Statics and dynamics of charge fluctuations in the *t*-*J* model

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The equation for the charge vertex γ of the *t-J* model is derived and solved in leading order of a 1/*N* expansion, working directly in terms of Hubbard operators. Various quantities which depend crucially on γ are then calculated, such as the lifetime and the transport lifetime of electrons due to a charge coupling to other degrees of freedom and the charge-charge correlation function. Our results show that the static screening of charges and the dynamics of charge fluctuations depend only weakly on *J* and are mainly determined by the constraint of having no double occupancies of sites. [S0163-1829(96)06737-9]

The charge-fluctuation spectrum and the screening properties of the t-J model are largely determined by the charge vertex $\gamma(k,q)$. Here, k denotes both the momentum **k** of an electron and the Matsubara frequency $i\omega_n$. Similarly, q stands for the transferred momentum \mathbf{q} and the frequency $i\nu_n$. A simple interpretation of γ has been given in Ref. 1: It multiplies the bare electron-phonon interaction g(k,q) to yield an effective electron-phonon interaction which takes into account screening effects due to the constraint of no double occupancies of sites. Another property of γ is that its poles in the second frequency argument determine the dispersion of collective density waves and thus is an important ingredient for the density-density correlation function D(q). For the case J=0 the properties of the static vertex γ has been investigated in Refs. 1 and 2. In particular, it has been shown that γ exhibits a strong momentum dependence in **q** at low frequencies and small and intermediate dopings which tends to suppress the effective electron-phonon interaction in the tt' model (t and t' denote hopping integrals between nearest- and second-nearest neighbor sites, respectively). This effect is especially pronounced in transport quantities. The frequency dependence of γ and D has been investigated, again for J=0, in Ref. 3. There it has been shown that D is nearly exclusively determined by collective effects and has an energy scale substantially larger than the effective bandwidth, in agreement with computer simulations.⁴ The purpose of this communication is to extend the above results to the t-J model and to investigate to what extent the above properties of γ and D depend on J.

The Hamiltonian of the t-J model reads

$$H = -\sum_{\substack{ij \ p=1,\dots,N}} \frac{t_{ij}}{N} X_i^{p0} X_j^{0p} + \sum_{\substack{ij \ p,q=1,\dots,N}} \frac{J_{ij}}{4N} X_i^{pq} X_j^{qp} .$$
(1)

The subscripts i, j stand for lattice sites; the superscripts p, q denote for p=0 the unoccupied and for $p=1, \ldots, N$ singly occupied states with a spin index p. This means that the original SU(2) spin space has been extended to a SU(N)

space which is a well-known procedure in slave-boson calculations.⁵ The Hubbard operators X_i^{pq} with p=0, q=0 and p>0, q>0 have bosonic and those with p=0, q>0 or p>0, q=0 have fermionic character. They obey the following commutation and anticommutation rules, respectively,

$$[X_i^{pq}, X_j^{rs}]_{\mp} = \delta_{ij} (\delta_{qr} X_i^{ps} \mp \delta_{sp} X_i^{rq}).$$
(2)

In the SU(N) model, considered here, the X operators are subject to the constraint

$$\sum_{p=0}^{N} X_{i}^{pp} = \frac{N}{2}.$$
 (3)

This means that at most N/2 of the N states at each site can be occupied at the same time. The first term in Eq. (1) describes the hopping of particles between the sites *i* and *j* with matrix elements t_{ij} . The second term in Eq. (1) denotes the Heisenberg interaction between the spin densities at site *i* and *j* with the exchange constants J_{ij} . In the following we consider J_{ij} only between nearest neighbors ($J_{ij}=J$) and t_{ij} between nearest ($t_{ij}=t$) and next-nearest ($t_{ij}=t'$) neighbors. The coupling constants in Eq. (1) have been scaled with N in such a way that the limit $N \rightarrow \infty$ describes an interesting physical case and that for N=2 the usual *t*-*J* model is, except for an overall factor 1/2, recovered.

Using a 1/N expansion the Hamiltonian Eq. (1) has been investigated for J=0 in Ref. 1 and, in more detail, in Ref. 2. These treatments can be generalized to a finite value of J in a straightforward way: The equation of motion for a fermionic X operator is, using Eq. (1),

$$\frac{\partial}{\partial \tau_1} X^{0q}(1) = \sum_{p_2, q_2, q_3} \int d2d3t \begin{pmatrix} 0p_1 & p_2q_2 & 0q_3\\ 1 & 2 & 3 \end{pmatrix} \times X^{p_2q_2}(2) X^{0q_3}(3)$$
(4)

with

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$$t \begin{pmatrix} 0q_1 & p_2q_2 & 0q_3 \\ 1 & 2 & 3 \end{pmatrix} = \delta(1-2)\,\delta_{p_20}\delta_{q_20}\delta_{q_1q_3}t(1-3)/N + \delta_{p_2q_3}\delta_{q_1q_2}[\,\delta(1-2)t(1-3) \\ - \,\delta(1-3)J(1-2)/2]/N.$$
(5)

