ORDER, DISORDER, AND PHASE TRANSITION IN CONDENSED SYSTEMS

Theory of Dynamic Spin Susceptibility in Terms of the t–J–V Model: Comparison with Neutron Scattering Data for $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ and $La_{2-x}Sr_xCuO_4$

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Abstract—A formula for the dynamic spin susceptibility is derived in terms of the t–J–V model. This formula makes it possible to explain the main features of recent experiments on neutron scattering in the electron-doped superconductor $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$. In particular, the proposed theory reproduces well a V-shaped relief in the frequency behavior of the imaginary part $\chi''(Q, \omega)$ of the susceptibility of the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ compound in the vicinity of the wave vector $Q = (\pi, \pi)$ and the scaling behavior of the position of the maxima in the dependence of the function $\chi''(Q, \omega)T$ on the quantity ω/T. The magnetism of the high-temperature superconductors is dual. These materials contain charge carriers, on the one hand, and localized spins in the copper ion sublattice, on the other hand. Both these systems are strongly coupled to each other. The mode of collective oscillations is common. The magnetism of localized spins "freezes" with the appearance of the superconducting gap. The recently revealed double-peak structure of the imaginary part $\chi''(Q, \omega)$ of the susceptibility in superconductors of the $La_{1.84}Sr_{0.16}CuO_4$ type is explained. The low-frequency absorption peak is located within the superconducting gap and interpreted as a manifestation of the branch of spin excitons, and the high-frequency absorption peak predominantly corresponds to renormalized collective oscillations of localized spins.

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1. INTRODUCTION

High-temperature superconductors based on layered cuprates have a rather rich phase diagram. These materials at low doping levels belong to the class of quasi-two-dimensional antiferromagnets. The temperature dependence of the magnetic susceptibility in the paramagnetic phase obeys the Curie–Weiss law. At high doping levels, these materials are metals with the Pauli–Landau paramagnetism. The description of the magnetism for the region intermediate between the insulator and metal phases is an important problems in physics [1]. The t–J model is considered the main model for describing the dual character of the magnetism in these compounds [2]. The parameter t corresponds to hopping of electrons (doped holes) from one site to another, and J is the parameter of the superexchange interaction between localized copper spins. The parameter V of the Coulomb interaction of electrons, as a rule, is considered insignificant in the theory of magnetism and is hence omitted for brevity. However, in the general case, the Coulomb interaction is undeniably important. In particular, this interaction is necessary for describing the spectrum of plasmon modes and phase separations in the systems under consideration.

The available works devoted to the study of the dual character of magnetism in the intermediate region of the phase diagram of high-temperature superconductors can be separated into two groups. The authors of [3–7] and other works (see references in [7]) begin with the dielectric phase in which the number of charge carriers is small and superconductivity is absent; they simply include the susceptibility of itinerant electrons as an additive component [3]. By contrast, in works of the other group [8–12], researchers consider the conducting phase as basic. Particular emphasis has been placed on the analysis of the magnetic susceptibility of itinerant electrons, for which the motion is correlated by the condition of the simultaneous absence of two charge carriers at the same site (lower Hubbard subband). In this case, the susceptibility of localized spins is ignored.

In this paper, we derive a new relationship for the dynamic spin susceptibility in terms of the t–J–V model. In the dielectric limit when the charge carrier concentration is zero, the derived relationship corresponds exactly to the spin susceptibility of a two-dimensional antiferromagnet. At the same time, our formula in the case where the spin–spin correlation

functions of localized spins are zero (metal phase) corresponds to the generalized random-phase approximation for metals with strong electron correlations. As an application of the derived relationship, we analyze the neutron scattering data for the electron-doped superconductor $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$. A short communication on this subject was published in our earlier work [13]. In the present paper, we thoroughly describe the derivation of the formula obtained in [13] for the dynamic spin susceptibility and compare it in detail with the experimental data on neutron scattering for this system [14]. We offer a new explanation for the scaling behavior of the imaginary part of the susceptibility multiplied by the temperature as a function of the ratio between the frequency and the temperature in both the normal and superconducting phases of the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ compound. This scaling phenomenon in the vicinity of the wave vector $Q = (\pi, \pi)$ in the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor was recently discovered by Wilson et al. [15]. Moreover, we demonstrate that the derived formula after the performance of the electron–hole transformation allows us to explain the origin of two peaks of neutron scattering in the vicinity of the wave vector $Q = (\pi, \pi)$ for p-type superconductors $La_{2-x}Sr_xCuO_4$.

2. DERIVATION OF THE FORMULA FOR THE SPIN SUSCEPTIBILITY

The Hamiltonian of the t–J–V model in the representation of the Hubbard operators has the form

$$H = H_t + H_J + H_V = \sum_{i,j,\sigma} t_{ij} X_i^{\sigma,0} X_j^{0,\sigma}$$

$$+ \sum_{i,j,\sigma} \frac{1}{4} J_{ij} (X_i^{\sigma,\bar{\sigma}} X_j^{\bar{\sigma},\sigma} - X_i^{\sigma,\sigma} X_j^{\bar{\sigma},\bar{\sigma}}) \qquad (1)$$

$$+ \sum_{i,j} \frac{1}{2} V_{ij} X_i^{0,0} X_j^{0,0}.$$

Here, the first term describes electron hops between sites of a two-dimensional lattice, the second term represents the superexchange interaction of spins, and the last term corresponds to the Coulomb interaction between charge carriers at different sites. In summation, it is assumed that $i \neq j$. In relationship (1), $X_i^{p,s}$ are the Hubbard operators; the indices p and s can take on values 0, σ, and $\bar{\sigma}$ ($\sigma = \uparrow$ and $\downarrow$, $\bar{\sigma} = -\sigma$); and $X_i^{\sigma,0}$ ($X_i^{0,\sigma}$) are the creation (annihilation) operators for electrons at the ith site with the spin σ.

In deriving the equation of motion for the Fourier transform of the spin operator

$$S_q^+ = \frac{1}{N} \sum_i X_i^{\uparrow,\downarrow} \exp(i\mathbf{q} \cdot \mathbf{R}_i)$$

we use the projection operator technique ($\mathbf{q}$ is the reciprocal lattice vector and $\mathbf{R}_i$ is the radius vector of the ith site). The anticommutation relations have the form

$$\{X_i^{0,\uparrow}, X_j^{\uparrow,0}\} = (X_i^{0,0} + X_i^{\uparrow,\uparrow})\delta_{ij}$$

$$= \left(\frac{1+\delta_i}{2} + S_i^z\right)\delta_{ij}, \qquad (2)$$

$$\{X_i^{0,\downarrow}, X_j^{\downarrow,0}\} = (X_i^{0,0} + X_i^{\downarrow,\downarrow})\delta_{ij}$$

$$= \left(\frac{1+\delta_i}{2} - S_i^z\right)\delta_{ij}, \qquad (3)$$

where δ_{ij} is the Kronecker symbol. These relations are obtained from the completeness condition $X_i^{0,0} + X_i^{\uparrow,\uparrow} + X_i^{\downarrow,\downarrow} = 1$ and the expressions for the spin operators

$$S_i^z = \frac{1}{2}(X_i^{\uparrow,\uparrow} - X_i^{\downarrow,\downarrow}), \quad S_i^+ = X_i^{\uparrow,\downarrow}, \quad S_i^- = X_i^{\downarrow,\uparrow}$$

and the operator of the charge carrier density per unit cell $X_i^{0,0} = \delta_i$. In the frequency representation, the Green's function $\langle\langle S_q^+ | S_{-q}^- \rangle\rangle$ is written in the form

$$\omega \langle\langle S_q^+ | S_{-q}^- \rangle\rangle = \langle\langle [S_q^+, H] | S_{-q}^- \rangle\rangle$$

$$= -\frac{1}{N} \sum_k (t_{k+q} - t_k) \langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle + \frac{1}{N} \qquad (4)$$

$$\times \sum_{i,j} J_{il} \exp(-i\mathbf{q} \cdot \mathbf{R}_i) \langle\langle (S_l^+ S_i^z - S_i^z S_l^+) | S_{-q}^- \rangle\rangle.$$

Here, as in [3–7], we took into account that the long-range magnetic order is absent; i.e., $\langle \sum_i S_i^z \rangle = 0$.

