The incoherent part of the spin-wave polarization operator in the \( t\)-\( J \) model

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Abstract

A calculation of the spin-wave polarization operator is very important for the analysis of the magnetic structure of high temperature superconductors. We analyze the significance of the incoherent part of the spin-wave polarization operator within the framework of the \( t\)-\( J \) model. This part is calculated analytically for small doping with logarithmic accuracy. We conclude that the incoherent part of the spin-wave polarization operator is negligible in comparison with the coherent part.

keywords: antiferromagnetic order, spin fluctuations.

I. INTRODUCTION

It is widely believed that the spin structure of the ground state of high-temperature copper oxide superconductors is of the type of the Anderson spin-liquid state \[1\]. On the other hand it is well known that at zero doping the materials under consideration are insulators with long-range antiferromagnetic (AF) order. The instability of long-range AF order under doping in the \( t\)-\( J \) model was probably first realized by Shraiman and Siggia \[2\]. It was later demonstrated in numerous works (see e.g. refs. \[3\]–\[7\]). The instability is due to the strong interaction of spin-waves with mobile holes. The spin-wave polarization operator is needed for the analysis of this instability and especially for the derivation of the spin-liquid ground state. The calculation of the so called coherent part of the polarization operator is straightforward. However there is also the incoherent part. The purpose of the present work is to calculate this part and to provide a rigorous proof of its smallness in comparison with the coherent part. It means that in the analysis of the magnetic properties one can neglect the incoherent contribution to the spin-wave polarization operator. This conclusion is in agreement with that of ref. \[8\] based on the numerical computation.

II. HAMILTONIAN

The \( t\)-\( J \) model is defined by the following Hamiltonian:

\[
H = H_t + H_J = -t \sum_{\langle nm \rangle, \sigma} (d_{n\sigma}^\dagger d_{m\sigma} + \text{H.c.}) + J \sum_{\langle nm \rangle} \mathbf{S}_n \cdot \mathbf{S}_m,
\]

where \( d_{n\sigma}^\dagger \) is the creation operator of a hole with spin \( \sigma \) (\( \sigma = \uparrow, \downarrow \)) at site \( n \) on a two-dimensional square lattice. The \( d_{n\sigma}^\dagger \) operators act in the Hilbert space with no double
electron occupancy. The spin operator is \( S_n = \frac{1}{2} d_{n\alpha}^\dagger \sigma_{\alpha\beta} d_{n\beta} \). \( <nm> \) are pairs of nearest-neighbor sites on the lattice. Below we set \( J \) as well as the lattice spacing equal to unity.

At half-filling (one hole per site) the \( t-J \) model is equivalent to the Heisenberg AF model \([3,10]\) which has long-range AF order in the ground state \([11,12]\). Let us denote the wave function of this ground state by \( |0> \). This is the undoped system. We consider the doped system based on the ground state of the undoped system. In spite of the destruction of the long-range AF order it is convenient to use \( |0> \) and corresponding quasiparticle excitations as a basis set for the doped system. The effective Hamiltonian for the \( t-J \) model was derived in terms of these quasiparticles in the papers \([3,13]\):

\[
H_{eff} = \sum_{k\sigma} \epsilon_k h_k^\dagger h_k + \sum_{q} \omega_q (\alpha_q h_q^\dagger + \beta_q h_q) + H_{hsw} + H_{HH}.
\]

It is expressed in terms of normal spin-waves on an AF background \( \alpha_q, \beta_q \) (see e.g. review \([10]\)) and composite hole operators \( h_k \). The summations over \( k \) and \( q \) are restricted inside the Brillouin zone of one sublattice where \( \gamma_q = \frac{1}{2} (\cos qx + \cos qy) \geq 0 \). The spin-wave dispersion relation is

\[
\omega_q = 2\sqrt{1 - \gamma_q^2}, \quad \omega_q \approx \sqrt{2|q|} \text{ for } q \ll 1.
\]