Here, 1 is an abbreviation for $i_1\tau_1$, i.e., $1=(i_1\tau_1)$, where τ_1 denotes the imaginary time. t(1-2) is equal to $t_{i_1i_2}\delta(\tau_1$ $(-\tau_2)$ and J(1-2) equal to $J_{i_1i_2}\delta(\tau_1-\tau_2)$. The first term in the parentheses on the right-hand side of Eq. (5) describes hopping without flip of the spin whereas the second term describes hopping with a spin flip. Comparing Eqs. (4) and (5) with Eqs. (9) and (10) of Ref. 2, one finds that the Heisenberg term in H just adds a contribution to the spin-flip hopping term. The perturbation expansion in Ref. 2 rests on two relations: The equation of motion for fermionic Hubbard operators and Eq. (31) in Ref. 2 which relates expectation values of bosonlike Hubbard operators to Green's functions. The first relation is modified by the Heisenberg term in the above way, the second relation is unchanged. As a result, it is straightforward to generalize the expressions for the selfenergy, the vertex, etc. in Ref. 2 to the case of a finite J.

Using the above procedure one obtains from Eq. (37) in Ref. 2 the following expression for the self-energy in O(1) of the *t*-*J* model:

$$\Sigma(1-2) = \delta(1-2) \int d3t(1-3)g(3^{+}-1)$$

-t(1-2)\lappa X^{00}(1)\rangle - \frac{J(1^{+}-2)}{2}g(1-2). (6)

The normalized Green's function g (denoted by \tilde{G} in²) is related to Σ via Dyson's equation

$$\int d3 \left(-\delta(1-3) \frac{\partial}{\partial \tau_1} - \Sigma(1-3) \right) g(3-2) = \delta(1-2).$$
(7)

 $\langle X^{00}(1) \rangle$ is the expectation value of $X^{00}(1)$. Both Σ and g are diagonal in the internal indices so we have omitted them in the above equations. The self-energy in Eq. (6) is instantaneous giving rise to a frequency-independent, but momentum-dependent renormalized one-particle energy $\epsilon(\mathbf{k})$. After a Fourier transformation Eqs. (6) and (7) yield $g(\mathbf{k},i\omega_n)=1/[i\omega_n-\xi(\mathbf{k})]$ with

$$\boldsymbol{\epsilon}(\mathbf{k}) = \Delta - q_0 t(\mathbf{k}) - \frac{1}{2N_c} \sum_p J(\mathbf{k} + \mathbf{p}) f(\boldsymbol{\xi}(\mathbf{p})). \quad (8)$$

Here we have $\xi(\mathbf{k}) = \epsilon(\mathbf{k}) - \mu$ and $\Delta = 1/N_c \Sigma_{\mathbf{p}} t(\mathbf{p}) f(\xi(\mathbf{p}))$, where f is the Fermi function, N_c is the number of primitive cells, and $q_0 = \delta/2$ with the doping δ .

Taking the Heisenberg interaction also into account the vertex equation (39) in Ref. 2 becomes

$$\widetilde{\Gamma}(12;3) = \delta(1-2)\,\delta(1-3) + t(1-2)\int d5d6g(1-5)\widetilde{\Gamma}(56;3)g(6-1^+) + \delta(1-2)\int d4d5d6t(1-4)g(4-5)\widetilde{\Gamma}(56;3)g(6-1) - \frac{J(1-2)}{2}\int d5d6g(1-5)\widetilde{\Gamma}(56;3)g(6-2).$$
(9)

Writing $\Gamma(12;3) = \gamma(1-2, 1-3)$ Eq. (9) becomes after a Fourier transformation

$$\gamma(k,q) = 1 + \frac{T}{N_c} \sum_{k'} \left(t(k) + t(k'+q) - \frac{J(k-k')}{2} \right) g(k')g(k'+q)\gamma(k',q). \quad (10)$$

Since the **k** dependence of J and t are given by trigonometric or products of trigonometric functions Eq. (10) represents an integral equation with a kernel consisting of six separable contributions. Equation (10) thus can be reduced to a 6×6 matrix equation with the solution

$$y(k,q) = 1 - \sum_{\alpha=1}^{6} F_{\alpha}(k) \sum_{\beta=1}^{6} \left[\delta_{\alpha\beta} + \chi(q) \right]_{\alpha\beta}^{-1} \chi_{\beta2}(q),$$
(11)

$$\chi_{\alpha\beta}(q) = \sum_{k'} G_{\alpha}(k',q) F_{\beta}(k').$$
(12)