Initially, we examine the Green's function

$$G_{it}(\omega, q) = -\frac{1}{N} \sum_k (t_{k+q} - t_k) \langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle. \qquad (5)$$

This function corresponds to the system of itinerant electrons. In order to calculate the Green's function, we consider the product of the operators

$$X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} = \frac{1}{N} \sum_{i,j} X_j^{0,\downarrow} X_i^{\uparrow,0}$$

$$\times \exp[-i(\mathbf{k}+\mathbf{q}) \cdot \mathbf{R}_j] \exp(i \cdot \mathbf{k}\mathbf{R}_i). \qquad (6)$$

It can be seen that these operators satisfy the following identity:

$$\sum_k X^{0,\downarrow}_{k+q} X^{\uparrow,0}_k = 0, \qquad (7)$$

which will be used in the form

$$\sum_k \langle\langle X^{0,\downarrow}_{k+q} X^{\uparrow,0}_k | S^-_{-q} \rangle\rangle = 0. \qquad (8)$$

In order to calculate the commutator $[X^{0,\downarrow}_{k+q} X^{\uparrow,0}_k, H]$, we use the decoupling scheme [16], in which the random-phase approximation is combined with the Zwanzig–Mori projection operator technique so that the results are obtained in the case of simple metals. For example, the product of the operators $X^{\uparrow,\downarrow}_j X^{\downarrow,0}_s$ in the site representation can be written in the form

$$
\begin{aligned}
t_{js} X^{\uparrow,\downarrow}_j X^{\downarrow,0}_s &= t_{js} X^{\uparrow,\downarrow}_j X^{\downarrow,0}_s (1 - F_t) + t_{js} F_t X^{\uparrow,\downarrow}_j X^{\downarrow,0}_s \\
&= t_{js}(1 - F_t) S^+_j X^{\downarrow,0}_s + (\varepsilon^{\mathrm{tr}}_{jsn} X^{\uparrow,0}_n + \Delta^{\mathrm{tr}}_{jsn} X^{0,\downarrow}_n).
\end{aligned}
\qquad (9)
$$

The coefficients $\varepsilon^{\mathrm{tr}}_{jsn}$ and $\Delta^{\mathrm{tr}}_{jsn}$ are found in the same way as in the conventional projection technique for the subspace of the creation and annihilation operators for electrons. Physically, the parameter F_t is intended to retain the molecular-field effects associated with spins and doped electrons and to provide the stability condition. The imaginary part of the susceptibility should be positive. In the general case, according to this scheme, it is possible to introduce three decoupling parameters: F_t, F_J, and F_V.

At $T > T_c$, using the above technique, we obtain

$$[X^{0,\downarrow}_{k+q} X^{\uparrow,0}_k, (H_t + H_J + H_V)]$$

$$= (\varepsilon_{k+q} - \varepsilon_k) X^{0,\downarrow}_{k+q} X^{\uparrow,0}_k + (1 - F_t)(t_k \langle X^{0,\uparrow}_k X^{\uparrow,0}_k \rangle$$

$$- t_{k+q} \langle X^{0,\downarrow}_{k+q} X^{\downarrow,0}_{k+q} \rangle) S^+_q \qquad (10)$$

$$+ \frac{J_q}{2} F_J (\langle X^{0,\uparrow}_k X^{\uparrow,0}_k \rangle - \langle X^{0,\downarrow}_{k+q} X^{\downarrow,0}_{k+q} \rangle) S^+_q$$

$$- \frac{1}{N} \sum_{k'} (\varepsilon_{k'+q} - \varepsilon_{k'}) X^{0,\downarrow}_{k'+q} X^{\uparrow,0}_{k'},$$

where

$$J_q = 2J_1 \gamma_q \equiv 2J_1[\cos(q_x a) + \cos(q_y a)],$$

$$t_k = \sum_j t_{lj} \exp[i\mathbf{k} \cdot (\mathbf{R}_l - \mathbf{R}_j)]$$

are the Fourier transforms of the superexchange interaction and the hopping integrals, respectively; a is the lattice constant; and

$$
\begin{aligned}
\varepsilon_k = &\left\{ \sum_l t_{li} \left[\frac{1+\delta}{2} + \frac{2}{1+\delta}(1 + 2F_t)\langle S^z_l S^z_i \rangle \right] \right. \\
&+ \sum_l J_{li}(1 - F_J)\frac{1}{1+\delta} \langle X^{0,\downarrow}_l X^{\downarrow,0}_i \rangle \\
&+ \left. \sum_l V_{li}(1 - F_V)\frac{2}{1+\delta} \langle X^{0,\uparrow}_l X^{\uparrow,0}_i \rangle \right\} \\
&\times \exp[i\mathbf{k} \cdot (\mathbf{R}_l - \mathbf{R}_j)]
\end{aligned}
\qquad (11)
$$

is the dispersion law for quasiparticles. This law is conveniently rewritten in the form typical of strong coupling:

$$
\begin{aligned}
\varepsilon_k = &\; 2t^{(1)}_{\mathrm{eff}}[\cos(k_x a) + \cos(k_y a)] \\
&+ 4t^{(2)}_{\mathrm{eff}} \cos(k_x a)\cos(k_y a) \\
&+ 2t^{(3)}_{\mathrm{eff}}[\cos(2k_x a) + \cos(2k_y a)].
\end{aligned}
\qquad (12)
$$

As can be seen, the effective band parameters are defined by the expressions

$$t^{(1)}_{\mathrm{eff}} = t_1 \left(P + \frac{1/2 + F_t}{1+\delta} K_1 \right)$$

$$- \frac{J_1(1-F_J) + 2V_1(1-F_V)}{2N} \sum_{k'} f_{k'} \cos(k'_x a),$$

$$t^{(2)}_{\mathrm{eff}} = t_2 \left(P + \frac{1/2 + F_t}{1+\delta} K_2 \right)$$

$$- \frac{V_2(1-F_V)}{N} \sum_{k'} f_{k'} \cos(k'_x a)\cos(k'_y a), \qquad (13)$$

$$t^{(3)}_{\mathrm{eff}} = t_3 \left(P + \frac{1/2 + F_t}{1+\delta} K_3 \right)$$

$$- \frac{V_3(1-F_V)}{N} \sum_{k'} f_{k'} \cos(2k'_x a),$$

where $P = (1 + \delta)/2$; δ is the mean number of charge carriers per unit cell; and V_1, V_2, and V_3 are the Coulomb interaction parameters for the nearest, next nearest, and third nearest neighbors, respectively.

The spin–spin correlation functions $K_n = 4\langle S^z_0 S^z_n \rangle$ are self-consistently calculated in terms of the dynamic spin susceptibility. The calculation procedure is described in Appendix A. In the course of calculations,

fulfillment of the condition $\langle S_i^+ S_i^- \rangle = (1 - \delta)/2$ (the sum rule) is verified.

