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DYNAMIC SPIN SUSCEPTIBILITY IN THE *t*-J MODEL NEAR TO THE LOCALIZED LIMIT

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1 INTRODUCTION

The unusual magnetic properties of high- T_c superconductors in the normal state [1] have attracted increasing attention. As revealed by neutron scattering [2] and nuclear magnetic resonance (NMR) [3] experiments, in the metallic state there exist pronounced antiferromagnetic (AFM) spin correlations reflected in an enhanced dynamic spin susceptibility at the AFM wave vector. It is widely believed that the essential characteristics of magnetic correlations in the CuO_2 plane may be described by effective one-band correlation models on the square lattice [4]; besides the Hubbard model, the t-J model is frequently used.

The hitherto existing theories of the dynamic spin susceptibility in the t-J model either in the paramagnetic or the ordered state make use of diagrammatic [5] and projection techniques [6], of slave-boson [7]-[9] and slave-fermion [10] methods, and of the extended Maleyev-Dyson representation [11]. In the slave-field approaches to the t-J model [7]-[11] the local constraints are treated in mean-field-type approximations which may restrict the validity of the theory. Therefore, it is tempting to investigate the spin susceptibility within a constraint-free theory. As a natural starting point, such a theory may be based on the representation of the t-J model in terms of Hubbard operators guaranteeing the exclusion of double occupancy, and on approximation schemes directly dealing with Hubbard operators.

Based on the Hubbard-operator representation of the t-J model, the aim of this paper is to calculate and to analyze the dynamic spin susceptibility $\chi^{+-}(\vec{q},\omega)$ in the paramagnetic phase within a Green's function decoupling procedure. The method can be understood as a generalization of the random phase approximation (RPA) to the case of Hubbard operators. The resulting expression for $\chi^{+-}(\vec{q},\omega)$ describes the kinematic enhancement (due to the transfer term in the t-J model) as well as the exchange enhancement (due to the exchange interaction). It generalizes some previous approaches treating the limits J = 0 (corresponding to the Hubbard model for $U \to \infty$ [12]-[14]) and t = 0, n = 1 (corresponding to the Heisenberg model [15]). In this paper we mostly restrict our analysis to small doping values $\delta = 1 - n$ near to the localized limit ($n \lesssim 1$)

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including this limit (n = 1). Within our decoupling scheme special care has to be taken of the calculation of the static susceptibility in the localized limit. To obtain reasonable results at n = 1, it turns out that an external magnetic field h in z-direction has to be included which is put equal to zero at the end of calculation. Then our decoupling coincides with that by Tyablikov [15] who has obtained a Curie-Weiß law for the uniform static susceptibility. Recently, Curie-type contributions to the static susceptibility were found by Izyumov et.al. [5] also for n < 1. Therefore, we will investigate the limits $h = 0, n \rightarrow 1$ and $n = 1, h \rightarrow 0$ in more detail.

The paper is organized as follows. In Sec. 2 analytical expressions for the transverse dynamic spin susceptibility in the paramagnetic phase with and without an external longitudinal magnetic field are derived by a decoupling procedure for two-time retarded Green's functions. Those expressions are evaluated and analyzed in the cases h = 0 (Sec. 3-5) and $h \neq 0$ (Sec. 6 and 7). In Sec. 3 the low-frequency susceptibility at large wave vectors is calculated at T = 0, and the hole contribution to the spin-fluctuation energy is derived. Sec. 4 is devoted to the calculation of the dynamic suceptibility at the AFM wave vector and at T = 0, where the resulting two-peak structure in the spin-fluctuation spectrum is investigated. The temperature dependence of the uniform static susceptibility is studied in Sec. 5. In the localized limit, considered in Sec. 6, the static spin susceptibility is calculated including an external magnetic field, where the problems with the limits $h = 0, n \rightarrow 1$ and $n = 1, h \rightarrow 0$ are pointed out. In Sec. 7 the static susceptibility for n < 1 and $h \rightarrow 0$ is examined, and the results of our approach are compared with those obtained by the diagrammatic technique [5]. The summary and conclusions of our investigation can be found in Sec. 8.

2 GREEN'S FUNCTIONS AND DECOUPLING PROCEDURE

Let us start with the t-J model in an external homogeneous magnetic field parallel to the z-axis,

$$H = \sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} + \frac{1}{2} \sum_{i,j} J_{ij} (\vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j) - h \sum_i S_i^z , \qquad (1)$$

where the summation is taken over the sites of the two dimensional square lattice with the transfer amplitude $t_{ij} = -t < 0$ and the exchange constant $J_{ij} = J > 0$ for nearest neighbours *i* and *j*. The spin and density operators are expressed by Hubbard operators as

$$S_i^{\sigma} = X_i^{\sigma\bar{\sigma}}, \quad S_i^z = \frac{1}{2} \sum_{\sigma} \sigma X_i^{\sigma\sigma}, \quad n_i = \sum_{\sigma} X_i^{\sigma\sigma}, \quad (2)$$

where $\bar{\sigma} = -\sigma$. As will be seen later on, within our approach the external magnetic field h is essential to obtain reasonable results in the localized limit n = 1. The transverse dynamic spin susceptibility $\chi^{+-}(\vec{q},\omega)$ describes the response to an additional space- and time-varying field $\vec{h}_1 \cos(\vec{q}\vec{R}_i - \omega t)$ which is perpendicular to the external field h. It is given by the two-time retarded Green's function

$$\chi^{+-}(\vec{q},\omega) = -\frac{1}{N} \langle \langle S_q^+ | S_{-q}^- \rangle \rangle_\omega \tag{3}$$

with

$$S_q^\sigma = \sum_i \exp(i \vec{q} \vec{R}_i) S_i^\sigma \; ,$$

where we use magnetic units $(g\mu_B = 1)$. Using the Fourier transform of Hubbard operators the transverse susceptibility can be written as

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$$\chi^{+-}(\vec{q},\omega) = -\frac{1}{N} \sum_{k} G_{kq}(\omega) , \qquad (4)$$

where the Green's function $G_{kq}(\omega)$ is defined by

$$G_{kq}(\omega) = \langle \langle X_k^{+0} X_{k+q}^{0-} | S_{-q}^{-} \rangle \rangle_{\omega}$$

= $\frac{1}{N} \sum_{i,j} e^{-i\vec{k}\vec{R}_i} e^{i(\vec{k}+\vec{q})\vec{R}_j} \langle \langle X_i^{+0} X_j^{0-} | S_{-q}^{-} \rangle \rangle_{\omega}.$ (5)

Now, we solve approximately the equation of motion for $G_{kq}(\omega)$. Decomposing the Hamiltonian (1) into $H = H_t + H_J + H_h$ we obtain the commutators (for the susceptibility (4) we have to set $\sigma = +$),

$$\begin{bmatrix} X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}}, H_{t} \end{bmatrix} = \sum_{m} t_{jm} \begin{bmatrix} X_{i}^{\sigma 0} X_{m}^{0\bar{\sigma}} (1 - X_{j}^{\sigma \sigma}) + X_{i}^{\sigma 0} X_{m}^{0\sigma} X_{j}^{\sigma \bar{\sigma}} \end{bmatrix} - \sum_{m} t_{im} \begin{bmatrix} (1 - X_{i}^{\bar{\sigma}\bar{\sigma}}) X_{m}^{\sigma 0} X_{j}^{0\bar{\sigma}} + X_{i}^{\sigma \bar{\sigma}} X_{m}^{0\bar{\sigma}} X_{j}^{0\bar{\sigma}} \end{bmatrix}, \quad (6)$$
$$\begin{bmatrix} X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}}, H_{J} \end{bmatrix} = \frac{1}{2} \sum_{m} J_{jm} \begin{bmatrix} X_{i}^{\sigma 0} X_{j}^{0\sigma} X_{m}^{\sigma \bar{\sigma}} - X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}} X_{m}^{\sigma \sigma} \end{bmatrix} - \frac{1}{2} \sum_{m} J_{im} \begin{bmatrix} X_{m}^{\sigma \bar{\sigma}} X_{i}^{\bar{\sigma}0} X_{j}^{0\bar{\sigma}} - X_{m}^{\bar{\sigma}\bar{\sigma}} X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}} \end{bmatrix}, \quad (7)$$
$$\begin{bmatrix} X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}}, H_{h} \end{bmatrix} = \sigma h X_{i}^{\sigma 0} X_{j}^{0\bar{\sigma}} . \quad (8)$$