The vectors F and G are given by

$$F_{\alpha}(k) = [t(\mathbf{k}), 1, J\cos k_{x}, J\sin k_{x}, J\cos k_{y}, J\sin k_{y}] \quad (13)$$

and

$$G_{\alpha}(k,q) = [1,t(\mathbf{k}+\mathbf{q}),\cos k_x,\sin k_x,\cos k_y,\sin k_y]\Pi(k,q)$$
(14)

with $\Pi(k,q) = -g(k)g(k+q)$. The frequency sum in Eq. (12) involves only Π and can easily be carried out:

$$\sum_{n'} \Pi(k',q) = \frac{f(\xi(\mathbf{q}+\mathbf{k}')) - f(\xi(\mathbf{k}'))}{\xi(\mathbf{k}') - \xi(\mathbf{q}+\mathbf{k}') - i\nu_n}.$$
 (15)

Calculation of $\gamma(k,q)$ thus requires essentially the calculation of the susceptibility matrix $\chi_{\alpha\beta}(q)$. For J=0 the matrix inversion in Eq. (11) can be done explicitly and one obtains Eqs. (12)–(15) of Ref. 2. In contrast to this special case, $\gamma(k,q)$ depends for $J\neq 0$ also on the vector **k** for a given doping.

The Green's function $\widetilde{D}(q)$ for density fluctuations is given by

FIG. 1. Zero-frequency vertex function $\gamma(\mathbf{k},\mathbf{q})$ as a function of aq with **k** fixed on the Fermi line along the (1,1) direction for three dopings δ .

$$\widetilde{D}(q) = \frac{T}{V} \sum_{k} \gamma(k,q) \Pi(k,q).$$
(16)

Using Eq. (11) we obtain

$$\widetilde{D}(q) = -\sum_{\beta=1}^{6} \left[1 + \chi(q) \right]_{1\beta}^{-1} \chi_{\beta 2}(q).$$
(17)

Carrying out the analytic continuation $i\omega_n \rightarrow \omega + i\eta$ the density-density correlation function $D(\mathbf{q},\omega)$ is equal to the negative imaginary part of $\widetilde{D}(\mathbf{q},\omega+i\eta)$.

We have evaluated numerically the susceptibility matrix $\chi_{\alpha\beta}(q)$ using a typical mesh of 1000×1000 points in the Brillouin zone for the summation over \mathbf{k}' . Figure 1 shows results for the zero-frequency vertex $\gamma(\mathbf{k},\mathbf{q})$ for J=0.2, t'=0(all energies are in units of the nearest-neighbor hopping energy t) and three different dopings δ . For each doping **k** is put on the Fermi line in the (1,1) direction and **q** is varied along the (1,1) direction from zero to the maximal momentum transfer for points on the Fermi line. Figure 1 should be compared with Fig. 1 of Ref. 1 where a similar plot for γ is given for the case J=t'=0. (The momentum scale in that reference should be scaled by a factor $\sqrt{2}$ in order to have the same absolute scale). The figures clearly show that the main property of the vertex found in Ref. 1 for J=0 is also present for J=0.2: For large dopings γ varies only smoothly with momentum whereas at smaller dopings γ develops a forward scattering peak with a width $\sim \delta$ due to a strong suppression of large momentum transfers. This implies that the effective charge interaction of electrons with other degrees of freedom (impurities, phonons, etc.) is essentially the bare one at small but heavily suppressed at large momenta. The curve for δ =0.10 in Fig. 1 shows a new feature: It passes through zero at a small momentum which means that the effective interaction is exactly zero at this point due to correlation effects. With increasing momentum it goes through a minimum with a negative value and approaches zero from below at large momenta. A similar, but less pronounced behavior, has been found² in the one-dimensional tmodel and in the two-dimensional tt' model with a finite t'. Finally, we have chosen in Fig. 1 a rather small value for J



and not too small values for δ in order to avoid singularities in γ due to instabilities of the homogenous phase.⁵

The above vertex function allows us to answer the following question: How much are the inverse lifetime $1/\tau$ and inverse transport lifetime $1/\tau_{tr}$ of an electron affected by electronic correlations if the coupling of the electron to additional degrees of freedom (phonons, impurities, etc.) is due to the interaction of charges? The answer becomes especially simple if one assumes that the bare coupling function is structureless, i.e., is independent of momentum and frequency. In Ref. 2 is has been shown that the quantities Λ_1, Λ_{tr} defined by

