Universal Charge and Spin Response in Optimally Doped Antiferromagnets

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Charge and spin response in the planar t-J model at finite temperatures are investigated numerically, in the regime corresponding to cuprates at intermediate doping. We show that the local spin correlation function is T independent, leading to $\chi''(\omega < J) \propto \tanh(\omega/2T)$. The current correlation function $C(\omega)$ appears to be T as well as ω independent, and the optical conductivity $\sigma \propto (1 - e^{-\omega/T})/\omega$. Such anomalous response functions are brought in connection with the large entropy persisting at $T < J$.

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Normal-state properties of cuprates offer a clear message that metals with strongly correlated itinerant electrons are not yet properly understood. Although the main goal remains to relate the correlation effects with the onset of superconductivity at high T_c, anomalous static and dynamical quantities at $T > T_c$ alone represent a challenging subject. From recent experiments testing normal-state properties, such as the dc resistivity [1], optical conductivity [2,3], neutron scattering [4,5], and the NMR and nuclear quadrupole resonance (NQR) relaxations [6], a unifying picture seems to emerge [1]. These properties mainly depend on the extent of doping, and the regimes have been classified into the underdoped, the "optimal" (intermediate doping), and the overdoped, respectively.

We investigate here the intermediate-doping (optimal) regime. In experiments the latter is usually defined by highest T_c, whereas we refer only to the characteristic normal-state properties [e.g., the linear $\rho(T)$ law], as summarized within the marginal Fermi liquid (MFL) hypothesis [7]. Consistent with experiments, the low-frequency dynamics in $\sigma(\omega)$ has been modeled within the Drude form by an anomalous effective relaxation rate $\tau^{-1} \propto \omega + \eta T$, and the spin susceptibility with $\chi''(\omega < T) \propto \omega/T$. Alternative phenomenological theories [8,9] have been also proposed, nevertheless the origin of these phenomena is not yet settled.

We discuss finite-T (normal-state) properties of doped antiferromagnets (AFM's) within the t-J model [10]

$$H = -t \sum_{\langle ij \rangle s} (c_{js}^\dagger c_{is} + \text{H.c.}) + J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j - \tfrac{1}{4} n_i n_j), \quad (1)$$

where $c_{is}^\dagger$ (c_{is}) are projected fermionic operators, prohibiting double occupancy of sites. The ground state of the t-J model and related properties have been intensively studied both by analytical [10] and numerical methods [11], nevertheless some basic questions, e.g., concerning possible pairing in the ground state, remain unsolved.

$T > 0$ properties have been approached by high-temperature series expansion [12], and recently by the present authors using a novel numerical method, based on the Lanczos diagonalization method combined with a random sampling [13]. The latter method has the advantage that it allows the study of dynamical response functions within the most challenging regime $T, \omega < J$, where one could hope for a universal behavior, as observed in the experiments on cuprates. Results concerning the charge [14] and spin [15] response in the intermediate-doping regime, obtained by this method, can be summarized as follows: (i) $\sigma(\omega)$ shows a non-Drude falloff, consistent with the ω-dependent relaxation rate within the MFL concept [7] and in cuprates [2,3], (ii) qualitative as well as quantitative results for $\sigma(\omega)$ and $\rho(T)$ agree reasonably well with the experimental ones, (iii) dynamical spin susceptibility $\chi''(\vec{q}, \omega)$ shows the coexistence of the high-frequency ($\omega \propto t$) free-fermion-like contribution and the low-ω spin-fluctuation contribution, and (iv) $\chi''(\vec{q}, \omega < T)$ shows a pronounced T dependence, consistent with the MFL form and (even quantitatively) with the NMR relaxation in cuprates.

The above results indicate that the t-J model represents a promising framework for the study of the anomalous metallic state in cuprates. In this Letter we present the evidence for some important features, which can lead to a more consistent picture of the intermediate-doping regime: (i) local spin (temporal) correlations appear to be particularly universal and thus fundamental to the understanding of $\chi(\vec{q}, \omega)$ response, (ii) conductivity $\sigma(\omega)$ is consistent with the fast-decaying T-independent current correlations, leading to a universal form for $\sigma(\omega)$, representing an alternative to the MFL ansatz, and (iii) both facts seem to be in a close connection with the large entropy persisting down to low temperatures $T \ll J$ in the optimal regime.