According to (6) and (7), there occur new Green's functions in the equation of motion for G_{kq} . We decouple these Green's functions in the following manner

$$\begin{bmatrix} X_i^{\sigma 0} X_j^{0\bar{\sigma}}, H_t \end{bmatrix} \simeq \sum_m t_{jm} \left[(1 - \langle X_j^{\sigma \sigma} \rangle) X_i^{\sigma 0} X_m^{0\bar{\sigma}} + \langle X_i^{\sigma 0} X_m^{0\sigma} \rangle X_j^{\sigma \bar{\sigma}} \right] - \sum_m t_{im} \left[(1 - \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle) X_m^{\sigma 0} X_j^{0\bar{\sigma}} + \langle X_m^{\bar{\sigma}0} X_j^{0\bar{\sigma}} \rangle X_i^{\sigma \bar{\sigma}} \right]$$
(9)
$$\begin{bmatrix} X_i^{\sigma 0} X_j^{0\bar{\sigma}}, H_J \end{bmatrix} \simeq \frac{1}{2} \sum_m J_{jm} \left[\langle X_i^{\sigma 0} X_j^{0\sigma} \rangle X_m^{\sigma \bar{\sigma}} - \langle X_m^{\sigma \sigma} \rangle X_i^{\sigma 0} X_j^{0\bar{\sigma}} \right] - \frac{1}{2} \sum_m J_{im} \left[\langle X_i^{\bar{\sigma}0} X_j^{0\bar{\sigma}} \rangle X_m^{\sigma \bar{\sigma}} - \langle X_m^{\bar{\sigma}\bar{\sigma}} \rangle X_i^{\sigma 0} X_j^{0\bar{\sigma}} \right].$$
(10)

Within this procedure we never split a density operator $X_i^{\sigma\sigma} (= X_i^{\sigma 0} X_i^{0\sigma})$ or a spin operator $X_i^{\sigma\bar{\sigma}} (= X_i^{\sigma 0} X_i^{0\bar{\sigma}})$ into two separate parts. Note that for coinciding indices i = j, the r.h.s. of Eq. (6) reduces to a more simpler form (due to $X_i^{\sigma 0} X_i^{\sigma\sigma} = 0$) which does not require the subsequent approximation (9). Dealing with the case i = j in a special manner we have carried out all the following analysis, and we have found only small quantitative corrections to the main results presented below. So, in the further discussion we will neglect these complications, i.e. we use (9) also for i = j. Some additional justification for this approximation will be presented also at the end of Sec. 2. The inhomogeneous term in the r.h.s. of the equation of motion for $G_{kq}(\omega)$ is expressed by the momentum distribution function n_k^{σ} as

$$\left\langle \left[X_k^{+0} X_{k+q}^{0-}, S_{-q}^{-} \right] \right\rangle = n_k^+ - n_{k+q}^- , \quad n_k^\sigma = \left\langle X_k^{\sigma 0} X_k^{0\sigma} \right\rangle . \tag{11}$$

Then, the equation of motion for $G_{kq}(\omega)$ reads

$$(\omega + i0^{+} + E_{k}^{+} - E_{k+q}^{-})G_{kq}(\omega) = n_{k}^{+} - n_{k+q}^{-} - (\varepsilon_{k}n_{k}^{+} - \varepsilon_{k+q}n_{k+q}^{-}) \times \\ \times \chi^{+-}(\vec{q},\omega) - J_{q}(n_{k}^{+} - n_{k+q}^{-})\chi^{+-}(\vec{q},\omega)$$
(12)

with

$$E_{k}^{\sigma} = \left(1 - \langle X_{i}^{\bar{\sigma}\bar{\sigma}} \rangle\right) \varepsilon_{k} - 2J \langle X_{i}^{\bar{\sigma}\bar{\sigma}} \rangle - \frac{\sigma h}{2}$$
(13)

and

$$J_q = 2J\gamma_q, \qquad \varepsilon_k = -4t\gamma_k, \qquad \gamma_k = \frac{1}{2}\left(\cos k_x + \cos k_y\right) . \tag{14}$$

In the paramagnetic phase the average $\langle X_i^{\sigma\sigma} \rangle$ does not depend on the site index and is given by

$$\langle X_i^{\sigma\sigma} \rangle = \frac{n}{2} + \sigma \langle S^z \rangle , \qquad (15)$$

where n is the electron concentration, $n \leq 1$, and $\langle S^z \rangle$ is the homogeneous magnetization due to the presence of the external magnetic field h. Finally, we obtain the transverse susceptibility

$$\chi^{+-}(\vec{q},\omega) = \frac{\chi_0(\vec{q},\omega)}{1-\chi_1(\vec{q},\omega)+J_q\chi_0(\vec{q},\omega)}, \qquad (16)$$

$$\chi_0(\vec{q},\omega) = -\frac{1}{N} \sum_k \frac{n_k^+ - n_{k+q}^-}{\omega + i0^+ + E_k^+ - E_{k+q}^-}, \qquad (17)$$

$$\chi_1(\vec{q},\omega) = \frac{1}{N} \sum_k \frac{\varepsilon_k n_k^+ - \varepsilon_{k+q} n_{k+q}^-}{\omega + i0^+ + E_k^+ - E_{k+q}^-} \,. \tag{18}$$

That is one of the main results of the present work. It generalizes several known expressions such as that by Hubbard and Jain [12] and others [13]-[14] (J = 0) or by Tyablikov [15] (n = 1, t = 0). The enhancement factor,

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i.e. the denominator in (16), includes two contributions. The enhancement term $\chi_1(\vec{q}, \omega)$, proportional to the hopping amplitude t, arises from the kinetic energy in the Hamiltonian (1) and will be called kinematic enhancement hereafter. This enhancement occurs even for J = 0 due to the nontrivial commutation relations for Hubbard operators. The other contribution, proportional to J, can be understood as an enhancement which is caused by the exchange interaction. The character of the contributions χ_0 and χ_1 is quite different. Due to the numerator $n_k^+ - n_{k+q}^$ in Eq. (17), the term $\chi_0(\vec{q}, \omega)$ is determined for $q \to 0$ by energies in the neighbourhood of the Fermi level, as is known from the itinerant theory of magnetism. In contrast, all the states below the Fermi level may contribute to $\chi_1(\vec{q}, \omega)$. Therefore, this term dominates the behaviour near to the localized limit $n \stackrel{<}{\sim} 1$.