The properties of single holes are well established (for a review see ref. \([17]\)). The wave function of a single hole can be represented as \( \psi_k = h_k^\dagger |0> \). At large \( t \) the composite hole operator \( h_k^\dagger h_k \) has a complex structure. For example at \( t/J = 3 \) the weight of the bare hole in \( \psi_k \) is about 25%, the weight of configurations of the type “bare hole + 1 magnon” is \(~50\%\) and for configurations of the type “bare hole + 2 or more magnons” it is \(~25\%\). The dressed hole is a normal fermion. The hole energy \( \epsilon_k \) has minima at \( k = k_0 \), where \( k_0 = (\pm\pi/2, \pm\pi/2) \). For \( t \leq 5 \) the dispersion can be well approximated by the expression \([18]\)

\[
\epsilon_k \approx E_0 + 2 - \sqrt{0.66^2 + 4.56t^2 - 2.8t^2\gamma_k - \frac{1}{4}\beta_2 (\cos k_x - \cos k_y)^2}.
\]

The numerical values in this formula are some combinations of the Heisenberg model spin correlators. The constant \( E_0 \) defines a reference level for the energy. To find \( \epsilon_k \) with respect to the undoped system one has to set \( E_0 = 0 \). However for the present work it is convenient to set \( \epsilon_{k_0} = 0 \) and therefore \( E_0 = \sqrt{0.66^2 + 4.56t^2} \). The coefficient \( \beta_2 \) is small and therefore the dispersion is almost degenerate along the face of the magnetic Brillouin zone \( \gamma_k = 0 \). According to refs. \([19,20]\) \( \beta_2 \approx 0.1t \) for \( t \geq 0.33 \). To avoid misunderstanding we note that formula (4) is not valid for very large \( t \) where the hole band width is saturated at the value of the order of unity and does not increase with \( t \). However, physically we are interested in \( t \approx 3 \) (see e.g. refs. \([21,22]\)) where (4) works well. Near the band minima, \( k_0 \) the dispersion (4) can be presented in the usual quadratic form:

\[
\epsilon_k \approx \frac{1}{2}\beta_1 p_1^2 + \frac{1}{2}\beta_2 p_2^2, \quad \beta_2 \ll \beta_1,
\]

where \( p_1 (p_2) \) is the projection of \( k - k_0 \) on the direction orthogonal (parallel) to the face of the magnetic Brillouin zone (fig. 1). From eq. (4) for \( t \gg 0.33 \) we find \( \beta_1 \approx 0.65t \), hence the mass anisotropy is \( \beta_1/\beta_2 \approx 7 \). For small hole concentrations, i.e. \( \delta \ll 1 \), the holes are localized in momentum space in the vicinity of the minima of the band \( k_0 = (\pm\pi/2, \pm\pi/2) \) and the Fermi surface consists of ellipses. (We recall that \( \delta = 0 \) corresponds to an insulator with long-range AF order.) The Fermi energy and Fermi momentum of non-interacting holes are
\[ \epsilon_F \approx \frac{1}{2} \pi (\beta_1 \beta_2)^{1/2} \delta \quad \text{and} \quad p_F \approx \sqrt{p_{1F} p_{2F}} \approx (\pi \delta)^{1/2}. \] (6)

The Fermi momentum \( p_F \) is measured from the center of the corresponding ellipse.

The interaction of a composite hole with spin-waves is of the form (see e.g. refs. [19,24,13])

\[ H_{h,sw} = \sum_{k,q} g_{k,q}(h^\dagger_{k+q} h_{k}^\alpha \alpha_q + h^\dagger_{k+q} h_{k}^\beta \beta_q + H.c.), \] (7)

\[ g_{k,q} = 2 \sqrt{2} f(\gamma_k U_q + \gamma_{k+q} V_q) \rightarrow 2^{1/4} f \sqrt{\frac{1}{q}}(q_x \sin k_x + q_y \sin k_y) \text{ for } q \ll 1. \]