It can be seen that the term involved in expression (10) leads to the appearance of a new Green's function:

$$D_{it}(\omega, q) = -\frac{1}{N}\sum_k (\varepsilon_{k+q} - \varepsilon_k)\langle\langle X_{k+q}^{0,\downarrow} X_k^{0,\downarrow} | S_{-q}^- \rangle\rangle.$$

Expression (10) is used to derive the relationship between the Green's functions:

$$\langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle = \frac{i}{2\pi}\chi_{0kq} + [(1 - F_t)\pi_{kq}$$
$$+ J_1\gamma_q F_J\chi_{0kq}]\langle\langle S_q^+ | S_{-q}^- \rangle\rangle + D_{it}(\omega, q)\zeta_{kq}. \tag{14}$$

By summing up over the index k and using condition (8), we obtain

$$D_{it}(\omega, q) = \frac{1}{\zeta(\omega, q)}$$
$$\times \left[-\frac{i}{2\pi}\chi_0(\omega, q) - \eta(\omega, q)\langle\langle S_q^+ | S_{-q}^- \rangle\rangle \right], \tag{15}$$

where

$$\eta(\omega, q) = (1 - F_t)\pi(\omega, q) + J_1\gamma_q F_J\chi_0(\omega, q),$$

$$\chi_0(\omega, q) = \frac{1}{N}\sum_k \chi_{0kq},$$

$$\chi_{0kq} = \frac{P(f_k^h - f_{k+q}^h)}{\omega + \varepsilon_k - \varepsilon_{k+q}},$$

$$\pi(\omega, q) = \frac{1}{N}\sum_k \pi_{kq}, \tag{16}$$

$$\pi_{kq} = \frac{P(t_k f_k^h - t_{k+q} f_{k+q}^h)}{\omega + \varepsilon_k - \varepsilon_{k+q}},$$

$$\zeta(\omega, q) = \frac{1}{N}\sum_k \zeta_{kq},$$

$$\zeta_{kq} = \frac{1}{\omega + \varepsilon_k - \varepsilon_{k+q}}.$$

Here, $Pf_k^h = n_k^h = \langle X_k^{0,\sigma} X_k^{\sigma 0} \rangle$ are the occupation numbers, $f_k^h = \{1 + \exp[(\mu - \varepsilon_k)/k_B T]\}^{-1}$ are the Fermi functions in the hole representation, and μ is the chemical potential. This representation is more convenient because the lower Hubbard band of states is completely occupied for the parent cuprate compound in which charge carriers are absent.

By differentiating relationship (4) with respect to time once more, the Fourier transform of the Green's function can be represented in the form

$$\omega^2 \langle\langle S_q^+ | S_{-q}^- \rangle\rangle = \omega\langle\langle [S_q^+, H] | S_{-q}^- \rangle\rangle$$
$$= \frac{i}{2\pi}\langle[[S_q^+, H], S_{-q}^-]\rangle$$
$$-\frac{1}{N}\sum_k (t_{k+q} - t_k)\langle\langle [X_{k+q}^{0,\downarrow} X_k^{\uparrow,0}, H] | S_{-q}^- \rangle\rangle$$
$$+\frac{1}{N}\sum_{i,l} J_{il}\exp(i\mathbf{q}\cdot\mathbf{R}_i)\langle\langle [(S_l^+ S_i^z - S_l^z S_i^+), H] | S_{-q}^- \rangle\rangle. \tag{17}$$

Here, we have

$$\langle [[S_q^+, H], S_{-q}^-]\rangle = -2J_1 K_1(2 - \gamma_q)$$
$$+\frac{P}{N}\sum_k (t_{k+q} - t_k)(f_{k+q}^h - f_k^h), \tag{18}$$

$$\frac{1}{N}\sum_{i,l} J_{il}\exp(-i\mathbf{q}\cdot\mathbf{R}_i)\langle\langle [(S_l^+ S_i^z - S_l^z S_i^+), H] | S_{-q}^- \rangle\rangle$$
$$= \Omega_q^2 \langle\langle S_q^+ | S_{-q}^- \rangle\rangle, \tag{19}$$

where

$$\Omega_q^2 = J_1^2(2 - \gamma_q)[1 - \delta + 2K_2 + K_3 - K_1(1 + 2\gamma_q)]$$

is the square of the frequency of oscillations of localized spins with allowance made for only the three nearest neighbors. The auxiliary Green's function involved in expression (17) is calculated using the aforementioned rules; that is,

$$-\frac{1}{N}\sum_k (t_{k+q} - t_k)\langle\langle [X_{k+q}^{0,\downarrow} X_k^{\uparrow,0}, H] | S_{-q}^- \rangle\rangle$$
$$= -\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle$$
$$-\frac{P}{N}\sum_k (t_{k+q} - t_k)\left\{\left[\frac{J_q}{2}F_J + (1 - F_t)\varepsilon_k\right]f_k^h\right.$$
$$\left.-\left[\frac{J_q}{2}F_J + (1 - F_t)\varepsilon_{k+q}\right]f_{k+q}^h\right\}\langle\langle S_q^+ | S_{-q}^- \rangle\rangle. \tag{20}$$

The last expression involves the new Green's function

$$\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle,$$

which can be calculated with the use of formula (14); that is,

$$\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\langle\langle X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} | S_{-q}^- \rangle\rangle$$

$$= \frac{i}{2\pi}\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\chi_{0kq}$$

$$+ \left[(1 - F_t)\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\pi_{kq} \right. \quad (21)$$

$$\left. + J_1\gamma_q F_J\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\chi_{0kq} \right]\langle\langle S_q^+ | S_{-q}^- \rangle\rangle$$

$$+ D_{it}(\omega, q)\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\zeta_{kq}.$$

By simultaneously solving Eqs. (15), (17), (20), and (21) with due regard for relationships (18) and (19) and making simplifications of the type

$$\frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k)\zeta_{kq}$$

$$= \frac{1}{N}\sum_k (t_{k+q} - t_k)(\varepsilon_{k+q} - \varepsilon_k - \omega)\frac{1}{\omega + \varepsilon_k - \varepsilon_{k+q}}$$

$$+ \frac{\omega}{N}\sum_k (t_{k+q} - t_k)\zeta_{kq} \quad (22)$$

$$= \frac{\omega}{N}\sum_k (t_{k+q} - t_k)\zeta_{kq} = \omega\zeta_t(\omega, q),$$

we obtain the following formula for the dynamic spin susceptibility:

$$\chi_{\text{total}}^{+,-}(\omega, q) = 2\pi i\langle\langle S_q^+ | S_{-q}^- \rangle\rangle = \frac{\omega\chi_0(\omega, q)\zeta_t(\omega, q) - [\omega\chi_t(\omega, q) + 2J_1 K_1(2 - \gamma_q)]\zeta(\omega, q)}{\omega\eta(\omega, q)\zeta_t(\omega, q) + [\Omega_q^2 - \omega^2 - \omega\eta_t(\omega, q)]\zeta(\omega, q)}, \quad (23)$$

where

$$\zeta_t(\omega, q) = \frac{1}{N}\sum_k (t_{k+q} - t_k)\zeta_{kq},$$

$$\chi_t(\omega, q) = \frac{1}{N}\sum_k (t_{k+q} - t_k)\chi_{0kq},$$

$$\eta_t(\omega, q) = \frac{1}{N}\sum_k (t_{k+q} - t_k)\eta_{kq}.$$

Let us discuss the specific features of relationship (23). In the absence of charge carriers, the functions $\chi_t(\omega, q)$, $\eta_t(\omega, q)$, $\chi_0(\omega, q)$, and $\eta(\omega, q)$ vanish and the function $\zeta(\omega, q)$ entering into the numerator and denominator of relationship (23) is canceled. As a result, we have the expression

$$\chi_{\text{local}}^{+,-}(\omega, q) = \frac{2J_1 K_1(2 - \gamma_q)}{\omega^2 - \Omega_q^2}, \quad (24)$$

which corresponds to a two-dimensional antiferromagnet. This formula coincides with that derived in [3–7, 17], where it is discussed in detail and compared with the results of cluster calculations.