The momentum distribution function n_k^{σ} (Eq. (11)) is determined by the one-particle Green's function

$$\mathcal{G}_{k}^{\sigma}(\omega) = \langle \langle X_{k}^{0\sigma} | X_{k}^{\sigma0} \rangle \rangle_{\omega} = \frac{1}{N} \sum_{i,j} e^{-i\vec{k}(\vec{R}_{i} - \vec{R}_{j})} \langle \langle X_{i}^{0\sigma} | X_{j}^{\sigma0} \rangle \rangle_{\omega}, \qquad (19)$$

which we calculate in the Hubbard-I approximation, i.e. by an analogous decoupling procedure as for the spin susceptibility (9-10). This yields

$$\mathcal{G}_{k}^{\sigma}(\omega) = \frac{1 - \langle X_{i}^{\bar{\sigma}\bar{\sigma}} \rangle}{\omega - E_{k}^{\bar{\sigma}} + i0^{+}}$$
(20)

with the renormalized band dispersion E_k^{σ} (13-14). From (20) we get

$$n_k^{\sigma} = \left(1 - \langle X_i^{\bar{\sigma}\bar{\sigma}} \rangle\right) f(E_k^{\sigma} - \mu) , \qquad (21)$$

where $f(x) = (e^{\beta x} + 1)^{-1}$ is the Fermi function, and $\beta = 1/T$. The chemical potential μ and the magnetization $\langle S^z \rangle$ are determined self-consistently by the equations

$$n = \frac{1}{N} \sum_{k\sigma} n_k^{\sigma}, \qquad \langle S^z \rangle = \frac{1}{2N} \sum_{k\sigma} \sigma n_k^{\sigma}.$$
(22)

The Hubbard-I approximation takes into account the effects of strong electron correlations by a reduction of the characteristic bandwidth (Eq.

(13)) and of the spectral weight for each \vec{k} -state (Eq. (20)). For very small electron concentrations $n \ll 1$, the momentum distribution function n_k^{σ} and the dispersion E_k^{σ} go over to their free electron values.

In the following we will analyze formula (16) first without magnetic field (h = 0) (Sec. 3-5) and after that for $h \neq 0$ (Sec. 6 and 7). For h = 0 the spin dependences in Eqs. (17) and (18) disappear, and we get

$$\chi_0(\vec{q},\omega) = -\frac{1}{N} \sum_k \frac{n_k - n_{k+q}}{\omega + i0^+ + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}}, \qquad (23)$$

$$\chi_1(\vec{q},\omega) = \frac{1}{N} \sum_k \frac{\varepsilon_k n_k - \varepsilon_{k+q} n_{k+q}}{\omega + i0^+ + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}}, \qquad (24)$$

where

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$$\tilde{\varepsilon}_{k} = (1 - \frac{n}{2})\varepsilon_{k},$$

$$n_{k} = (1 - n/2)f(\tilde{\varepsilon}_{k} - \tilde{\mu}), \qquad \tilde{\mu} = \mu + nJ.$$
(25)

The dynamic spin susceptibility $\chi^{+-}(\vec{q},\omega)$ for h = 0 is then given by (16) with (23) and (24). Putting J = 0 in (16), only the kinematic enhancement $\chi_1(\vec{q},\omega)$ remains. This result was also obtained by Hubbard and Jain [12] (see also [13, 14]), starting from the Hubbard model (with h = 0) and taking the limit $U \to \infty$. Note that the t-J model may be derived from the Hubbard model in the strong correlation limit $U \gg t$, where $J = 4t^2/U$. These previous works [12]-[14] did not indicate an antiferromagnetic (AFM) instability near the half-filled limit $n \stackrel{<}{\sim} 1$. In our derivation based on the t-J model an additional contribution to the enhancement factor appears due to the exchange interaction. Below we present an analysis of the expression (16) and show that the t-J model has such an AFM instability near the half-filled limit $n \stackrel{<}{\sim} 1$.

The method of Hubbard and Jain does not deal with the two-particle Green's function, instead the linear response of the magnetization to a weak longitudinal, space- and time-varying field is examined. For completeness and for a better comparison, in Appendix A we calculate the longitudinal dynamic spin susceptibility $\chi^{zz}(\vec{q},\omega)$ of the *t-J* model for h = 0 within the Hubbard-Jain technique. We obtain $\chi^{zz}(\vec{q},\omega) = \frac{1}{2}\chi^{+-}(\vec{q},\omega)$ with $\chi^{+-}(\vec{q},\omega)$ given by (16,23,24) which is in complete coincidence with

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our previous calculation. Let us emphasize that in the Hubbard-Jain procedure the problem of coinciding indices i = j in our decoupling (9) does not occur. That gives further support for our approximation.

3 LOW-FREQUENCY SPIN DYNAMICS

Now, we consider the low-frequency dynamics for $\omega \ll t$ and for large momenta \vec{q} at zero temperature and without magnetic field (h = 0). We choose a particular direction $q_x = q_y = q$. For small doping, $\delta \ll 1$, the Fermi surface covers nearly the whole Brillouin zone (BZ) except for small spherical hole pockets located at the corners of the BZ at $\vec{Q} = (\pm \pi, \pm \pi)$. The characteristic radius $k_{\rm F}$ of the hole pockets can be estimated from (22) written as

$$\delta = \frac{1}{N} \sum_{k} \bar{n}_{k} , \qquad \bar{n}_{k} = \left(1 - \frac{n}{2}\right) \left(1 - f(\tilde{\varepsilon}_{k} - \tilde{\mu})\right) , \qquad (26)$$

where the hole distribution function \bar{n}_k is introduced, and we obtain

$$k_{\rm F} \simeq \sqrt{8\pi\delta}$$
 (27)

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The function $\chi_0(\vec{q},\omega)$, Eq. (23), can be easily rewritten in terms of \bar{n}_k . For further use we introduce the functions

$$F_1(\vec{q},\omega) = \sum_k \frac{1}{\omega + i0^+ + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}}$$
(28)

$$F_2(\vec{q},\omega) = \sum_k \frac{\varepsilon_k \bar{n}_k - \varepsilon_{k+q} \bar{n}_{k+q}}{\omega + i0^+ + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}} .$$
(29)

Then we may write

$$1 - \chi_1(\vec{q}, \omega) = \omega F_1(\vec{q}, \omega) + F_2(\vec{q}, \omega) .$$
 (30)

Now, we expand the functions χ_0 , F_1 and F_2 for small frequencies ω (up to first order in ω) and large enough momenta $q > 2k_{\rm F}$. We take into

account all contributions up to second order in the doping δ . The result is given in Appendix B, and it is valid for all frequencies which obey

$$|\omega| \ll \omega_m(q) , \qquad \omega_m(q) = 2\tilde{W}\sin^2\frac{q}{2} , \qquad (31)$$

where $\tilde{W} = (4-2n)t$ is the half width of the correlated conduction band. Note that $\omega_m(q)$ is of the order of t. Under all these conditions, i.e. $q > 2k_{\rm F}, \omega \ll \omega_m(q)$ and $\delta \ll 1$, we obtain the dynamic spin susceptibility

$$\chi^{+-}(q,\omega) \simeq \frac{\delta(1+\pi\delta)}{4t\delta + J_q\delta(1+\pi\delta) + i\frac{\omega}{\pi}\sin(q/2)\ln|\omega/(16t\sin(q/2))|} \ . \tag{32}$$

The logarithmic contribution results from the singularity in the density of states at the centre of the band. In the static limit, $\omega = 0$, the expression (32) simplifies to

$$\chi^{+-}(q,0) = \frac{1+\pi\delta}{4t + J_q(1+\pi\delta)} \equiv \chi(q)$$
(33)

which indicates an instability of the paramagnetic state against AFM ordering at $\vec{q} = \vec{Q}$. The static susceptibility (33) diverges at the critical . value J_c of the exchange interaction given by

$$J_c = \frac{2t}{1+\pi\delta} \simeq 2t(1-\pi\delta) . \tag{34}$$

Above J_c , one finds AFM order within our approximation. Of course, this value of J_c which is of the order of t is much too large to be realistic for the t-J model, since we also expect AFM order in the parameter region $J \ll t$. The reason that J_c is too large consists in our mean-field like decoupling in the equation of motion (9,10). On the other hand, it is an important improvement of the Hubbard and Jain approach that we find AFM near n = 1 at all. It allows us to study the dynamic spin susceptibility in the vicinity of the phase boundary, i.e. for values of J slightly below J_c (Eq. (34)). Irrespective of the actual value of J_c which is suggested to be strongly renormalized from its mean-field value (34) by better approximations we expect that the qualitative picture near to the phase boundary is correctly given by our procedure.