Here \( U_q = \sqrt{\frac{1}{\omega_q} + \frac{1}{2}} \) and \( V_q = -\text{sign}(\gamma_q) \sqrt{\frac{1}{\omega_q} - \frac{1}{2}} \) are the parameters of the Bogoliubov transformation diagonalizing the spin-wave Hamiltonian. The hole spin-wave coupling constant \( f \) is a function of \( t \) evaluated in the work [13]. For large \( t \) the coupling constant is \( t \)-independent, \( f \approx 2 \). Let us stress that even for \( t > J \) the quasihole-spin-wave interaction \([7]\) has the same form as for \( t \ll J \) (i.e. as for bare hole operators) with an added renormalization factor (of the order \( J/t \) for \( t \gg J \)). This remarkable property of the \( t-J \) model is due to the absence of a single loop correction to the hole-spin-wave vertex. It was first stated implicitly by Kane, Lee and Read [25]. In refs. [19,24,13] it was explicitly demonstrated that the vertex corrections with different kinematic structure are of the order of a few percent at \( t/J \approx 3 \). There is also some \( q \)-dependence of the coupling constant \( f \). For example \( f(q = \pi) \approx 1.15 f(q = 0) \) at \( t/J = 3 \) (see refs. [13,20]). However this dependence is weak and is beyond the accuracy of the calculation of the renormalized value of \( f \). Therefore we neglect this dependence.

Finally there is the contact hole-hole interaction \( H_{hh} \) in the effective Hamiltonian \([2]\). \( H_{hh} \) is discussed in detail in refs. [14,13,26]. It is proportional to some function \( A(t) \). For small \( t \) this function approaches the value \(-0.25\), which gives the well known hole-hole attraction induced by the reduction of the number of missing antiferromagnetic links. However for realistic superconductors \( t \approx 3 \) (see e.g. refs. [21,23]). Surprisingly the function \( A(t) \) vanishes exactly at \( t \approx 3 \) and this means that the mechanism of contact hole-hole attraction is switched off. In contrast the spin-wave exchange mechanism \( H_{h,sw} \) is negligible for small \( t \) for which \( f \sim t \) and it is most important for large \( t \) for which \( f \) approaches 2. We are interested in “physical” values of \( t \): \( t \approx 3 \). Therefore in the present work we neglect the contact interaction (\( H_{hh} = 0 \)) and consider only the hole-spin-wave interaction at \( t = 3 \). The corresponding value of \( f \) according to \([13]\) is \( f = 1.8 \). Thus all numerical values in the present work are calculated at \( t = 3 \), \( \beta_1/\beta_2 = 7 \) and \( f = 1.8 \).

### III. POLARIZATION OPERATOR

There are two types of spin-waves in the \( t-J \) model, \( \alpha \) and \( \beta \). Therefore, one generally has to introduce a set of spin-wave Green’s functions [27,23]: \( D_{\alpha\alpha}, D_{\alpha\beta}, D_{\beta\alpha}, \) and \( D_{\beta\beta} \). However if we restrict ourselves to the long wavelength limit, the consideration can be simplified. It is well known that in the long wavelength limit the Heisenberg model is equivalent to the nonlinear \( \sigma \)-model (see e.g. review paper [16]). Therefore the usual field theory crossing symmetry is valid. The same is valid for the \( t-J \) model. This is evident from eq. \([7]\): at \( q \ll 1 \) the vertex \( g_{k,q} \approx g_{k-q,q} \). This means that instead of considering a set of Green’s functions one can introduce a single combined Green’s function of vector excitation:

\[ D(\omega, q) = \frac{2 \omega_q}{\omega^2 - \omega_q^2 - 2 \omega_q \Pi(\omega, q)}, \] (8)
where $\Pi(\omega, \mathbf{q})$ (or $P(\omega, \mathbf{q})$) is the mobile holes polarization operator. For the system to be stable the condition

$$\omega_q + 2\Pi(0, \mathbf{q}) > 0$$

(9)

should be fulfilled. Otherwise the Green’s function (8) would possess poles with imaginary $\omega$.

In the single loop approximation for dressed quasiholes the polarization operator is given by the diagram in fig. 2. The quasihole Green’s function in this diagram is determined by the effective Hamiltonian [2]. Let us call this contribution to the polarization operator the “coherent part”. The meaning of this term is elucidated below. In this paper we neglect the interaction between quasiholes and consider them as a normal Fermi-liquid. In this approximation the calculation of a single loop polarization operator is very simple. In the static long wavelength limit the result is [7]

$$\Pi_{coh}(0, \mathbf{q}) \approx -\sqrt{2}f^2/\pi \sqrt{\beta_1 \beta_2} q$$

(10)

for $q \ll p_F$.

