of the «zero-order GF» \hat{G}^0 for the ideal system (without impurity or vacancy)

$$\Delta\hat{G} = \sum_{\mu} \hat{G}^0 \hat{T}_{\mu} \hat{M}_{\mu} \hat{T}_{\mu}^+ \hat{G}^0 = \sum_{\mu} \Delta G^{(\mu)}, \quad (15)$$

where summation runs over the possible irreducible representation μ . The corresponding block-diagonal matrices are

$$\hat{M}_{\mu} = \hat{V}_{\mu} \left[1 - \hat{G}_{\mu}^0 \hat{V}_{\mu} \right]^{-1} \quad (16)$$

with $\hat{V}_{\mu} \equiv \hat{T}_{\mu}^+ \hat{V} \hat{T}_{\mu}$ and $\hat{G}_{\mu}^0(\omega) \equiv \hat{T}_{\mu}^+ \hat{G}^0(\omega) \hat{T}_{\mu}$, where \hat{T}_{μ} are rectangular matrices, that are columns of the corresponding unitary matrix that «block-diagonalizes» the perturbation matrix \hat{V} . In such a way, one obtains the symmetrized scattering additions to «zero-order GF», as was written in paper [1] for the present model.

1.4. Useful Formulae and Approximations. Using Eqs. (9), (10) one has for charge-transfer

$$\langle X_m^{\sigma 0} X_n^{0\sigma} \rangle = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} \langle \langle X_n^{0\sigma} | X_m^{\sigma 0} \rangle \rangle_{\omega}}{e^{\beta\omega} + 1} \equiv -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} G_{nm}(\omega)}{e^{\beta\omega} + 1} \quad (17)$$

and for the spin-fluctuation correlation function

$$\langle S_m^- S_n^+ \rangle = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} \langle \langle S_n^+ | S_m^- \rangle \rangle_{\omega}}{e^{-\beta\omega} - 1} \equiv \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega \frac{\text{Im} \mathcal{S}_{nm}(\omega)}{e^{-\beta\omega} - 1}. \quad (18)$$

Using Eq. (12) one has

$$(S_m^+, S_n^-) \equiv -\langle \langle S_m^+ | S_n^- \rangle \rangle_{\omega=0} = \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\text{Im} \mathcal{S}_{mn}(\omega')}{\omega'}. \quad (19)$$

To evaluate the multisite correlation functions, one can use mean-field approximations [8], where

$$(X_i^{\sigma 0} X_j^{0\sigma} S_m^+, S_n^-) \simeq \lambda \langle X_i^{\sigma 0} X_j^{0\sigma} \rangle (S_m^+, S_n^-) \quad (20)$$

and

$$(S_i^+ S_j^- S_m^+, S_n^-) \simeq \alpha_1 \langle S_m^+ S_j^- \rangle (S_i^+, S_n^-) + \alpha_2 \langle S_i^+ S_j^- \rangle (S_m^+, S_n^-), \quad (21)$$

where one renormalizes the corresponding vertices: λ takes into account the spin-hole interactions; and α_1 and α_2 , spin-flip processes in the n.n. and n.n.n. lattice sites. In the considered paramagnetic phase of the CuO₂ system, one has the following relations:

$$\langle \langle S_m^z | S_n^z \rangle \rangle = \frac{1}{2} \langle \langle S_m^+ | S_n^- \rangle \rangle, \quad \langle S_m^- S_n^+ \rangle = \langle S_m^+ S_n^- \rangle = 2 \langle S_m^z S_n^z \rangle \quad (22)$$

and also

$$\langle X_i^{+0} X_j^{0-} S_l^- \rangle \simeq 0, \quad \langle X_i^{++} \rangle \simeq \langle X_i^{--} \rangle = n/2, \quad \langle X_i^{-0} X_j^{0-} \rangle \simeq \langle X_i^{+0} X_j^{0+} \rangle. \quad (23)$$

As the considered square lattice with the vacant $i = 0$ site has the central point (or, inversion) symmetry under that vacant site, all physical quantities relating to that system are invariant under the $\mathbf{r} \rightarrow -\mathbf{r}$ transformation. As a consequence, one also has

$$\langle X_0^{\sigma 0} X_n^{0\sigma} \rangle = \langle X_n^{\sigma 0} X_0^{0\sigma} \rangle, \quad \langle S_0^+ S_n^- \rangle = \langle S_n^+ S_0^- \rangle. \quad (24)$$

2. CALCULATIONS OF THE GENERAL EXPRESSION

Firstly, one should derive the general identity, where static spin susceptibility $\chi_{ij} = \langle S_i^+ S_j^- \rangle$ appears as a factor.