Now, we consider the wide band limit. In this case, the function $\zeta(\omega, q)$ becomes small, the terms with factors in square brackets in relationship (23) can be omit-

ted, and the function $\omega\zeta_t(\omega, q)$ is canceled. This leads to the expression

$$\chi_{\text{itinerant}}^{+,-}(\omega, q)$$

$$= \frac{\chi_0(\omega, q)}{(1 - F_t)\pi(\omega, q) + J_1\gamma_q F_J\chi_0(\omega, q)}. \quad (25)$$

At $F_t = 0$ and $F_J = 1$, this expression exactly coincides with the formula obtained in [8, 10–12]. According to the terminology accepted in [1], this is the generalized random-phase approximation formula for the lower subband. The corresponding formula for the upper Hubbard subband was derived in [9]. However, it should be emphasized that, at $F_t = 0$, expression (25) does not satisfy the stability condition. In the given case, the imaginary part of the function at the band parameters determined from the angle-resolved photoemission spectroscopic data according to our calculations appears to be negative. This justifies the introduction of the parameter $F_t \neq 0$ in order to satisfy the stability conditions with respect to the spin and charge susceptibilities.

Formula (23) has much in common with the expression obtained in [6] for the susceptibility:

$$\chi_{[6]}^{+,-}(\omega, q) = \frac{2(\gamma_q - 1)(J_1 K_1 + t F_1/2)}{\omega^2 - \omega\Pi(\omega, q) - \Omega_q^2}. \quad (26)$$

It can be seen that this expression does not contain the susceptibility function $\chi_0(\omega, q)$ characteristic of itinerant electrons. A similar situation occurs for the formulas derived in [18]. This is explained by different pro-

jection methods used for deriving the corresponding relationships. In [6], as in our study, the dispersion law for quasiparticles was derived using the average value of the anticommutators as the scalar product. However, the expression for the spin susceptibility in [6, 18] was obtained from the Kubo correlation functions. In our case, the dispersion and the susceptibility function were determined with the use of the same projection method. Moreover, in our case, we can generalize formula (23) to the superconducting phase. At $T < T_c$, the general scheme of deriving the relationship for the susceptibility remains the same; however, the technical calculations are substantially complicated. They are presented in Appendix B.

In closing this section, it should be noted that, when the aforementioned projection technique is used, the expression for the charge susceptibility has the form

$$\chi_{\mathrm{ch}}(\omega, q) = 2\pi i \langle\langle X_q^{0,0} | X_{-q}^{0,0}\rangle\rangle$$

$$= \frac{\chi_0(\omega, q)\zeta_t(\omega, q) - \chi_t(\omega, q)\zeta(\omega, q)}{[1 + \varphi(\omega, q)]\zeta_t(\omega, q) - [\omega/2 + \varphi_t(\omega, q)]\zeta(\omega, q)}, \quad (27)$$

where

$$\varphi_{kq} = \frac{M_{k,q} n_k^h - M_{k+q,q} n_{k+q}^h}{\omega + \varepsilon_k - \varepsilon_{k+q}}, \quad \varphi(\omega, q) = \frac{1}{N}\sum_k \varphi_{kq},$$

$$\varphi_t(\omega, q) = \frac{1}{N}\sum_k (t_{k+q} - t_k)\varphi_{kq},$$

$$M_{k,q} = F_V V_q - \frac{1}{4}F_J J_q - \frac{1}{2}(1 - F_t)t_k.$$

The other designations are identical to those for the spin susceptibility.

3. COMPARISON WITH INELASTIC NEUTRON SCATTERING DATA FOR THE $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ SUPERCONDUCTOR

The experimental data obtained by Wilson et al. [14] are characterized by two pronounced features: (1) the imaginary part of the spin susceptibility in the superconducting state exhibits a sharp peak at low energies (Fig. 1); and (2) the scattering intensity peak with an increase in the neutron energy is split, acquires a V-shaped form in the vicinity of the wave vector $Q = (\pi, \pi)$, and resembles strongly weakened magnon scattering for the parent compound La_2CuO_4.

In our calculations, the effective band parameters were taken according to the experimentally observed Fermi surface: $t_{\mathrm{eff}}^{(1)} = 270$ meV, $t_{\mathrm{eff}}^{(2)} = -108$ meV, and $t_{\mathrm{eff}}^{(3)} = 27$ meV. The Hamiltonian parameters, which were self-consistent when formulas (13) were used,
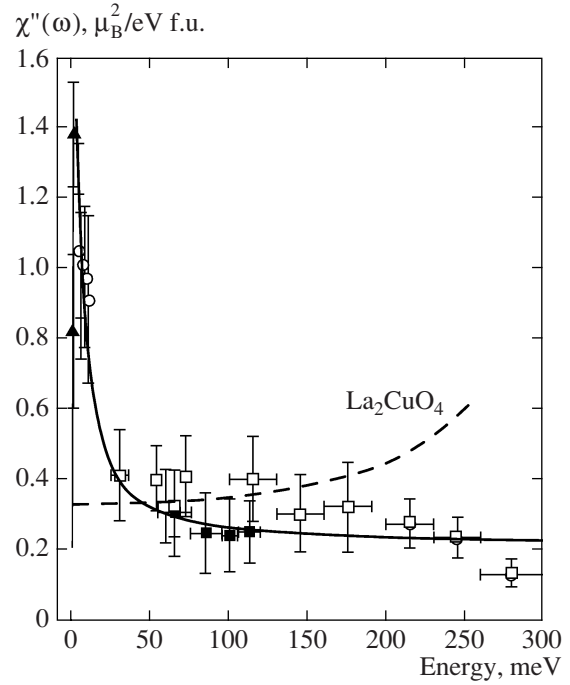

$\chi''(\omega)$, μ_B^2/eV f.u.

Fig. 1. Frequency dependence of the imaginary part of the susceptibility for the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor according to the data taken from [14].

were as follows: $t_1 = 473$ meV, $t_2 = -136.1$ meV, $t_3 = 34.7$ meV, and $\mu = 50$ meV.

The dependence of the screened Coulomb interaction on distance was defined by the relationship $V(R) = (e^2/R)\exp(-\sigma_0 R)$, where $\sigma_0 \approx 10^{10}$ m^{-1} is the screening parameter. It should be noted that the results of the calculations are weakly sensitive to possible changes in the form of the Coulomb pseudopotential. As in [6], the square of the frequency of localized spins at copper sites in the absence of charge carriers was taken to be $\Omega_q^2 = 2J_1^2 \alpha |K_1|(2 - \gamma_q)(2\Delta + 2 + \gamma_q)$. As a result of the self-consistent calculations (see Appendix A), we obtained the spin–spin correlation function for the nearest neighbors $K_1 = 4\langle S_0^z S_1^z \rangle = -0.4$, the decoupling parameter $\alpha = 1.5$, and the spin gap parameter $\Delta = 5 \times 10^{-4}$. For numerical estimates, we used the parameter $J_1 = 140$ meV (i.e., the same parameter as for the parent compound La_2CuO_4) and the dependence of the superconducting gap on the wave vector was specified according to the experimental data (as in [19]):

$$\Delta_k = \Delta_1[\cos(k_x a) - \cos(k_y a)]$$
$$+ \Delta_4[\cos(3k_x a) - \cos(3k_y a)],$$