This is independent of the hole concentration! Using this result one can easily prove that the stability condition (9) is violated because

$$-2\Pi(0, \mathbf{q})/\omega_q = 2f^2/(\pi \sqrt{\beta_1 \beta_2}) \approx 2.8$$

This is a well known fact concerning the instability of long-range AF order under doping (see e.g. refs. [2–7]).

Let us now explain the obtained result in terms of bare $d_{nr}$ which enter into the bare Hamiltonian (1). The Green’s function of a bare hole is of the form

$$G(\epsilon, \mathbf{k}) = \frac{Z}{\epsilon - \epsilon_k + i0} + G_{inh},$$

(11)

where $Z$ is the quasiparticle residue. If we use the bare hole Green’s function we also have to use the bare hole-spin-wave coupling constant $f_{bare} = 2t$ in the vertex $g_{k,\mathbf{q}}$ (7). Substitution of the pole (coherent) part of (11) into the single loop polarization operator gives the combination $f_{bare} Z$, but this is exactly the effective coupling constant $f$ [13]. Thus in the single loop approximation the effective theory with Hamiltonian (2) only takes into account the coherent (pole) part of the bare hole Green’s function (11). Because of this the contribution (10) is called the coherent part.

The incoherent part of the polarization operator which comes from $G_{inh}$ in (11) is proportional to the hole concentration $\delta$. Therefore it is negligible for $\delta \ll 1$. This conclusion agrees with that of Becker and Muschelknautz [8].

Now we will calculate $P_{inh}$ explicitly. We give two different calculations of $P_{inh}$. The first calculation is based on the self-energy approach. It is well known that the self-energy as well as the polarization operator is in essence an energy shift of the system. Let us consider the diagram in fig. 3a which represents the energy shift of a hole (solid line) in an external spin-wave (wavy line). If we join up the wavy lines and integrate over the momenta of the spin-wave we get the usual hole self energy (fig. 3b) which is already taken into account in the correct (renormalized) hole dispersion (4) and the renormalized value of the spin-wave coupling constant $f$. If we join up the solid lines and integrate over the momenta of the hole we get the coherent polarization operator (fig. 3c) which has also already been taken into account. Let us consider now the first correction to the diagram fig. 3a. It is given by the diagrams in fig. 4. (We remind the reader that there is no one loop correction to the spin-wave vertex.) This is the correction to the hole energy in an external spin-wave or the correction to the energy of the spin-wave in the presence of a single hole. The calculation
of this correction is very simple if one uses Schrödinger perturbation theory. Consider for example the case when the external spin-wave is of the \( \beta \)-type, i.e. for this wave the \( z \)-projection of spin is \( S_z = +1 \). The arrows in fig. 4 indicate the projections of hole spin (note that there is a spin flip at each vertex). It is evident that for spin up diagram 4b vanishes and similarly for spin down diagram 4a vanishes. We will see that the integral over \( Q \) is logarithmically divergent. Therefore we set \( q \ll Q \ll 1 \). Near the band minimum the hole energy is quadratic in momenta \( (\delta) \). Therefore it can be neglected in comparison with the energy of the intermediate spin-wave \( \omega_Q \) which is linear in momentum. This means that the energies of all three intermediate states in fig. 4a as well as in fig. 4b are approximately equal to \( \omega_Q \). Therefore the energy correction corresponding to fig. 4 is independent of the hole spin projection and equals

\[
\delta \epsilon = -g^2_{k,q} \sum_Q \frac{g^2_Q}{\omega_Q^2} = -\frac{f^4}{\sqrt{2q}} (q_x \sin k_x + q_y \sin k_y)^2 \int \frac{(Q_x \sin k_x + Q_y \sin k_y)^2}{Q^4} \frac{d^2Q}{(2\pi)^2}. \tag{12}
\]