If one introduces the «spin-current» $J_j \equiv i\dot{S}_j^+ = [S_j^+, H]$ and the «spin-force» $F_j = -\ddot{S}_j^+ = i\dot{J}_j = [[S_j^+, H], H]$ operators [8], one can write Eq. (7) in a shorter form

$$m_{ij} = \langle [J_i, S_j^-] \rangle = (F_i, S_j^-). \quad (25)$$

To arrange the calculation procedure of the commutation relations, one can introduce useful denotation to separate different terms of Hamiltonians (4), (5)

$$H_{t-J} = H_t + H_\mu + H_J, \quad V = V_t + V_J, \quad (26)$$

where

$$H_t = \sum_{i \neq j, \sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma}, \quad H_J = \frac{1}{4} \sum_{i \neq j, \sigma} J_{ij} (X_i^{\sigma \bar{\sigma}} X_j^{\bar{\sigma} \sigma} - X_i^{\sigma \sigma} X_j^{\bar{\sigma} \bar{\sigma}}) \quad (27)$$

and

$$V_t = -t \sum_{\Delta \sigma} (X_0^{\sigma 0} X_{\Delta}^{0\sigma} + \text{h.c.}), \quad V_\mu = -\epsilon \sum_{\sigma} X_0^{\sigma \sigma}, \quad V_J = -\frac{J}{4} \sum_{\Delta \sigma} (X_0^{\sigma \bar{\sigma}} X_{\Delta}^{\bar{\sigma} \sigma} - X_0^{\sigma \sigma} X_{\Delta}^{\bar{\sigma} \bar{\sigma}} + \text{h.c.}) \quad (28)$$

and, as a consequence, one has different terms in the spin-current

$$J_j = J_j^t + \delta J_j^t + J_j^J + \delta J_j^J \quad (29)$$

with

$$J_j^t = [S_j^+, H_t], \quad \delta J_j^t = [S_j^+, V_t], \quad J_j^J = [S_j^+, H_J], \quad \delta J_j^J = [S_j^+, H_J] \quad (30)$$

and the spin-force operators [8]

$$F_j = F_j^{tt} + \delta F_j^{tt} + \delta^2 F_j^{tt} + F_j^{JJ} + \delta F_j^{JJ} + \delta^2 F_j^{JJ} \quad (31)$$

with

$$F_j^{tt} = [J_j^t, H_t], \quad \delta F_j^{tt} = [J_j^t, V_t], \quad \delta^2 F_j^{tt} = [\delta J_j^t, V_t], \quad F_j^{JJ} = [J_j^J, H_J], \quad (32)$$

and

$$\delta F_j^{JJ} = [\delta J_j^J, H_J], \quad \delta^2 F_j^{JJ} = [\delta J_j^J, V_J], \quad (33)$$

respectively. Any of the commutators of S_j^+ and J_j with H_μ and V_μ are equal to zero.

In such a way, one has in the new denotation

$$m_{jk} = \langle [J_j, S_k^-] \rangle = \langle [J_j^t + J_j^J, S_k^-] \rangle + \langle [\delta J_j^t + \delta J_j^J, S_k^-] \rangle = \\ = (F_j^{tt} + F_j^{JJ}, S_k^-) + (\delta F_j^{tt} + \delta^2 F_j^{tt} + \delta F_j^{JJ} + \delta^2 F_j^{JJ}, S_k^-). \quad (34)$$

As in the ideal system, one has $\langle [J_j^t + J_j^J, S_k^-] \rangle = (F_j^{tt} + F_j^{JJ}, S_k^-)$, which leads to the following relations

$$\langle [\delta J_j^t + \delta J_j^J, S_k^-] \rangle = (\delta F_j^{tt} + \delta^2 F_j^{tt} + \delta F_j^{JJ} + \delta^2 F_j^{JJ}, S_k^-). \quad (35)$$

Specifying the sites j and k and developing the commutators contained in the spin-force terms F_j^{aa} with $a = (t, J)$, one obtains self-consistent relation where, the sought static spin susceptibility $\chi_{jk} = (S_j^+, S_k^-)$ appears as a factor.