Let us consider the dynamical spin response as given by the susceptibility $\chi(\vec{q}, \omega)$ and the corresponding dynamical spin correlation function $S(\vec{q}, \omega)$

$$\chi''(\vec{q}, \omega) = (1 - e^{-\beta\omega}) S(\vec{q}, \omega),$$
$$S(\vec{q}, \omega) = \text{Re} \int_0^\infty dt\, e^{i\omega t} \langle S_{\vec{q}}^z(t) S_{-\vec{q}}^z \rangle, \quad (2)$$

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with $\beta = 1/T$ (we use units with $\hbar = k_B = 1$). We first analyze the local spin correlation function $S_L(\omega)$ and its symmetric part $\bar{S}(\omega)$

$$S_L(\omega) = \frac{1}{N} \sum_{\vec{q}} S(\vec{q}, \omega),$$
$$\bar{S}(\omega) = S_L(\omega) + S_L(-\omega) = (1 + e^{-\beta\omega}) S_L(\omega). \tag{3}$$

It should be pointed out that $S_L(\omega)$ and the related susceptibility $\chi_L(\omega)$ are directly measured (in cuprates) by neutron scattering [4,5]. The NMR relaxation as well yields the information on $S_L(\omega \rightarrow 0)$ [6,8], provided the AFM spin fluctuations $\vec{q} \sim \vec{Q} = (\pi, \pi)$ are dominant.

An important restriction for $\bar{S}(\omega)$ is the sum rule

$$\int_0^\infty \bar{S}(\omega) d\omega = \pi \langle (S_i^z)^2 \rangle = \frac{\pi}{4}(1 - c_h), \tag{4}$$

where $c_h = N_h/N$ is the hole concentration. Since in any finite system $S(\vec{q} = 0, \omega)$ is ill defined (due to conservation of total S^z), the $\vec{q} = \vec{0}$ term is omitted in Eq. (3), and the sum rule (4) serves as a useful test.

We perform the evaluation of $\bar{S}(\omega)$ via Eq. (3) by calculating $S(\vec{q}, \omega)$ using the finite-T diagonalization method for small systems, in this case for the t-J model on the square lattice with $N = 16-20$ sites. We fix $J/t = 0.3$ to remain in the regime of cuprates [10]. For the description of the method we refer to Ref. [13]; its application to the spin dynamics is given in Ref. [15]. We stress again that the method yields macroscopiclike results for $T > T^*$, while below T^* finite-size effects become pronounced. Within the intermediate regime $2/16 \leq c_h \leq 4/16$, we find typically $T^* \sim 0.1t$. T^* is larger within both the underdoped and the overdoped regions (at fixed N).

In Fig. 1 we display the $\bar{S}(\omega)$ for $c_h = 1/20, 3/16$, and several T in the range $0.1 \leq T/t \leq 0.7$. It is immediately evident that $\bar{S}(\omega)$ at optimal doping $c_h = 3/16$ is essentially T independent in a wide T range, although one crosses the exchange-energy scale $T \sim J$. For the underdoped case $c_h = 1/20$ the behavior is analogous for higher $T > T_0 \sim 0.7J$ (the same holds for the undoped AFM, and to some extent for $c_h = 2/16$), consistent with the quantum critical regime within the AFM's [16]. Deviations at lower $T < T_0$ (where the renormalized classical regime [16] is expected in the AFM's) could be an indication for the onset of a "pseudogap," but we cannot exclude that these phenomena are finite-size artifacts, since $T_0 \gtrsim T^*(c_h)$.

To follow the doping dependence we present in Fig. 2 the variation with c_h at fixed $T = 0.2t < J$. Here we plot the integrated intensity

$$I_S(\omega) = \int_0^\omega \bar{S}(\omega') d\omega', \tag{6}$$

since the latter does not require any smoothing. Again, we notice that for chosen T results are most reliable at intermediate doping, being poorer otherwise. The most striking message is that the initial slope of $I_S(\omega)$ and consequently $S_L(\omega \rightarrow 0)$ is nearly doping independent for $0 \leq c_h \leq 0.25$ (as well as T independent at intermediate doping). This is consistent with the NMR (NQR) relaxation rates T_1^{-1} as measured in $La_{2-x}Sr_xCuO_4$ in the range $x = 0-0.15$ [6,15].

Only for the overdoped systems with $c_h > 0.25$ does the low-frequency behavior change qualitatively, where the latter part is strongly suppressed as expected in (more) normal Fermi liquids. $I_S(\omega > J)$ is doping dependent even for $c_h < 0.25$, consistent with the c_h dependence of the sum rule, Eq. (4). In addition, at the intermediate doping $\bar{S}(\omega)$ decreases smoothly (see Fig. 1) up to $\omega \sim 4t$, this being the consequence of a free-fermion-like component [15]. On the other hand, in the underdoped regime the dynamics is restricted to $\omega < 3J < t$.

How can one explain the universality of $\bar{S}(\omega)$ at intermediate c_h? First we note that up to $c_h \sim 0.3$ the dominant scale of spin fluctuations remains related to J.

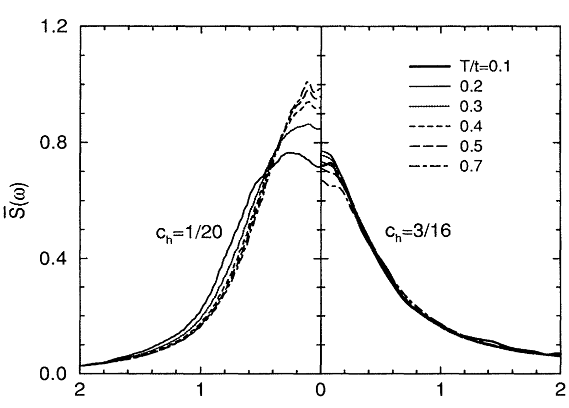

FIG. 1. Local spin correlation function $\bar{S}(\omega)$ for $c_h = 1/20$, 3/16, and various T.