To compare with phenomenological approaches it is appropriate to fit the logarithmic dependence in Eq. (32) by a linear one. It turns out that a good fit may be obtained by

$$\chi^{+-}(q,\omega) = \chi(q) \frac{\Gamma_q}{\Gamma_q - i\omega} , \qquad \Gamma_q = 4\delta \frac{4t + J_q(1+\pi\delta)}{\pi \sin(q/2)} .$$
(35)

That is shown in Fig. 1, where the ω -dependence of $\text{Im}\chi^{+-}(q,\omega)$ from Eq. (32) is compared with the fit (35). Both curves have a maximum at around the spin-fluctuation energy Γ_q . On the other hand, similar expressions as (35) are already known to explain the NMR-data from a phenomenologically given spin-susceptibility [16]. The important point is a strong maximum of the q-dependence of $\text{Im}\chi^{+-}(q,\omega)$ around the AFM wave vector $\vec{Q} = (\pi, \pi)$. For illustration, in Fig. 2 we show the q-dependence of $\text{Im}\chi^{+-}$ and of Γ_q which arise from Eq. (35).

We can interpret our result (35) as the magnetic response of a collection of nearly localized spins which are coupled to the itinerant degrees of freedom with a characteristic energy $\varepsilon(\delta) = tk_{\rm F}^2/2 \simeq 4\pi t\delta$ (hole Fermi energy). There is also a contribution from the exchange interaction which . is mediated, however, only via these itinerant degrees of freedom. According to that, the spin fluctuation energy Γ_q contains two parts. The first one is governed by the energy scale $\varepsilon(\delta)$ and the second term, proportional to $J_q \varepsilon(\delta)/t$, strongly suppresses the value of Γ_q at $\vec{q} \simeq \vec{Q}$. Nevertheless, due to the static part $\chi(q)$, we obtain the strong maximum of $\text{Im}\chi^{+-}(q,\omega)$. The peak in Fig. 1 with a position proportional to δ collapses at the ordinate axis for $n \rightarrow 1$. That is a drawback of our theory because in that limit one expects the existence of low-frequency spin fluctuations due to paramagnons with a characteristic energy of the order of J. This contribution is not captured, however, in our procedure. The reason is clear since we decoupled in Eqs. (9,10) the spin operators of neighbouring sites, i.e. we neglected spin-correlations.

4 DYNAMIC SPIN SUSCEPTIBILITY AT THE ANTIFERROMAGNETIC WAVE VECTOR

Here we consider the particular case $\vec{q} = \vec{Q}$ and calculate $\chi^{+-}(\vec{Q},\omega)$ near half-filling at T = 0 not restricting ourselves to low frequencies ω . The function $\chi_0(\vec{Q},\omega)$ now takes the form

$$\chi_{0}(\vec{Q},\omega) = \frac{1-n/2}{N} \sum_{|\vec{k}| < k_{\rm F}} \left\{ \frac{1}{\omega - 2\tilde{\varepsilon}_{k}} - \frac{1}{\omega + 2\tilde{\varepsilon}_{k}} \right\} .$$
(36)

Integrating in (36) over $|\vec{k}| < k_{\rm F} = \sqrt{8\pi\delta}$ and noting that $\tilde{\varepsilon}_k \simeq -\tilde{W} + \frac{1}{4}\tilde{W}\vec{k}^2$ we obtain for the real and the imaginary parts of $\chi_0(\vec{Q},\omega)$ the following results, respectively,

$$\chi_0'(\vec{Q},\omega) = \frac{1-n/2}{2\pi\tilde{W}} \ln \left| \frac{\omega^2 - (2\tilde{W})^2}{\omega^2 - (2\tilde{W} - \frac{1}{2}\tilde{W}k_{\rm F}^2)^2} \right| , \qquad (37)$$

$$\chi_0''(\vec{Q},\omega) = \frac{1}{8t} \Theta\left(\omega - 2\tilde{W} + \frac{1}{2}\tilde{W}k_{\rm F}^2\right) \Theta(2\tilde{W} - \omega) ; \qquad \omega > 0 ,$$

where $\chi_0''(\vec{Q}, -\omega) = -\chi_0''(\vec{Q}, \omega)$ and $\Theta(x)$ is the Heaviside step function. Analogously, for $F_2(\vec{Q}, \omega)$ we obtain

$$F_{2}'(\vec{Q},\omega) = \frac{k_{\rm F}^{2}}{4\pi} + \frac{\omega}{4\pi\tilde{W}} \left\{ \ln \left| \frac{\omega - 2\tilde{W}}{\omega + 2\tilde{W}} \right| + \ln \left| \frac{\omega + 2\tilde{W} - \frac{1}{2}\tilde{W}k_{\rm F}^{2}}{\omega - 2\tilde{W} + \frac{1}{2}\tilde{W}k_{\rm F}^{2}} \right| \right\}$$
(38)

$$F_2''(\vec{Q},\omega) = \frac{\omega}{4\tilde{W}} \Theta\left(\omega - 2\tilde{W} + \frac{1}{2}\tilde{W}k_{\rm F}^2\right) \Theta(2\tilde{W} - \omega) \; ; \qquad \omega > 0 \; .$$

It can be easily checked that the Kramers-Kronig relation is fulfilled for each pair in (37) and (38).

Further, to calculate $\omega F_1(\vec{Q}, \omega)$ we notice that the real part is given by (B8) with $\sin(q/2) = 1$, and the density of states (DOS) is defined by

J,

$$\rho(\varepsilon) = \frac{1}{N} \sum_{k} \delta(\varepsilon - \tilde{\varepsilon}_{k}) .$$
(39)

The function which is integrated in (B8) with the DOS is a rather flat one. It tends to unity, if the van Hove singularity in the DOS is reached at $\varepsilon = 0$. So we may estimate (B8) with the square DOS, $\rho(\varepsilon) \to \bar{\rho}(\varepsilon) =$ $(2\tilde{W})^{-1}\Theta(\tilde{W} - |\varepsilon|)$, that leads to the result

$$\left[\omega F_1(\vec{Q},\omega)\right]' = \frac{\omega}{4\tilde{W}} \ln \left| \frac{\omega + 2\tilde{W}}{\omega - 2\tilde{W}} \right| .$$
(40)

The imaginary part resulting from (B10) is given by

$$\left[\omega F_1(\vec{Q},\omega)\right]'' = -\pi \frac{\omega}{2} \rho\left(\frac{\omega}{2}\right) . \tag{41}$$

Collecting the results (37)-(41) and using Eqs. (16) and (30) we obtain a rather complicated analytical expression for $\chi^{+-}(\vec{Q},\omega)$. The results of the numerical analysis are presented in Fig. 3 for J = 0 and J =1.2t. For comparison, we also show $\text{Im}\chi_0(\vec{Q},\omega)$. There occur two peaks in the ω -dependence of Im χ^{+-} . The first one, at low frequencies, is due to a relaxation process of nearly localized spins originating from the presence of holes as described in the previous section. The structure at higher frequencies of the order of 4t is mainly given by χ''_0 which describes a continuum of electron-hole pairs. Because $\chi_0'' = 0$ beyond the high frequency region, one may infer that the low-frequency part of $Im\chi^{+-}$ is mainly caused by χ_1'' , i.e. by the kinematic enhancement. Indeed, this peak is already present at J = 0. If we approach the magnetic phase boundary, the maximum of the low-energy peak will be greatly enhanced. For decreasing doping the high-energy peak vanishes, whereas the low-energy one collapses on the ordinate axis, as already discussed in the previous section.