2.1. Local Static Spin Susceptibilities. For $j = k = 1$, Eq. (35) becomes

$$-2t \langle X_0^{\sigma 0} X_1^{0\sigma} \rangle + 2J \langle S_0^+ S_1^- \rangle = (\delta F_1^{tt} + \delta^2 F_1^{tt}, S_1^-) + (\delta F_1^{JJ} + \delta^2 F_1^{JJ}, S_1^-) \quad (36)$$

with

$$(\delta F_1^{tt} + \delta^2 F_1^{tt}, S_1^-) = \left\{ 2\lambda t^2 [\langle X_0^{\sigma 0} X_{2a_X}^{0\sigma} \rangle + 2\langle X_0^{\sigma 0} X_{a_X+a_Y}^{0\sigma} \rangle] + \right. \\ \left. + 4\lambda t t' [\langle X_0^{\sigma 0} X_{2a_X+a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_Y}^{0\sigma} \rangle] + \left(\frac{3}{2}n\lambda + 1 \right) t^2 \right\} (S_1^+, S_1^-) + \left(\frac{n\lambda}{2} + 1 \right) t^2 (S_0^+, S_1^-) \quad (37)$$

and

$$(\delta F_1^{JJ} + \delta^2 F_1^{JJ}, S_1^-) = \alpha_1 J^2 \{ \langle S_0^- S_1^+ \rangle [\langle S_{1+a_X}^+, S_1^- \rangle + \langle S_{1+a_Y}, S_1^- \rangle + \langle S_{1-a_Y}, S_1^- \rangle - \\ - \langle S_{1-a_X+a_Y}, S_1^- \rangle - \langle S_{1-a_X-a_Y}, S_1^- \rangle - \langle S_{1-2a_X}, S_1^- \rangle] - \left[\langle S_0^- S_{a_Y}^+ \rangle + \frac{1}{2} \langle S_0^- S_{-a_X}^+ \rangle \right] \times \\ \times \langle S_1^+, S_1^- \rangle \} + \alpha_2 J^2 \{ \langle S_{1-a_X+a_Y}^-, S_1^+ \rangle + \langle S_{1-a_X-a_Y}^-, S_1^+ \rangle + \langle S_{1-2a_X}^-, S_1^+ \rangle \} \langle S_0^+, S_1^- \rangle - \\ - [\langle S_{2a_X}^-, S_0^+ \rangle + 2\langle S_{a_X+a_Y}^-, S_0^+ \rangle] \langle S_1^+, S_1^- \rangle \} + \lambda J^2 \langle S_1^+, S_1^- \rangle + \lambda J^2 \frac{n}{2} \langle S_0^+, S_1^- \rangle, \quad (38)$$

where $a_X = a$ and $a_Y = a$ are lattice translation constants along the x - and y -axes.

For $j = k = 1'$, Eq. (35) becomes

$$-2t' \langle X_0^{\sigma 0} X_{1'}^{0\sigma} \rangle + 2J \langle S_0^+ S_{1'}^- \rangle = (\delta F_{1'}^{tt} + \delta^2 F_{1'}^{tt}, S_{1'}^-), \quad (39)$$

where in the right-hand side there are no corresponding terms containing $F_{1'}^{JJ}$, as in Eq. (36), because it gives zero contribution $(\delta F_{1'}^{JJ} + \delta^2 F_{1'}^{JJ}, S_{1'}^-) = 0$ which is a consequence of the fact that $J_{01'}^J = 0$ in the considered model (5). For the right-hand side of Eq. (39), one has

$$(\delta F_{1'}^{tt} + \delta^2 F_{1'}^{tt}, S_{1'}^-) = \\ = 2\lambda t' t [\langle X_0^{\sigma 0} X_{2a_X+a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_X+2a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_Y}^{0\sigma} \rangle] \langle S_{1'}^+, S_{1'}^- \rangle + 2\lambda t'^2 [\langle X_0^{\sigma 0} X_{2a_X+2a_Y} \rangle + \\ + \langle X_0^{\sigma 0} X_{2a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{2a_X}^{0\sigma} \rangle] \langle S_{1'}^+, S_{1'}^- \rangle + t'^2 \left(\frac{3}{2}n\lambda + 1 \right) \langle S_{1'}^+, S_{1'}^- \rangle + t'^2 \left(\frac{n\lambda}{2} + 1 \right) \langle S_0^+, S_{1'}^- \rangle. \quad (40)$$