where $\Delta_1 = 3.9$ meV and $\Delta_4 = -2.0$ meV. The decoupling parameters F_t, F_J, and F_V were taken equal to 0.65, 1.00, and 1.00, respectively. These parameters were consistent with the positivity condition for the imaginary parts of the spin and charge susceptibilities.
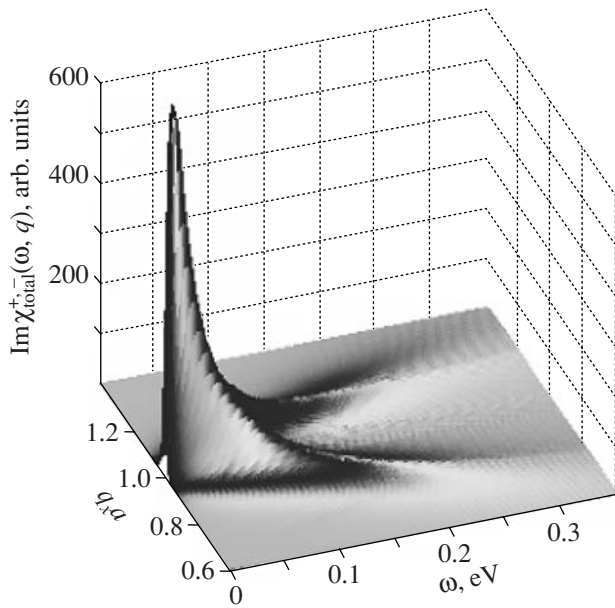
Fig. 2. Imaginary part of the susceptibility calculated from relationship (23) as a function of the frequency and the wave vector $q_x a$ (in terms of π) at $q_y = q_x$ for the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor.

The results of the numerical calculation of the imaginary part of the spin susceptibility for the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor with the use of the occupation parameter $P = 0.7$ at a temperature of $T = 10$ K are presented in Fig. 2. It can be seen from this
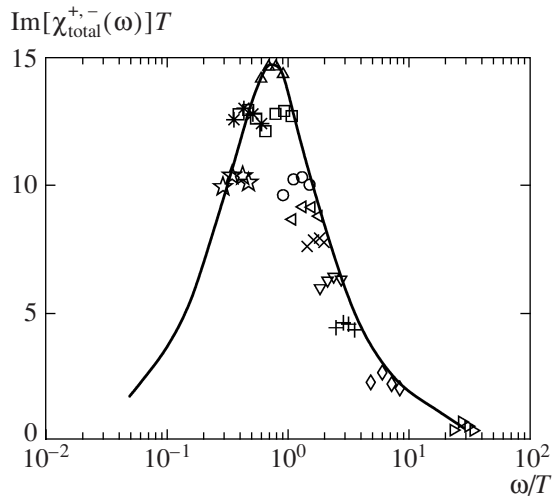

Fig. 3. Scaling behavior of the imaginary part of the spin susceptibility multiplied by the temperature as a function of the ratio between the frequency and the temperature. Shown are the positions of the maxima of the function $Im[\chi_{total}^{+,-}(\omega)]T$ at different temperatures in the superconducting ($T = (\triangleright)$ 2, $(\diamond)$ 10, $(+)$ 20 K) and normal ($T = (\triangledown)$ 30, $(\times)$ 40, $(\triangleleft)$ 50, $(\circ)$ 60, $(\square)$ 90, $(\triangle)$ 120, $(*)$ 300, $(\star)$ 600 K) phases.

figure that the imaginary part of the spin susceptibility at the wave vector $Q = (\pi, \pi)$ in the low-frequency range exhibits a pronounced peak, which is in agreement with the experimental data [14]. The diverging V-shaped relief resembles the corresponding relief associated with the magnon mode for the parent compound La_2CuO_4.

The scaling behavior of the imaginary part of the spin susceptibility multiplied by the temperature as a function of the ratio between the frequency and the temperature in the normal and superconducting phases according to the calculations at the same parameters is illustrated in Fig. 3. As in [7], it was assumed that the damping parameter is proportional to the temperature: $\Gamma = \beta T$, where $\beta = (1/3) \times 10^{-4}$ eV/K.

For comparison, the data taken from [15] are presented in Fig. 4. It can be seen from this figure that the results of our calculation reproduce the specific features of the frequency–temperature dependence of the neutron scattering for the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor.

4. ON THE ORIGIN OF TWO PEAKS IN NEUTRON SCATTERING FOR THE $La_{2-x}Sr_xCuO_4$ SUPERCONDUCTOR AND CONCLUDING REMARKS

As one more example of the application of the developed theory, let us analyze new data on neutron scattering for superconductors of the $La_{2-x}Sr_xCuO_4$ type. Recent experiments [20, 21] with the use of the $La_{1.84}Sr_{0.16}CuO_4$ and $La_{1.90}Sr_{0.10}CuO_4$ compounds demonstrated that the inelastic neutron scattering intensity is characterized not by one (as was previously believed) but by two peaks (Fig. 5a). One of them (the low-frequency peak) is most pronounced for the superconducting phase. For samples corresponding to optimum doping ($x = 0.16$), this peak is observed at an energy of
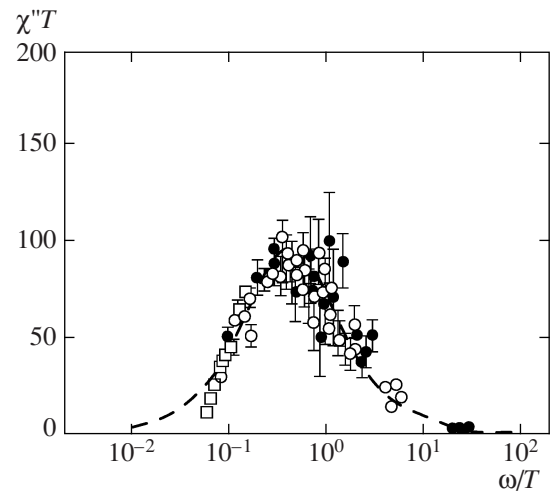

Fig. 4. Neutron scattering data taken from [15].

approximately 18 meV [20]. As was emphasized in [21], none of the existing theories of spin susceptibility can explain the simultaneous observation of these peaks. In this respect, it is of interest to reveal whether the observed phenomenon can be described using relationship (23).

The $La_{2-x}Sr_xCuO_4$ compound belongs to the group of *p*-type superconductors. The charge carriers are distributed over oxygen sites. The most simplified initial Hamiltonian for *p*-type high-temperature superconductors has the form [16]

$$H = \sum_{i, j, \sigma} t_{ij} \psi_i^{\sigma, pd} \psi_j^{pd, \sigma}$$

$$+ \sum_{i, j, \sigma} \frac{1}{4} J_{ij} (\psi_i^{\sigma, \bar{\sigma}} \psi_j^{\bar{\sigma}, \sigma} - \psi_i^{\sigma, \sigma} \psi_j^{\bar{\sigma}, \bar{\sigma}}) \qquad (28)$$

$$+ \sum_{i, j} \frac{1}{2} V_{ij} \psi_i^{pd, pd} \psi_j^{pd, pd}.$$

Here, $\psi_i^{pd, \sigma}$ ($\psi_j^{\sigma, pd}$) are the creation (annihilation) operators for composite quasiparticles in the conduction band. For example, the operator $\psi_i^{pd, \uparrow}$ can be approximately written in the form

$$\psi_i^{pd, \uparrow} \approx \frac{1}{\sqrt{2}} (X_i^{\uparrow, \downarrow} P_i^{\uparrow, 0} - X_i^{\uparrow, \uparrow} P_i^{\downarrow, 0}),$$

where $X_i^{p, q}$ and $P_i^{p, q}$ are the Hubbard operators corresponding to Cu^{2+} *d* holes and O^{1-} *p* holes, respectively. Formally, the energy operator (28) can be obtained from Hamiltonian (1) through the transformation