A similar two-peak structure was also suggested phenomenologically by Takahashi and Zhang [17]. Also the recently published exact diagonalization studies of the dynamic spin susceptibility [18] show a similar distinction between structures, determined by the electron-hole continuum, and the relaxation behaviour for small energies.

5 TEMPERATURE DEPENDENCE OF THE SPIN SUSCEPTIBILITY

Here we calculate the temperature dependence of the uniform static spin susceptibility without an external magnetic field and for any filling $n \neq 1$. We determine the chemical potential from Eq. (22) approximating the density of states (39) by a square one. This approximation is especially justified for small doping values $\delta \ll 1$, since then the chemical potential is far from the van Hove singularity. But once we have chosen the square density of states, the following derivations are valid for any filling n. From (22) we get

$$e^{4t\beta n} = \frac{1 + e^{\beta(W + \tilde{\mu})}}{1 + e^{-\beta(\bar{W} - \tilde{\mu})}},$$
 (42)

which determines $\tilde{\mu}$. Then we calculate χ_0 and χ_1 from their formulas for h = 0 (23,24). In the static limit ($\omega = 0$) and for $\vec{q} \to 0$ we obtain

$$\chi_0(0,0) = (1-\frac{n}{2})\frac{1}{N}\sum_k \left(-\frac{\partial f(\tilde{\varepsilon}_k-\tilde{\mu})}{\partial \tilde{\varepsilon}_k}\right) , \qquad (43)$$

$$\chi_1(0,0) = \frac{n/2}{1-n/2} - \frac{1}{N} \sum_k \tilde{\varepsilon}_k \left(-\frac{\partial f(\tilde{\varepsilon}_k - \tilde{\mu})}{\partial \tilde{\varepsilon}_k} \right) .$$
(44)

For the square density of states we get

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$$\chi_0(0,0) = \frac{1}{8t} \left(f(-\tilde{W} - \tilde{\mu}) - f(\tilde{W} - \tilde{\mu}) \right) , \qquad (45)$$

$$\chi_1(0,0) = \frac{1}{2} \left(f(-\tilde{W} - \tilde{\mu}) + f(\tilde{W} - \tilde{\mu}) \right) . \tag{46}$$

By (42) we finally obtain the uniform static spin susceptibility

$$\chi^{+-}(0,0) = \frac{1}{4t \coth(2nt\beta) + 2J} . \tag{47}$$

At $T \to 0$, the susceptibility tends to a constant value. Hence, in our approach, there is no indication for a ferromagnetic instability for any n. This was derived up to now from the analysis for h = 0. We will see in Sec. 7 that the inclusion of a magnetic field will modify (47), but will

not lead to ferromagnetism. For large T the susceptibility (47) decreases like a Curie law only at rather high temperatures $T \gg 2nt$,

$$\chi^{+-}(0,0) = \frac{1}{2} \cdot \frac{n}{T+nJ} .$$
(48)

The result (48) with J = 0 ($U \to \infty$) agrees with that obtained by Hubbard and Jain [12]. They pointed out that the temperature range, $T \gg 2t$ (for *n* near to unity), for which (48) holds is in contrast with the general expectation. Near to the localized limit $n \to 1$ one expects that the Curie law has to be reached already at T > J.

To clarify this contradiction we note that the previous analysis without a magnetic field h becomes meaningless in the localized limit n = 1. In the next section we will see that one can calculate the susceptibility in the localized limit n = 1 within the present approach only if one includes a weak magnetic field, i.e. if one starts from the general expressions (16-18).

6 THE LOCALIZED LIMIT

Now, we consider the limit n = 1 at finite temperature in the presence of a longitudinal magnetic field h which will tend to zero in the end of the calculation. We have to start with the representation (16-18). Before we restrict the analysis to the case n = 1, let us rewrite the general formula. Note that, due to the presence of a static magnetic field, both the electron dispersion E_k^{σ} and the spectral weight of each \vec{k} -state depend on the spin σ (see Eq. (20)). For convenience, we change the notation by rewriting

$$n_{k}^{\sigma} = \left(1 - \frac{n}{2} + \sigma \langle S^{z} \rangle\right) - \bar{n}_{k}^{\sigma} , \qquad (49)$$

where \bar{n}_k^{σ} is the hole momentum distribution function. In this notation the susceptibility (16) can be expressed by

$$\chi^{+-}(\vec{q},\omega) = \frac{-2\langle S^z \rangle \bar{F}_1(\vec{q},\omega) + \bar{\chi}_0(\vec{q},\omega)}{[\omega + i0^+ - h - 2\langle S^z \rangle (J_q - 2J)] \bar{F}_1(\vec{q},\omega) + \bar{F}_2(\vec{q},\omega) + J_q \bar{\chi}_0(\vec{q},\omega)}$$
(50)

Here, $\bar{\chi}_0(\vec{q},\omega)$ is given by (17) with n_k^{σ} replaced by $-\bar{n}_k^{\sigma}$. The functions $\bar{F}_1(\vec{q},\omega)$ and $\bar{F}_2(\vec{q},\omega)$ are determined by Eqs. (28) and (29), respectively, with the substitutions $\tilde{\varepsilon}_k \to E_k^+$, $\tilde{\varepsilon}_{k+q} \to E_{k+q}^-$ and $\bar{n}_k \to \bar{n}_k^+$, $\bar{n}_{k+q} \to \bar{n}_{k+q}^-$.

In the limit n = 1, all \vec{k} -states in the BZ are occupied which gives $\bar{n}_k^{\sigma} = 0$. Therefore, $\bar{\chi}_0(\vec{q},\omega) = \bar{F}_2(\vec{q},\omega) = 0$, and only the terms $\propto \bar{F}_1(\vec{q},\omega)$ in Eq. (50) survive. Accordingly, the susceptibility takes the form

$$\chi^{+-}(\vec{q},\omega) = \frac{-2\langle S^z \rangle}{\omega + i0^+ - h - 2\langle S^z \rangle (J_q - 2J)}$$
(51)

and describes the response of localized spins to a weak transverse magnetic field in the presence of a finite longitudinal field h. The same formula was also obtained by Tyablikov [15] (for J < 0) starting directly from a Green's functions decoupling in the Heisenberg model. Thus, in the localized limit n = 1, the general formulas (16-18) reduce to the Tyablikov approach. Therefore, we may follow him to calculate the magnetization $\langle S^z \rangle$. Using the operator identity $S_i^z = \frac{1}{2} - S_i^- S_i^+$ (for spin s = 1/2), the average $\langle S^z \rangle$ can be calculated from

$$\langle S^z \rangle = \frac{1}{2} - \frac{1}{N} \sum_{q} \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \frac{\mathrm{Im}\chi^{+-}(\vec{q},\omega)}{\exp(\beta\omega) - 1} \,. \tag{52}$$

With (51), $\langle S^z \rangle$ can be transformed to give the self-consistency equation

$$\frac{1}{2\langle S^z \rangle} = \frac{1}{N} \sum_q \coth\left[\beta \frac{h + 2\langle S^z \rangle (J_q - 2J)}{2}\right] .$$
(53)