The integral over \( Q \) is restricted by the limits \( Q_{\text{min}} \sim p_F = \sqrt{\pi \delta} \) and \( Q_{\text{max}} \sim \pi \). The integral over \( Q \) is logarithmically divergent and therefore it gives a big logarithm: \( \ln(Q_{\text{max}}/Q_{\text{min}}) \approx 0.5 \ln(1/\delta) \). When the momentum of the hole is close to the band minimum, \( k \approx k_0 = (\pi/2, \pm \pi/2) \), one gets

\[
\delta \epsilon = -\frac{f^4}{4\sqrt{2\pi}} \frac{(q_x \pm q_y)^2}{q} \ln \delta. \tag{13}
\]

To find the incoherent spin-wave polarization operator we now need to sum \( (13) \) over all occupied hole states (i.e. sum over \( k \)). Thus for \( \omega \ll \epsilon_F \) and \( q \ll p_F \) the result is

\[
P_{\text{incoh}}(\omega, q) \approx -\frac{f^4}{4\sqrt{2\pi}} \cdot \delta \cdot \ln \frac{1}{\delta} \cdot q. \tag{14}
\]

There are also higher order diagrams which contribute to \( P_{\text{incoh}} \). An example is presented in fig. 5. However all of these diagrams do not contain the big logarithm (\( \ln(1/\delta) \)) and therefore can be neglected according to the accepted accuracy.

To elucidate the meaning of \( P_{\text{incoh}} \) we will now give a different derivation of \( (14) \). The first correction to the single loop polarization operator arises from the diagram presented in fig. 6. After integration over the energies in the closed loops one gets the following expression for the contribution of this diagram:

\[
P_0(\omega, q) = \int \frac{d^2k}{(2\pi)^2} \frac{d^2Q}{(2\pi)^2} g^2_{k,Q} \sum_Q \frac{g^2_Q}{\omega_Q^2} \times
\]

\[
\left( \frac{n_{k-q}(1-n_{k-Q}) - n_k(1-n_{k-q})}{(\epsilon_{k-q} - \epsilon_k + \omega)(\epsilon_{k-q} - \epsilon_k - \omega_Q + \omega)} \right) + \frac{n_{k-q}n_{k-Q} - n_k n_{k-q}}{(1-n_k)\omega_Q} + \left( \epsilon_{k-Q} - \epsilon_k - \omega_Q \right)^2 \left( \epsilon_{k-Q} - \epsilon_{k-q} - \omega_Q - \omega \right),
\]

where \( n_k \) is the ground state occupation number. The first two terms in the expression \( (13) \) have second powers of \( (\epsilon_{k-q} - \epsilon_k + \omega) \) in the denominator. This factor is exactly the denominator of the one-loop polarization operator fig. 2. It means that the first two terms correspond to the renormalization of the pole (coherent) part of the hole Green’s function \( P_{\text{coh}} \). They are actually already taken into account in \( P_{\text{coh}} \) because for the calculation of \( P_{\text{coh}} \) we have used the dressed hole Green’s function which absorbs all of the corrections to
the pole part. Thus the new contribution, corresponding to \(P_{\text{incoh}}\), arises from the last two terms in (13). After carrying out some algebraic manipulation and using the fact that \(q\) is small (and so, for example \(\epsilon_{k-q} \approx \epsilon_k\)) \(P_{\text{incoh}}\) can be written as

\[
P_{\text{incoh}}(0, q) = -2 \int \frac{d^2k}{(2\pi)^2} \frac{d^2Q}{(2\pi)^2} g_{k,Q}^2 g_{k,q}^2 \frac{n_k(1 - n_{k-Q})}{(\omega_Q + \epsilon_{k-Q} - \epsilon_k)^3}.
\]  

(16)

It is evident that this expression is equivalent to (12). Neglecting \(\epsilon_{k-Q} - \epsilon_k\) in comparison with \(\omega_Q\) and carrying out the integration over \(Q\) with logarithmic accuracy we once more come to the result (14) for \(P_{\text{incoh}}\).