$$X^{0, \uparrow} \longrightarrow \psi^{pd, \downarrow}, \quad \psi^{pd, \uparrow} \longrightarrow -X^{0, \downarrow},$$

$$X_i^{0, 0} \longrightarrow \psi_i^{pd, pd}$$

and the change in the sign of the hopping integral; i.e., $t_{ij} \longrightarrow -t_{ji}$. It is easy to check that the functions $\chi_0(\omega, q)$ and $\xi(\omega, q)$ in expressions (16) are invariant with respect to this transformation. However, it should be emphasized that, upon the given transformation, the function $\pi(\omega, q)$ in expressions (16) changes sign. In particular, this function for the $La_{2-x}Sr_xCuO_4$ superconductors is represented in the form (for brevity, we write it only for the normal phase)

$$\pi(\omega, q) = \frac{1}{N} \sum_k \frac{P(t_k f_k - t_{k+q} f_{k+q})}{\omega - \varepsilon_k + \varepsilon_{k+q}},$$

where $f_k = \{1 + \exp[(\varepsilon_k - \mu)/k_B T]\}^{-1}$ is the electron Fermi function and the quantity P is determined by the value of the anticommutator

$$\{\psi_i^{pd, \uparrow}, \psi_j^{\uparrow, pd}\} = (\psi_i^{pd, pd} + \psi_i^{\uparrow, \uparrow})\delta_{ij} = (P + S_i^z)\delta_{ij}.$$

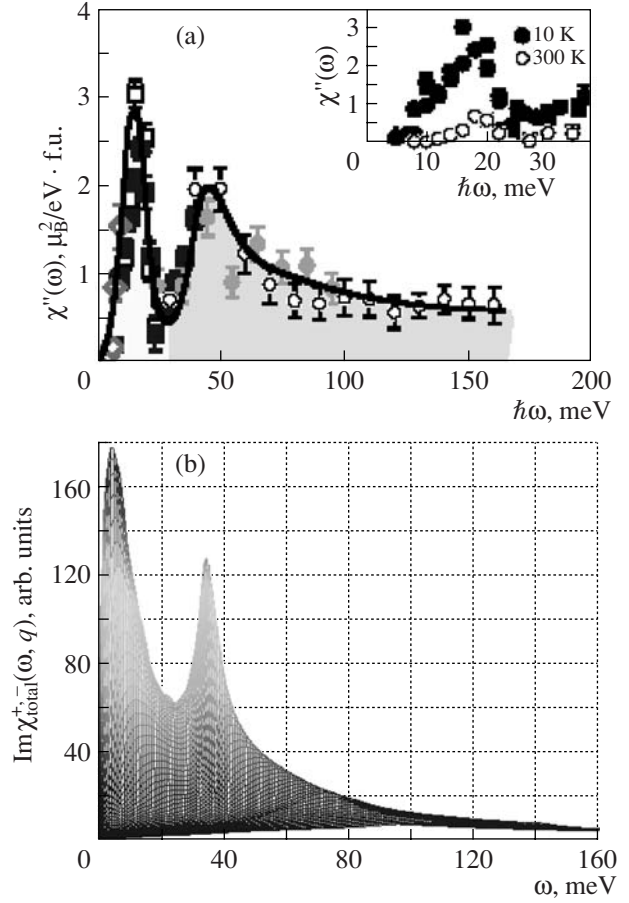With allowance made for these transformations, formula (23) can be used for analyzing magnetic suscepti-

Fig. 5. Imaginary parts of the susceptibility for the $La_{1.84}Sr_{0.16}CuO_4$ superconductor according to (a) the neutron scattering data taken from [20] and (b) the results of the numerical calculations from relationship (23).

bility of the $La_{2-x}Sr_xCuO_4$ superconductors. In order to avoid misunderstandings, it should be noted that the given transformation should be differentiated from the standard electron–hole transformation within states of one conduction band. Now, the case in point is the properties of symmetry between the formulas for the susceptibilities from different bands, namely, the Hubbard subbands of the lower and upper types.

The shape of the Fermi surface was specified according to the data obtained by Yoshida et al. [22]. The effective hopping integrals were as follows: $t_{eff}^{(1)} = 250$ meV, $t_{eff}^{(2)} = -37.5$ meV, and $t_{eff}^{(3)} = 18.75$ meV. The results of the numerical calculations of the imaginary part of the susceptibility for the superconducting phase are presented in Fig. 5. In the calculations, we used the following parameters: the superexchange interaction parameter $J_1 = 0.13$ eV, the damping parameter $\Gamma = 0.003$ eV, the gap parameter $\Delta_1 = 0.01$ eV in the expression $\Delta_k = \Delta_1[\cos(k_x a) - \cos(k_y a)]$, $K_1 = -0.424$, $K_2 = 0.178$, $K_3 = K_2$, $F_t = 0.01$, $F_J = 0.80$, the number of

charge carriers per unit cell $\delta = 0.25$, $P = 0.6250$, and the chemical potential $\mu = 202.5$ meV.

A comparison of Figs. 5a and 5b demonstrates that the results of our calculations reproduce the double-peak structure of the neutron scattering intensity for the $La_{2-x}Sr_xCuO_4$ superconductor. The low-frequency peak is located within the energy range corresponding to the superconducting gap. This peak will disappear if the functions $\eta(\omega, q)$ and $\eta_t(\omega, q)$ in the denominator of relationship (23) vanish. This corresponds to the absence of correlations in the motion of itinerant holes. It is interesting to note that, in this case, the function $\zeta(\omega, q)$ located before the frequencies of oscillations of localized spins blocks their manifestation. The coherence factors in the function $\zeta(\omega, q)$ are responsible for the shift in the contribution from the localized oscillations to the susceptibility toward the high-frequency range outside the energy gap. In other words, the susceptibility at low frequencies "freezes." Therefore, as in the framework of the random-phase approximation, the origin of the low-frequency peak can be interpreted as a manifestation of collective spin oscillations within the superconducting gap (spin excitons according to the terminology proposed in [23]). The dispersion of the high-frequency peak in the vicinity of the wave vector $Q = (\pi, \pi)$ resembles the magnon scattering in the two-dimensional system of localized spins with strong antiferromagnetic correlations. It should be noted that these oscillations are significantly renormalized as a result of coupling with itinerant spins. The relief of the high-frequency peak is similar to the V-shaped relief depicted in Fig. 1. However, in the case of the $La_{2-x}Sr_xCuO_4$ superconductor, the position of this peak is considerably shifted toward the high-frequency range. The factor responsible for this shift becomes clear taking into account that the effective radius of charge carriers (oxygen holes correlated with the copper spins in a singlet manner) is considerably larger than that for the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ superconductor, in which the charge carriers are distributed over copper sites. In the last case, the perturbation of antiferromagnetic correlations is weaker and the spin gap parameter Δ_1 is smaller than that for the $La_{2-x}Sr_xCuO_4$ superconductor.

Thus, the performed analysis demonstrates that the derived relationship permits us to describe the recently revealed features of the neutron scattering in the $Pr_{0.88}LaCe_{0.12}CuO_{4-x}$ and $La_{2-x}Sr_xCuO_4$ superconductors. It is hoped that the proposed formula for the susceptibility turns out to be useful for interpreting the data not only on neutron scattering but also on the magnetic resonance at different nuclei in high-temperature superconductors, as well as for evaluating the efficiency of the mechanism of pairing of quasiparticles through spin fluctuations.

APPENDIX A

SPIN–SPIN CORRELATION FUNCTIONS

The spin–spin correlation functions are calculated as follows:

$$\langle S_i^- S_j^+ \rangle = \frac{1}{N^2} \sum_q \langle S_{-q}^- S_q^+ \rangle \exp(i\mathbf{q} \cdot \mathbf{R}_{ij}), \qquad (A.1)$$

where $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$.