Following the lines indicated by Tyablikov, for $h \ll T$ we expand the r.h.s. of Eq. (53) in terms of the small parameters h/(2T) and $2\langle S^z \rangle J/T$ to obtain a solution for $\langle S^z \rangle$. This expansion is well convergent for T > J. Using the definition of the longitudinal susceptibility

$$\chi^{zz} = \partial \langle S^z \rangle / \partial h |_{h \to 0} , \qquad (54)$$

for T > J we obtain the Curie law

$$\chi^{zz} = \frac{1}{4(T+T_N)}, \qquad T_N = J,$$
(55)

where T_N is the Néel temperature. Substituting this result into (51) $(\langle S^z \rangle = \chi^{zz} h)$, the static transverse susceptibility is given by

$$\chi^{+-}(\vec{q},0) = \frac{1}{2} \cdot \frac{1}{T+J\gamma_q} , \qquad T > J .$$
 (56)

For the AFM wave vector \vec{Q} one has

$$\chi^{+-}(\vec{Q},0) = \frac{1}{2(T-T_N)} , \qquad (57)$$

which manifests an AFM instability at $T = T_N$. For $\vec{q} = 0$ we have $\chi^{+-}(0,0) = 2\chi^{zz}$. In contrast to the expansion (48) of the previous section, the Curie law (55) shows a decay like $(T + T_N)^{-1}$ already for T > J which is more preferable.

Let us emphasize that we do not obtain Eq. (56) for $\vec{q} = 0$, if we let n go to unity in Eq. (47). With other words, for $\vec{q} = 0$ the limits $h = 0, n \rightarrow 1$ and $n = 1, h \rightarrow 0$ do not give the same result within our method. In the present section we fixed n = 1 and let h tend to zero. That seems to be the correct approach. In Sec. 3 to 5 we have performed the calculations at finite doping for zero magnetic field. The question is, if we obtain another result also for n < 1 dealing with a weak magnetic field. That will be answered in the next section. Another question is, if the necessity of a longitudinal magnetic field h in our approach results only from the present approximations. We think that this is the case, since the magnetic field h only breaks the symmetry. For h = 0 we would obtain zero in the r.h.s. of the equation of motion (12) after decoupling it at n = 1. But we suggest that an improved decoupling scheme does not need a magnetic field to obtain a nontrivial result for n = 1.

7 CURIE-TYPE CONTRIBUTION FOR FINITE DOPING ?

In the last step of our analysis we consider the general expressions (16-18) at finite magnetic field h and for n < 1. We have seen in the previous section that within our approach for n = 1 we need a magnetic field to obtain reasonable results. The question is, if the magnetic field also changes the results of our first analysis (Sec. 3-5) for n < 1 which we carried out for h = 0. We will now show that this is not the case, except for the uniform static susceptibility.

The formula (50) clearly indicates two contributions to the susceptibility. Namely, the first term in the numerator of (50) proportional to $\langle S^z \rangle$ describes the response of a localized spin and was discussed in Sec. 6. The second term in the numerator is due to an itinerant component at n < 1. The contribution of a localized spin disappears, if one takes h = 0 in the very beginning. Then we come to the description on the basis of Eqs. (23) and (24) which was analyzed above. Now we examine, if the contribution of a localized spin survives in the itinerant regime, n < 1, for h tending to zero.

One easily sees that at $\omega \neq 0$ and $h \rightarrow 0$ the equations (23) and (24) are restored. So all the results obtained above for the dynamical susceptibility at h = 0 remain valid.

To analyze the static case, $\omega = 0$, at $h \rightarrow 0$ we note that

$$E_k^+ - E_{k+q}^- = \left(\tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}\right) - h\left[1 - \frac{\langle S^2 \rangle}{h}(\varepsilon_k + \varepsilon_{k+q} + 4J)\right] .$$
(58)

So, in the integrands of (17) and (18) at $\omega = 0$ and $h \to 0$ we have

$$\frac{n_k^+ - n_{k+q}^-}{E_k^+ - E_{k+q}^-} \to \frac{n_k - n_{k+q}}{\tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}}, \qquad (\vec{k} \notin \mathbf{L})$$
(59)

for all \vec{k} except for $\vec{k} \in L$ at which $\tilde{\varepsilon}_k = \tilde{\varepsilon}_{k+q}$. For $\vec{k} \in L$, we have

$$\frac{n_k^+ - n_{k+q}^-}{E_k^+ - E_{k+q}^-} \to \left(1 - \frac{n}{2}\right) \frac{\partial f(\tilde{\varepsilon}_k - \tilde{\mu})}{\partial \tilde{\varepsilon}_k} - \frac{2\langle S^z \rangle}{h} \Big|_{h \to 0} \frac{f(\tilde{\varepsilon}_k - \tilde{\mu})}{1 - \frac{2\langle S^z \rangle}{h} \Big|_{h \to 0} \left(\varepsilon_k + 2J\right)}$$
(60)

Then we divide the summation over the BZ into a summation over L and the remaining part. If $\vec{q} \neq 0$, L is a line in \vec{k} -space with N_L \vec{k} -points and, hence, the summation over L gives a correction of order N_L/N $\ll 1$ which vanishes in the thermodynamic limit. Therefore, for $\vec{q} \neq 0$, $\omega = 0$ and $h \rightarrow 0$ we restore the result (23)-(24) obtained at h = 0. The situation is another one for $\vec{q} = 0$. In this case, all the \vec{k} -points belong to L (L is equal to the BZ), and at $h \to 0$ we have

$$\chi_0(0,0,h\to 0) = \chi_0(0,0,h=0) + \frac{2\langle S^z \rangle}{h} \mid_{h\to 0} \cdot C(\delta,T) , \qquad (61)$$

where $\chi_0(0, 0, h = 0)$ is given by Eq. (43), and $C(\delta, T)$ is defined as

$$C(\delta,T) = \frac{1}{N} \sum_{k} \frac{f(\tilde{\varepsilon}_{k} - \tilde{\mu})}{1 - \frac{2\langle S^{\star} \rangle}{h}} \Big|_{h \to 0} (\varepsilon_{k} + 2J)$$
(62)

The function $C(\delta, T)$ also occurs in the enhancement factor, and we obtain

$$\chi^{+-}(0,0,h\to 0) = \frac{\chi_0(0,0,h=0) + \frac{2\langle S^* \rangle}{h}}{1-\chi_1(0,0,h=0) + 2J\chi_0(0,0,h=0) + C(\delta,T)},$$
(63)

where χ_0 and χ_1 at h = 0 are given by (43,44) (see also (45,46)). The previously derived result (47) at h = 0 can be obtained from (63) only by putting $C(\delta, T)$ equal to zero. However, the local contribution $C(\delta, T)$ changes the result considerably. The formula (63) resembles the spin susceptibility which was derived by Izyumov and Letfulov [5] by means of a diagrammatic technique for Hubbard operators. They predicted, for n < 1 at $h \to 0$ and $\omega = 0$, a local contribution for any \vec{q} . In contrast to them, we obtain such a contribution in the limit $h \to 0$ only for $\vec{q} = 0$.

To analyze formula (63) one has to determine $\langle S^z \rangle$ in a self-consistent way. Let us give here only a rough estimate for small doping $8t\beta\delta \ll 1$. Using the square density of states we obtain

$$\chi_0(0,0,h=0) \simeq \frac{\delta}{T}$$
, $1-\chi_1(0,0,h=0) \simeq \frac{4t\delta}{T}$. (64)

Since $C(\delta, T)$ remains finite, the contribution of a localized spin becomes dominant at $\delta \to 0$,

$$\chi^{+-}(0,0,h\to 0) \simeq \frac{2\langle S^z \rangle}{h} \mid_{h\to 0} .$$
(65)

This result is in agreement with the definition of the longitudinal spin susceptibility (54). A self-consistent calculation of $\langle S^z \rangle$ similar as in Sec.