Using the usual parameter value $t \simeq 0.4$ eV, $J = 0.3t$ and $t = -0.3t$ [3, 12], one can write Eqs. (36), (40) in simpler forms and one finally obtains local spin susceptibilities, respectively, at the n.n.n. and the n.n. sites with respect to the Cu-vacancy (or, Zn impurity ion) in the CuO₂ plane as

$$\chi_{1'1'} \equiv (S_{1'}^+, S_{1'}^-) = \frac{-t'/t \langle X_0^{\sigma 0} X_{1'}^{0\sigma} \rangle + J/t \langle S_0^- S_{1'}^+ \rangle}{\lambda t' [\langle X_0^{\sigma 0} X_{2a_X+a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_X+2a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_Y}^{0\sigma} \rangle]} \quad (41)$$

and

$$\begin{aligned} \chi_{11} \equiv (S_1^+, S_1^-) &= \\ &= \frac{-2 \langle X_0^{\sigma 0} X_1^{0\sigma} \rangle + 2J/t \langle S_0^- S_1^+ \rangle - (1 + n\lambda/2)t(S_0^+, S_1^-)}{2\lambda t [\langle X_0^{\sigma 0} X_{2a_X}^{0\sigma} \rangle + 2 \langle X_0^{\sigma 0} X_{a_X+a_Y}^{0\sigma} \rangle] + 4\lambda t' [\langle X_0^{\sigma 0} X_{2a_X+a_Y}^{0\sigma} \rangle + \langle X_0^{\sigma 0} X_{a_Y}^{0\sigma} \rangle] + \left(1 + \frac{3n\lambda}{2}\right)t}, \end{aligned} \quad (42)$$

which for $\lambda t \gg 1$ becomes

$$\chi_{11} \equiv (S_1^+, S_1^-) = \frac{-(1/\lambda + n/2)(S_0^+, S_1^-)}{2[\langle X_0^{\sigma 0} X_{2a_X}^{0\sigma} \rangle + 2 \langle X_0^{\sigma 0} X_{a_X+a_Y}^{0\sigma} \rangle] + 1/\lambda + 3n/2}. \quad (43)$$

As one can see from Eqs. (41), (43), one has to calculate also (S_0^+, S_1^-) and the correlation functions $\langle S_0^+ S_1^- \rangle$ and $\langle X_0^{0\sigma} X_m^{\sigma 0} \rangle$. For them one should use Eqs. (18) and (17), respectively, and for the GF's, which appear there, one should use equations $S_{0m} = S_{0m}^0 + \Delta S_{0m}^\mu$ and $G_{0m} = G_{0m}^0 + \Delta G_{0m}^{(\mu)}$. The additions ΔS_{0m}^μ and $\Delta G_{0m}^{(\mu)}$ to the «zero-order GF's» S_{0m}^0 and G_{0m}^0 , respectively, have the same symmetrized form in terms of the latter, as given in [1]. Finally, one can use Eq. (19) to calculate (S_0^+, S_1^-) .

CONCLUSIONS

In this paper, the analytical expressions for local spin susceptibilities in the n.n. and n.n.n. sites to the vacant $i = 0$ site of the $t - J$ model were derived, as proposed in the model of Zn doped superconducting cuprates.

A special variant of the memory function technique, developed in [8] was applied. To obtain complete self-consistent equations, one should use also the results of the symmetry analysis for the present model, which is performed in [1] and also «zero-order GF's». For charge-transfer GF and their F.T. $G^0(\mathbf{q}, \omega) = \langle \langle X_{\mathbf{q}}^{0\sigma} X_{-\mathbf{q}}^{\sigma 0} \rangle \rangle^0(\omega)$ one can use the renormalized band energy $E(\mathbf{q})$ obtained in [1] or [11]. For zero-order spin-fluctuation GF and their F.T. $S^0(\mathbf{q}, \omega) = \langle \langle S_{\mathbf{q}}^+ | S_{-\mathbf{q}}^- \rangle \rangle^0(\omega)$ one can use some of the well-justified models [11].

Further work will be aimed at obtaining the impurity induced staggered spin susceptibilities around $i = 0$ site and the numerical calculations, which will be published elsewhere.

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