Then, we use the Green's function

$$
\begin{aligned}
\langle S_{-q}^- S_q^+ \rangle &= \int \frac{d\omega}{e^{\beta\omega} - 1} \\
&\times [\langle\langle S_q^+ | S_{-q}^- \rangle\rangle_{\omega + i\varepsilon} - \langle\langle S_q^+ | S_{-q}^- \rangle\rangle_{\omega - i\varepsilon}] \\
&= \frac{N}{2\pi i} \int \frac{d\omega}{e^{\beta\omega} - 1} [\chi^{+,-}(q, \omega + i\varepsilon) - \chi^{+,-}(q, \omega - i\varepsilon)] \\
&= \frac{N}{\pi} \int \frac{d\omega}{e^{\beta\omega} - 1} \mathrm{Im}\chi^{+,-}(q, \omega).
\end{aligned}
\tag{A.2}
$$

Since the following equality is satisfied,

$$\mathrm{Im}\chi^{+,-}(q, \omega) = -\mathrm{Im}\chi^{+,-}(q, -\omega), \qquad (A.3)$$

the integration can be carried out only over positive frequencies. With due regard for this circumstance, we find

$$
\begin{aligned}
\langle S_i^- S_j^+ \rangle &= \frac{1}{N\pi} \sum_q \frac{d\omega}{e^{\beta\omega} - 1} \mathrm{Im}\chi^{+,-}(q, \omega) \\
&\times \exp(i\mathbf{q} \cdot \mathbf{R}_{ij}) = \frac{1}{\pi}\left(\frac{a}{2\pi}\right)^2 \\
&\times \iiint \left[\frac{d\omega}{e^{\beta\omega} - 1} \mathrm{Im}\chi^{+,-}(q, \omega) \right. \\
&\left. - \frac{d\omega}{e^{-\beta\omega} - 1} \mathrm{Im}\chi^{+,-}(q, -\omega) \right] \exp(i\mathbf{q} \cdot \mathbf{R}_{ij}) dq_x dq_y \\
&= \frac{1}{\pi}\left(\frac{a}{2\pi}\right)^2 \iiint \coth\left(\frac{\beta\omega}{2}\right) \mathrm{Im}\chi^{+,-}(q, \omega) \\
&\times \exp(i\mathbf{q} \cdot \mathbf{R}_{ij}) d\omega dq_x dq_y.
\end{aligned}
\tag{A.4}
$$

In the general case, the dependence of the correlation functions (like the exchange integral in the Ruderman–

Kittel–Kasuya–Yoshida interaction) on the distance exhibits an oscillatory behavior.

It should be noted that, when the indices of sites coincide with each other ($i = j$), the left-hand side of relationship (A.4) should be represented in the form

$$\langle S_i^- S_i^+ \rangle = \frac{1}{2}(1-\delta),$$

rather than 1/2 as in [17]. In order to calculate the integral over frequencies, according to [17] we can change over to summation over the Matsubara frequencies $\omega_n = 2n\pi/\beta$, where $n = 0, \pm 1, \pm 2, \ldots$ are integer numbers. For this purpose, we use the expansion

$$\frac{1}{e^{\beta\omega} - 1} - \frac{1}{e^{-\beta\omega} - 1}$$

$$= \frac{1}{\beta}\left[\sum_i \frac{1}{2\pi n_i/\beta - \omega} - \sum_i \frac{1}{2\pi n_i/\beta + \omega}\right]. \quad \text{(A.5)}$$

Then, we carry out the term-by-term integration with the use of the Kramers–Kronig relations. In this case, the integral of the imaginary part of the susceptibility over frequencies is expressed through the real part and the formula takes the form

$$\langle S_i^- S_j^+ \rangle = k_B T \left(\frac{a}{2\pi}\right)^2$$

$$\times \iint \sum_n \operatorname{Re}\chi^{+,-}(q, i\omega_n)\exp(i\mathbf{q}\cdot\mathbf{R}_{ij}). \quad \text{(A.6)}$$

The term on the right-hand side with $\omega_n = 0$ corresponds to the high-temperature approximation [24]. Since the characteristic frequencies in our case can be approximately 40 meV, i.e., they can be higher than $k_B T_c$, the next terms of the sum should also be taken into account.

APPENDIX B

DERIVATION OF THE FORMULA AT $T < T_c$

Generally speaking, since the mechanism of pairing remains unknown, the formulation of this problem can appear to be premature. However, it is possible to analyze a heuristic variant based on the assumption that the creation and annihilation operators for quasiparticles in high-temperature superconductors are Bogoliubov operators. By writing the energy operator through the Bogoliubov operators as the initial operator, it only remains to account for the correction terms proportional to he magnetization. It should be noted that, within the single-band model, the changeover to Bogoliubov operators of the composite type does not violate the commutation relations.

Therefore, we seek the equation of motion for the operator $X_{k+q}^{0,\downarrow} X_k^{\uparrow,0}$ expressed through the Bogoliubov operators; that is,

$$X_{k+q}^{0,\downarrow} X_k^{\uparrow,0} = u_{k+q} u_k \alpha_{k+q}^{0,\downarrow} \alpha_k^{\uparrow,0} - u_{k+q} v_k \alpha_{k+q}^{0,\downarrow} \alpha_{-k}^{0,\downarrow}$$
$$+ v_{k+q} u_k \alpha_{-(k+q)}^{\uparrow,0} \alpha_k^{\uparrow,0} - v_{k+q} v_k \alpha_{-(k+q)}^{\uparrow,0} \alpha_{-k}^{0,\downarrow}, \quad \text{(B.1)}$$

where

$$x_k = u_k^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_k - \mu}{E_k}\right),$$

$$y_k = v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{E_k}\right), \quad z_k = u_k v_k = \frac{\Delta_k}{2E_k},$$

$$E_k = \sqrt{(\varepsilon_k - \mu)^2 + |\Delta_k|^2}, \quad \alpha_k^{0,\uparrow} = u_k X_k^{0,\uparrow} - v_k X_{-k}^{\downarrow,0},$$

$$\alpha_k^{\downarrow,0} = u_k X_k^{\downarrow,0} + v_k X_{-k}^{0,\uparrow}.$$

For the Green's functions constructed from the Bogoliubov operators, we have

$$(\omega - E_k + E_{k+q})\langle\langle \alpha_{k+q}^{0,\downarrow} \alpha_k^{\uparrow,0}|S_{-q}^-\rangle\rangle$$

$$= \frac{i}{2\pi}(u_{k+q} u_k - v_{k+q} v_k)(n_k^h - n_{k+q}^h)$$

$$+ (u_{k+q} u_k - v_{k+q} v_k)\left\{\left[F_J\frac{J_q}{2} + (1 - F_t)t_k\right]n_k^h \quad \text{(B.2)}\right.$$

$$\left. - \left[F_J\frac{J_q}{2} + (1 - F_t)t_{k+q}\right]n_{k+q}^h\right\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle$$

$$- (u_{k+q} u_k - v_{k+q} v_k)\frac{1}{N}\sum_{k'}(t_{k'+q} - t_{k'})\langle\langle X_{k'+q}^{0,\downarrow} X_{k'}^{\uparrow,0}|S_{-q}^-\rangle\rangle,$$

$$(\omega + E_{-k} + E_{k+q})\langle\langle \alpha_{k+q}^{0,\downarrow} \alpha_{-k}^{0,\downarrow}|S_{-q}^-\rangle\rangle$$