6 gives then a uniform static susceptibility which goes continuously to the result (55) if n tends to unity. But this works only for $\vec{q} = 0$. For $\vec{q} \neq 0$ a discontinuity remains.

Finally we would like to stress that within our approach there appears a contribution of a localized spin for any \vec{q} if we consider a magnetic field such that h > t, J. In that case the second term in Eq. (58) proportional to h would dominate the energy difference $\tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}$ independently on the wave vector \vec{q} . But the condition h > t, J is an unrealistic limit, since hshould tend to zero in the end. In this respect it should be mentioned that the diagrammatic technique [5] is based on a perturbation expansion which treats H_t and H_J as perturbation and considers H_h as zero-order part. That might give an explanation for the difference between our result and that given in Ref. [5].

8 CONCLUSION

The main results of our Green's functions decoupling approach to the dynamic spin susceptibility in the t-J model are the following.

(i) Within a RPA-like decoupling in the Hubbard operator representation, we have derived analytical expressions for the dynamic spin susceptibility which reveal both a kinematic and an exchange enhancement and generalize some previous results obtained in the limits J = 0 [12]-[14] and t = 0, n = 1 [15].

(ii) The low-frequency susceptibility near to the localized limit $(n \lesssim 1)$ and at T = 0 can be calculated analytically in the case of large enough wave vectors in the (1,1)-direction. We have obtained an instability against AFM ordering at a critical exchange interaction and a relaxation of spins due to the presence of holes. Near to the phase boundary, the \vec{q} -dependence shows a strong exchange enhancement around the AFM wave vector. The absence of spin relaxation in the localized limit n = 1is ascribed to the neglect of spin-correlations within our approach.

(iii) The spin-fluctuation spectrum at the AFM wave vector, which we have calculated analytically for $n \stackrel{<}{\sim} 1$ and T = 0, exhibits two peaks, where, besides the low-frequency relaxation peak, there appears a struc-

ture at frequencies of the order of 4t due to the electron-hole continuum. Those structures are in qualitative agreement with phenomenological suggestions [17]. Note that the two-peak structure is not obtained by slaveboson methods [7]-[9].

(iv) The temperature dependence of the static susceptibility at n = 1and of the uniform static susceptibility at $n \leq 1$ have to be calculated, within our approach, by means of an external magnetic field which is put equal to zero in the end. In the localized limit, a Curie law behaviour with the Néel temperature $T_N = J$ is found. At $n \leq 1$ there appears a contribution to the uniform static susceptibility which describes the response of a localized spin. The local contribution resembles the result obtained within the diagrammatic technique by Izyumov et. al. [5] who have found, however, such a contribution for any \vec{q} .

Besides the physical insights, the analysis of our constraint-free RPAlike approach and the discussion of its drawbacks may give a basis for the development of improved constraint-free theories of the spin susceptibility in the t-J model. From our results we conclude that the main problem to be solved is the appropriate treatment of spin-correlations so that the qualitative features of the localized (Heisenberg) limit can be reproduced.

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FIG. 1: Imaginary part of the spin susceptibility $\text{Im}\chi^{+-}$ in dependence on frequency for t = 1, $\delta = .05$, J = 1.2 and at the antiferromagnetic wave vector \vec{Q} . Compared is the correct expression (thick line) with a fitted one (thin line).







FIG. 3: Frequency dependence of $\text{Im}\chi^{+-}(\vec{Q},\omega)$ at the antiferromagnetic wave vector \vec{Q} for t = 1, $\delta = .05$, J = 1.2 and J = 0 (thick lines). For comparison we show $\chi_0''(\vec{Q},\omega)$ (thin line).

APPENDIX A

In the Hubbard and Jain approach [12] a linear response to a weak longitudinal magnetic field is calculated. So we have to replace the H_h term in (1) by $H_h(t) = -h \sum_i S_i^z \cos(\vec{q}\vec{R}_i - \omega t)$. After decoupling in the Hubbard-I approximation the equation of motion for $X_i^{0\sigma}(t)$ reads

$$i\frac{\partial}{\partial t}X_{i}^{0\sigma}(t) = \langle 1 - X_{i}^{\bar{\sigma}\bar{\sigma}}(t)\rangle \sum_{l} t_{il}X_{l}^{0\sigma}(t) - \sum_{l} J_{il}\langle X_{l}^{\bar{\sigma}\bar{\sigma}}(t)\rangle X_{i}^{0\sigma}(t) - \frac{h\sigma}{2}X_{i}^{0\sigma}(t)\operatorname{Re} e^{i(\vec{q}\vec{R}_{i}-\omega t)}.$$
(A1)

Analogously to [12] we make the ansatz

$$\langle X_l^{\sigma\sigma}(t)\rangle = \frac{n}{2} + \sigma \langle S_l^z(t)\rangle = \frac{n}{2} + \sigma \operatorname{Re}\left[m(\vec{q},\omega)e^{i(\vec{q}\vec{R}_l - \omega t)}\right] , \qquad (A2)$$

where $m(\vec{q}, \omega)$ measures the linear response of $\langle X_l^{\sigma\sigma}(t) \rangle$ to the applied field. The magnetization can be also written as $(g\mu_{\beta} = 1)$

$$m(\vec{q},\omega) = \chi^{zz}(\vec{q},\omega)h , \qquad (A3)$$

where $\chi^{zz}(\vec{q},\omega)$ is the longitudinal spin susceptibility. After making a Fourier transformation and solving Eq. (A1) we obtain the result

$$X_{k}^{0\sigma}(t) = e^{-iE_{k}t} + \frac{\sigma}{2} \cdot \frac{m(\vec{q},\omega) (\varepsilon_{k+q} + J_{q}) - h/2}{\omega + E_{k+q} - E_{k} + i0^{+}} e^{-i(\omega + E_{k+q})t} X_{k+q}^{0\sigma} - \frac{\sigma}{2} \cdot \frac{m^{*}(\vec{q},\omega) (\varepsilon_{k-q} + J_{q}) - h/2}{\omega - E_{k-q} + E_{k} - i0^{+}} e^{i(\omega - E_{k-q})t} X_{k-q}^{0\sigma} , \qquad (A4)$$

with $E_k = \tilde{\varepsilon}_k - nJ$. Substituting this expression for $X_k^{0\sigma}(t)$ into

$$X_{l}^{\sigma\sigma}(t)\rangle = \frac{1}{N} \sum_{k,k'} \langle X_{k'}^{\sigma0}(t) X_{k}^{0\sigma}(t) \rangle e^{i(\vec{k'} - \vec{k})\vec{R}_{l}}$$
(A5)

and comparing with (A2) we determine $m(\vec{q}, \omega)$. Using Eqs. (A3) and (A2) one finally obtains

$$\chi^{zz}(\vec{q},\omega) = \frac{1}{2} \frac{-\frac{1}{N} \sum_{k} \frac{n_{k} - n_{k+q}}{\omega + \tilde{\epsilon}_{k} - \tilde{\epsilon}_{k+q} + i0^{+}}}{1 - \frac{1}{N} \sum_{k} \frac{\varepsilon_{k} n_{k} - \varepsilon_{k+q} n_{k+q}}{\omega + \tilde{\epsilon}_{k} - \tilde{\epsilon}_{k+q} + i0^{+}} - J_{q} \frac{1}{N} \sum_{k} \frac{n_{k} - n_{k+q}}{\omega + \tilde{\epsilon}_{k} - \tilde{\epsilon}_{k+q} + i0^{+}}}, \quad (A6)$$

where the identity $E_{k} - E_{k+q} = \tilde{\epsilon}_{k} - \tilde{\epsilon}_{k+q}$ is used.