IV. CONCLUSION

In the present work we have analytically calculated the incoherent contribution to the spin-wave polarization operator. This analytical calculation is possible because of the logarithmic enhancement of the corresponding diagrams. The ratio of the incoherent contribution (14) to the coherent one (10) is

\[
\frac{P_{\text{incoh}}(0, q)}{P_{\text{coh}}(0, q)} = \frac{1}{8} f^2 \sqrt{\beta_1/\beta_2} \cdot \delta \cdot \ln \frac{1}{\delta}.
\]  

(17)

For the parameters of the \(t-J\) model corresponding to realistic high-\(T_c\) superconductors and for hole concentration \(\delta \leq 0.2\) this ratio does not exceed 10%. It means that in the analysis of the magnetic properties one can neglect the incoherent contribution to the spin-wave polarization operator.
REFERENCES

[1] P. W. Anderson, Science 235 (1987) 1196.
[2] B. Shraiman and E. Siggia, Phys. Rev. Lett. 62 (1989) 1564.
[3] T. Dombre, J. Physique 51 (1990) 847.
[4] A. Singh and Z. Tesanovic, Phys. Rev. B 41 (1990) 614.
[5] R. Eder, Phys. Rev. B 43 (1991) 10706.
[6] J. Igarashi and P. Fulde, Phys. Rev. B 45 (1992) 10419.
[7] O. P. Sushkov and V. V. Flambaum, Physica C 206 (1993) 269.
[8] K. W. Becker and U. Muschelknautz, Phys. Rev. B 48 (1993) 13826.
[9] J. E. Hirch, Phys. Rev. Lett. 54 (1985) 1317.
[10] C. Gross, R. Joynt and T. M. Rice, Phys. Rev. B 36 (1987) 381.
[11] J. Oitmaa and D. D. Betts, Can. J. Phys. 56 (1971) 897.
[12] D. A. Huse, Phys. Rev. B 37 (1988) 2380.
[13] O. P. Sushkov, Phys. Rev. B 49 (1994) 1250.
[14] A. L. Chernyshev, A. V. Dotsenko and O. P. Sushkov, Phys. Rev. B 49 (1994) 6197.
[15] M. Yu. Kuchiev and O. P. Sushkov, Physica C 218 (1993) 197.
[16] E. Manousakis, Rev. Mod. Phys. 63 (1991) 1.
[17] E. Dagotto, Rev. Mod. Phys. 66 (1994) 763 and references therein.
[18] O. P. Sushkov, Solid State Communications 83 (1992) 303.
[19] G. Martínez and P. Horsch, Phys. Rev. B 44 (1991) 317.
[20] T. Giamarchi and C. Lhuillier, Phys. Rev. B 47 (1993) 2775.
[21] H. Eskes, G. A. Sawatzky and L. F. Feiner, Physica C 160 (1989) 424.
[22] V. V. Flambaum and O. P. Sushkov, Physica C 175 (1991) 347.
[23] V. I. Belinicher and A. L. Chernyshev, Phys. Rev. B 47 (1993) 390.
[24] Z. Liu and E. Manousakis, Phys. Rev. B 45 (1992) 2425.
[25] C. L. Kane, P. A. Lee and N. Read, Phys. Rev. B 39 (1989) 6880.
[26] V. I. Belinicher, A. L. Chernyshev, A. V. Dotsenko and O. P. Sushkov, Phys. Rev. B 51 (1995) 6076.
[27] J. Igarashi and P. Fulde, Phys. Rev. B 45 (1992) 12357.
[28] G. Khaliullin and P. Horsch, Phys. Rev. B 47 (1993) 463.

FIGURE CAPTIONS

FIG. 1. The magnetic Brillouin zone.
FIG. 2. The coherent spin-wave polarization operator.
Fig. 3. a) The leading order contribution to the energy shift of a hole (solid line) in an external spin-wave (dashed line). b) The hole self-energy. c) The coherent spin-wave polarization operator.
FIG. 4. The fourth order correction to the energy of a hole in an external spin-wave.
FIG. 5. A typical fifth order diagram for the energy of a hole in an external spin-wave.
FIG. 6. The two loop correction to the spin-wave polarization operator.