$$= \frac{i}{2\pi}(u_{k+q} v_k - v_{k+q} u_k)(n_{-k}^h - n_{k+q}^h - P)$$

$$+ (u_{k+q} v_k - v_{k+q} u_k)\left\{\left[F_J\frac{J_q}{2} + (1 - F_t)t_{k+q}\right]n_{k+q}^h\right.$$

$$\left. - \left[F_J\frac{J_q}{2} + (1 - F_t)t_k\right](P - n_{-k}^h)\right\}\langle\langle S_q^+|S_{-q}^-\rangle\rangle \quad \text{(B.3)}$$

$$+ (u_{k+q} v_k - v_{k+q} u_k)\frac{1}{N}\sum_{k'}(t_{k'+q} - t_{k'})\langle\langle X_{k'+q}^{0,\downarrow} X_{k'}^{\uparrow,0}|S_{-q}^-\rangle\rangle,$$

$$(\omega - E_k - E_{-(k+q)})\langle\langle \alpha_{-(k+q)}^{\uparrow,0} \alpha_k^{\uparrow,0}|S_{-q}^-\rangle\rangle$$

$$= \frac{i}{2\pi}(u_{k+q}v_k - v_{k+q}u_k)(P - n_k^h - n_{-(k+q)}^h)$$

$$+ (u_{k+q}v_k - v_{k+q}u_k)\left\{\left[F_J\frac{J_q}{2} + (1 - F_t)t_{k+q}\right]\right.$$

(B.4)

$$\times (P - n_{-(k+q)}^h) - \left[F_J\frac{J_q}{2} + (1 - F_t)t_k\right]n_k^h\right\}$$

$$\times \langle\langle S_q^+|S_{-q}^-\rangle\rangle + (u_{k+q}v_k - v_{k+q}u_k)$$

$$\times \frac{1}{N}\sum_{k'}(t_{k'+q} - t_{k'})\langle\langle X_{k'+q}^{0,\downarrow}X_{k'}^{\uparrow,0}|S_{-q}^-\rangle\rangle,$$

$$(\omega + E_{-k} - E_{-(k+q)})\langle\langle \alpha_{-(k+q)}^{\uparrow,0}\alpha_{-k}^{0,\downarrow}|S_{-q}^-\rangle\rangle$$

$$= \frac{i}{2\pi}(u_{k+q}u_k + v_{k+q}v_k)(n_{-k}^h - n_{-(k+q)}^h)$$

$$+ (u_{k+q}u_k + v_{k+q}v_k)\left\{\left[F_J\frac{J_q}{2} + (1 - F_t)t_{k+q}\right]\right.$$

(B.5)

$$\times (P - n_{-(k+q)}^h) - \left[F_J\frac{J_q}{2} + (1 - F_t)t_k\right](P - n_{-k}^h)\right\}$$

$$\times \langle\langle S_q^+|S_{-q}^-\rangle\rangle + (u_{k+q}u_k + v_{k+q}v_k)$$

$$\times \frac{1}{N}\sum_{k'}(t_{k'+q} - t_{k'})\langle\langle X_{k'+q}^{0,\downarrow}X_{k'}^{\uparrow,0}|S_{-q}^-\rangle\rangle.$$

In relationships (B.2)–(B.5), the occupation numbers are calculated according to the rule

$$n_k^h = \langle X_k^{0,\uparrow}X_k^{\uparrow,0}\rangle = P\langle(u_k\alpha_k^{0,\uparrow} - v_k\alpha_{-k}^{\downarrow,0})$$

$$\times (u_k\alpha_k^{\uparrow,0} - v_k\alpha_{-k}^{0,\downarrow})\rangle = u_k^2 P(1 - f_k^h) + v_k^2 P f_k^h,$$

where $f_k^h = [1 + \exp(-E_k/k_B T)]^{-1}$.

By combining these four equations according to relationship (B.1), we obtain the generalization of expression (14) to the case of the superconducting phase; that is,

$$\langle\langle X_{k+q}^{0,\downarrow}X_k^{\uparrow,0}|S_{-q}^-\rangle\rangle = \frac{i}{2\pi}\chi_{0kq} + \left[F_J\frac{J_q}{2}\chi_{0kq}\right.$$

(B.6)

$$+ (1 - F_t)\pi_{kq}\left]\langle\langle S_q^+|S_{-q}^-\rangle\rangle + \zeta_{kq}D_{it}(\omega, q),$$

where

$$\chi_{0kq}(\omega, q) = S_{xx}\frac{P(f_k^h - f_{k+q}^h)}{\omega + E_k - E_{k+q}}$$

$$+ S_{yy}\frac{P(f_{k+q}^h - f_k^h)}{\omega - E_k + E_{k+q}} + S_{yx}^{(-)}\frac{P(1 - f_k^h - f_{k+q}^h)}{\omega - E_k - E_{k+q}} \quad (B.7)$$

$$+ S_{xy}^{(+)}\frac{P(f_k^h + f_{k+q}^h - 1)}{\omega + E_k + E_{k+q}},$$

$$\pi_{kq}(\omega, q) = S_{xx}\frac{P(t_k f_k^h - t_{k+q}f_{k+q}^h)}{\omega + E_k - E_{k+q}}$$

$$+ S_{yx}^{(-)}\frac{P(t_k(1 - f_k^h) - t_{k+q}f_{k+q}^h)}{\omega - E_k - E_{k+q}}$$

(B.8)

$$+ S_{xy}^{(+)}\frac{P(t_k f_k^h - t_{k+q}(1 - f_{k+q}^h))}{\omega + E_k + E_{k+q}}$$

$$+ S_{yy}\frac{P(t_k(1 - f_k^h) - t_{k+q}(1 - f_{k+q}^h))}{\omega - E_k + E_{k+q}},$$

$$\zeta_{kq}(\omega, q) = \frac{S_{xx}}{\omega + E_k - E_{k+q}} + \frac{S_{yx}^{(-)}}{\omega - E_k - E_{k+q}}$$

(B.9)

$$+ \frac{S_{xy}^{(+)}}{\omega + E_k + E_{k+q}} + \frac{S_{yy}}{\omega - E_k + E_{k+q}}.$$

Here, in order to write the above expressions in a more compact form, we introduced the coherence factors

$$S_{xx} = x_k x_{k+q} + z_k z_{k+q}, \quad S_{yy} = y_k y_{k+q} + z_k z_{k+q},$$

$$S_{xy}^{(+)} = x_k y_{k+q} - z_k z_{k+q}, \quad S_{yx}^{(-)} = y_k x_{k+q} - z_k z_{k+q}.$$

Formulas (17)–(22) for the superconducting phase somewhat transform, so that the quantity ε_k in them should be formally replaced by the quantity E_k and functions (16) should be replaced by functions (B.7)–(B.9). Moreover, relationship (B.1) should be taken into account in Eqs. (17)–(21). In this case, the formula for the spin susceptibility has a form identical to expression (23); however, the functions

$$\zeta(\omega, q) = \frac{1}{N}\sum_k \zeta_{kq}, \quad \chi_0(\omega, q) = \frac{1}{N}\sum_k \chi_{0kq},$$

$$\pi(\omega, q) = \frac{1}{N}\sum_k \pi_{kq},$$

$$\zeta_t(\omega, q) = \frac{1}{N}\sum_k(t_{k+q} - t_k)\zeta_{kq},$$

$$\chi_t(\omega, q) = \frac{1}{N}\sum_k(t_{k+q} - t_k)\chi_{0kq},$$

$$\pi_t(\omega, q) = \frac{1}{N}\sum_k(t_{k+q} - t_k)\pi_{kq},$$

$$n_t(\omega, q) = F_J J_1 \gamma_q \chi_t(\omega, q) + (1 - F_t)\pi_t(\omega, q)$$

in it are determined by relationships (B.7)–(B.9).

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