APPENDIX B

Here we calculate the functions χ_0 , F_1 and F_2 defined by (23),(28) and (29) for small frequencies ω without magnetic field (h = 0) and for zero temperature (T = 0). We consider wave vectors with $|\vec{q}| > 2k_F$ and assume a small doping value δ such that only small hole pockets with a radius k_F given by (27) are occupied. In this limit the hole distribution function (26) is given by

$$\bar{n}_k = \left(1 - \frac{n}{2}\right)\Theta(\tilde{\mu} - \tilde{\varepsilon}_k) . \tag{B1}$$

The function $\chi_0(\vec{q},\omega)$ may be represented in the form

$$\chi_0(\vec{q},\omega) = \frac{1-n/2}{N} \sum_{|\vec{k}| < k_{\rm F}} \left\{ \frac{1}{\omega - \tilde{\varepsilon}_k + \tilde{\varepsilon}_{k+q} + i0^+} - \frac{1}{\omega + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k-q} + i0^+} \right\}$$
(B2)

For the particular direction $q_x = q_y = q$ and $k < k_F$ we expand

$$\tilde{\varepsilon}_k - \tilde{\varepsilon}_{k\pm q} \simeq -2\tilde{W} \left(1 - \frac{1}{4}k^2\right) \sin^2(q/2) \pm \tilde{W}(k_x + k_y)\sin q$$
, (B3)

where $\tilde{W} = (4 - 2n) t$ is the half width of the conduction band $\tilde{\varepsilon}_k$. Then, in the low-frequency limit $|\omega| \ll \omega_m(q) \equiv 2\tilde{W} \sin^2(q/2)$ it can be easily seen that $\chi_0''(q,\omega) = \text{Im}\chi_0(q,\omega) = 0$. In this limit we obtain

$$\frac{1}{\omega + \tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q}} \simeq \frac{1}{\omega - \omega_m(q)} \left\{ 1 - \frac{1}{4} \frac{\omega_m(q)}{\omega - \omega_m(q)} \vec{k}^2 + \right] \\ + \frac{\omega_m(q)}{\omega - \omega_m(q)} \operatorname{ctg}(\frac{q}{2})(k_x + k_y) \right\}.$$
(B4)

Integrating in (B2) over $|\vec{k}| < k_{\rm F}$ we get

$$\chi_0(q,\omega) \simeq \frac{\delta(1+\pi\delta)}{2t\sin^2(q/2)} \left\{ 1 + O\left[\left(\frac{\omega}{2t\sin(q/2)}\right)^2\right] \right\} .$$
(B5)

In the same manner as above, for $|\omega| < \omega_m(q)$ we obtain ${
m Im} F_2(q,\omega) = 0$ and

$$F_2(q,\omega) = 4t \frac{\delta}{2t \sin^2(q/2)} + O\left[\left(\frac{\omega}{2t \sin(q/2)}\right)^2\right] + O(\delta^3) .$$
 (B6)

To evaluate the function $\omega F_1(q,\omega)$ we have to integrate over the full BZ. We note that for $q_x = q_y = q$ one has $\tilde{\varepsilon}_k - \tilde{\varepsilon}_{k+q} = 2\tilde{\varepsilon}_{k'}\sin(q/2)$ with $k'_{\alpha} = k_{\alpha} - q/2 + \pi/2$, $(\alpha = x, y)$. This yields

$$\omega F_1(q,\omega) = \frac{1}{N} \sum_k \frac{\omega}{\omega + i0^+ + 2\tilde{\varepsilon}_k \sin(q/2)} . \tag{B7}$$

The real part which is a symmetric function of ω , is given by

$$\omega F_1(q,\omega)]' = P \int d\varepsilon \rho(\varepsilon) \frac{\omega/(2\sin(q/2))}{\omega/(2\sin(q/2)) + \varepsilon} , \qquad (B8)$$

and we estimate it as

$$[\omega F_1(q,\omega)]' \simeq O\left[\left(\frac{\omega}{2t\sin(q/2)}\right)^2\right]$$
(B9)

The imaginary part is given by

$$[\omega F_1(q,\omega)]'' = -\pi \frac{\omega}{2\sin(q/2)} \cdot \rho\left(\frac{\omega}{2\sin(q/2)}\right). \tag{B10}$$

For small frequencies ω we have to take the density of states $\rho(\varepsilon)$ near to the centre of the band. At this energy it has a logarithmic singularity which is well known from the two dimensional tight binding model with nearest neighbour hopping (see e.g. [19]). We have to take into account the renormalization of the bandwidth by a factor of two and obtain

$$\rho(\varepsilon) = \frac{1}{\pi^2 t} \ln \left| \frac{8t}{\varepsilon} \right| . \tag{B11}$$

Using this expression in (B10) we result in

$$[\omega F_1(q,\omega)]'' = \frac{\omega}{2\pi t \sin(q/2)} \ln \left| \frac{\omega}{16t \sin(q/2)} \right|$$
(B12)

Now we can put all together to obtain the dynamic spin susceptibility according to (16) and (30). The formula is given in the main text in Eq. (32).

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Received by Publishing Department on January 22, 1996. Юшанхай В.Ю., Хайн Р., Иле Д. Динамическая спиновая восприимчивость в *1–J* модели вблизи половинного заполнения

- Динамическая спиновая восприничивость в парамагнитной фазе вычислена на основе расцепления уравнений для функции Грипа в обобщенном приближении случайных фаз в рамках t-J модели. Полученное аналитическое выражение выявляет наличие как кинематического, так и обменного успления восприимчивости. Вблизи половинного заполнения (n < 1) найдена антифер-

ромагнитная нестабильность при критическом значении обменного интеграла. Дан анализ вида спин-флуктуационного спектра и его зависимости от концентрации электронов. При иоловинном заполнении, n = 1, температурная зависимость статической восприимчивости следует закону Кюри с температурой Нееля $T_N = J$. При n < 1 одпородная статическая восприимчивость содержит вклад, описывающий отклик локализованных снинов подобно тому, как представлено в работе Изюмова и др. Одпако локальный вклад найден только для $\vec{q} = 0$.

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Yushankhai V.Yu., Hayn R., Ihle D. Dynamic Spin Susceptibility in the t-J Model Near to the Localized Limit

Based on the representation of the t-J model in terms of Hubbard operators, the dynamic spin susceptibility in the paramagnetic phase is calculated by an RPA-like Green's functions decoupling. The analytical expression reveals both a kinematic and an exchange enhancement. Near to the localized limit (n < 1), an antiferromagnetic

instability at a critical exchange interaction is found. The spin-fluctuation spectrum consists of a low-frequency part at $\omega \ll t$, which, near to the phase boundary, is strongly exchange enhanced around the antiferromagnetic wave vector, and a high-frequency part at $\omega \cong 4t$. In our approach, both parts of the spectrum strongly depend on the electron concentration and disappear at n = 1. In the localized limit, the temperature dependence of the static susceptibility is investigated, where a Curie law behaviour with the Neel temperature $T_N = J$ is obtained. At n < 1 the uniform static susceptibility

contains a contribution which describes the response of a localized spin, similar to recent results by Izyumov et al. (J. Phys. Condens. Matter 2 (1990), 8905). However, in difference to them, the local contribution is found only at $\vec{q} = 0$.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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