$$\Lambda_{1} = C \ll \frac{|\boldsymbol{\gamma}(\mathbf{k}, \mathbf{k} - \mathbf{k}')|^{2}}{q_{0}} \geq_{\mathbf{k}} \geq_{\mathbf{k}'}, \qquad (18)$$
$$\Lambda_{tt} = C \ll \frac{|\boldsymbol{\gamma}(\mathbf{k}, \mathbf{k} - \mathbf{k}')|^{2}}{q_{0}} \times [\mathbf{v}(\mathbf{k}) - \mathbf{v}(\mathbf{k}')]^{2} \geq_{\mathbf{k}} \geq_{\mathbf{k}'} / (2 \ll \mathbf{v}^{2}(\mathbf{k}) \geq_{\mathbf{k}} \geq_{\mathbf{k}'}, \qquad (19)$$

describe changes in the inverse lifetime $1/\tau$ [or, in the Eliashberg function $\alpha^2 F(\omega)$ for s-wave superconductivity] and the inverse transport lifetime $1/\tau_{\rm tr}$ due to correlation effects. The overall factor C is chosen such that $\Lambda_1 = \Lambda_{tr} = 1$ for $\delta \rightarrow 1$, i.e., the empty band limit. If γ in Eqs. (18) and (19) depends only weakly on momentum we have $\Lambda_1 \sim \Lambda_{tr}$. On the other hand, if γ is nonzero only for $\mathbf{k} \sim \mathbf{k}' \Lambda_{tr}$ is much smaller than Λ_1 . Figure 2 shows Λ_1 and Λ_{tr} as a function of δ for J=0.3 and t' = -0.25. With decreasing doping Λ_1 and Λ_{tr} first pass through a maximum at around $\delta \sim 0.8$ and then decrease monotonically by around a factor 2 and 4, respectively, until $\delta \sim 0.2$. The more and more pronounced appearance of a forward scattering peak in γ at still smaller dopings would cause a further decrease in Λ_1 and Λ_{tr} and especially in the ratio Λ_{tr}/Λ_1 . However, we exclude this low-doping region from our considerations because of the occurrence of instabilities of the homogenous phase in that region. Figure 2 suggests that correlation effects suppress Λ_1 and, even stronger, Λ_{tr} , moving from the overdoped towards the maximal doped regime. Figure 10 in Ref. 2 presents results for Λ_1 and $\Lambda_{\rm tr}$ and for (using our energy units) J=0 and t'=-0.20. Comparing this figure with our present Fig. 2 one concludes





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FIG. 3. Density-density correlation function $D(\mathbf{q},\omega)$ as a function of energy ω for $\delta=0.2$ and J=0.1 (left panel) and J=0.3 (right panel) using $\eta=0.1$.

that Λ_1 and Λ_{tr} depend only very weakly on *J*. (The additional interpretation of the quantity $\delta \cdot \Lambda_{tr}$ as being proportional to the resistivity in Ref. 2 should be dropped since the Drude weight entering the static part of the resistivity depends strongly on δ and the resistivity near half-filling is characterized by Λ_{tr}/δ rather than by $\Lambda_{tr} \cdot \delta$).

Figure 3 shows the density-density correlation function $D(\mathbf{q}, \omega)$ for J=0.1 (left panel) and J=0.3 (right panel) for various momenta \mathbf{q} . Curves corresponding to the same momentum practically coincide with each other demonstrating that $D(\mathbf{q}, \omega)$ and thus also the dynamic part of the vertex are nearly independent of J. This implies that D is dominated by

collective effects in the form of an infinitely sharp, dispersive sound peak also in the presence of the Heisenberg interaction. This peak has been broadened in Fig. 3 by using a finite value of 0.1 for η . The energy of this peak is in general much larger than the width of the renormalized band (which is 0.96 for J=0.1 and 1.28 for J=0.3). The contribution of the particle-hole continuum to D is nearly invisible if the sound peak is well above the particle-hole spectrum like, for instance, in the case $\mathbf{q} = (\pi, \pi)$. In the other cases like $\mathbf{q} = (2\pi/2)$ $(\pi/5, \pi/5)$, $(\pi/5, 3\pi/5)$, or $(\pi, 0)$ the collective peak is not so well separated from the particle-hole continuum and D has structure also at the low-frequency reflecting density of states of single particle-hole excitations. The absence of a noticeable dependence of the peak position on J as well as the quite different energy scales for charge and spin fluctuations³ remind one of the spin-charge separation found in onedimensional models.

In conclusion, the equation for the charge vertex γ of the *t*-*J* model has been derived in leading order of an 1/*N* expansion, reduced to a 6×6 system of linear equations, and solved numerically. Our results for the momentum and frequency dependence of γ show only a weak dependence on *J*. We also discussed various properties which depend sensitively on γ , namely, the effect of correlations on the inverse lifetime and the inverse transport lifetime of electrons and the dynamics of charge fluctuations. Our conclusion is that these quantities depend only weakly on *J* and are mainly determined by the constraint of having no double occupancies of sites. These findings are consistent with recent exact numerical results from small clusters.^{4,6}

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