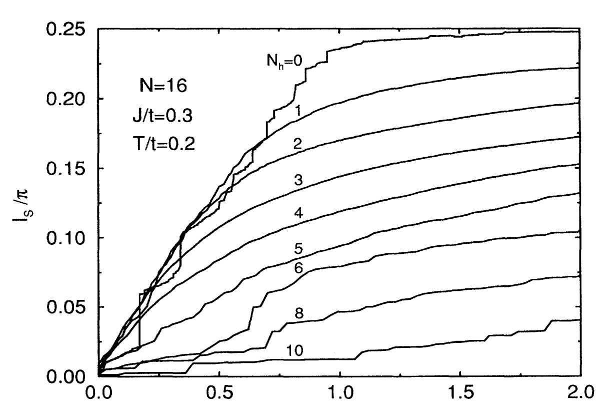

FIG. 2. Integrated spectra $I_S(\omega)$ at fixed $T = 0.2t$ and various c_h.

From the explicit expression in terms of the eigenstates of the system

$$\bar{S}(\omega) = (1 + e^{-\beta\omega})\frac{\pi}{Z}\sum_{n,m} e^{-\beta E_n}|\langle n|S_i^z|m\rangle|^2 \times \delta(\omega - E_m + E_n), \quad (6)$$

one would conjecture (quite generally) a T independence of response for $\omega \gg T$. Although such plausibility arguments have been used previously, their validity clearly depends on the character and the density of low-lying many-body states (further on we present evidence that the optimally doped AFM has a particularly large density of low-lying states). To explain also the T independence of $\bar{S}(\omega < T)$, we only need to recall the sum rule Eq. (4) and to assume that there is no characteristic scale $\omega_c < T$ which could introduce an additional low-ω structure in $\bar{S}(\omega)$.

A natural scale for an AFM is the (gap) frequency $\omega_c \sim c/\xi$, where c is the spin wave velocity and ξ the AFM correlation length. Here originates the essential difference between the undoped and the optimally doped AFM. While for an AFM in the renormalized classical regime ξ is exponentially large for $T \ll J$, and consequently $\omega_c < T$ [16], in the doped case $\xi < 1/\sqrt{c_h}$ is determined predominantly by c_h, so ξ is rather T independent for $T < J$, excluding $\omega_c < T < J$.

We conclude the discussion of spin dynamics by consequences of the universality of $\bar{S}(\omega)$. The local susceptibility is given by

$$\chi_L''(\omega) = \tanh\left(\frac{\omega}{2T}\right)\bar{S}(\omega). \quad (7)$$

Since neutron scattering probes only $\omega < J$, one can simplify Eq. (7) further by $\bar{S}(\omega) \sim \bar{S}_0$. Such a form, consistent with the MFL [7], has been recently used to describe experiments [5]. Here, one should take into account that we are not able to establish within the t-J model the existence of the pseudogap $\omega_g \sim 0.1J$ [5], observed in cuprates at low $T > T_c$. Further it follows from Eq. (7) that for $T < J$ the relevant scale for $\chi_L''(\omega)$ is $\omega \sim 2T$. The same should hold for the response at fixed $\vec{q}$. So one can generalize Eq. (7):

$$\chi''(\vec{q},\omega) \sim \frac{\chi_{\vec{q}}}{\chi_L}\chi_L''(\omega) \sim \frac{2\pi \ln^{-1}(\xi q_m)}{|\vec{q} - \vec{Q}|^2 + \xi^{-2}}\chi_L''(\omega), \quad (8)$$

where the cutoff $q_m \sim \pi$. The scaling Eq. (8) is expected to hold only for $|\vec{q} - \vec{Q}| \lesssim \xi^{-1}$, where one should take into account that in the optimal regime of the t-J model $\xi < 1$ [12,15]. Nevertheless, ξ remains T dependent (becoming even shorter at higher T), introducing additional T variation in Eq. (8). Outside the mentioned regime, in particular, for $q \sim 0$, the response is more free-fermion-like, i.e., $\chi''(\vec{q},\omega)$ is T independent [15].

Let us investigate in an analogous way the dynamical conductivity $\sigma(\omega)$

$$\sigma(\omega) = \frac{1 - e^{-\beta\omega}}{\omega}C(\omega), \quad C(\omega) = \mathrm{Re}\int_0^\infty dt\, e^{i\omega t}\langle j(t)j\rangle, \quad (9)$$

where j is the current density (we put $e_0 = 1$). Unlike $\bar{S}(\omega)$, $C(\omega)$ does not obey a T-independent sum rule. Nevertheless, motivated by universal spin dynamics we reexamine our results on $\sigma(\omega)$, obtained by the same finite-T numerical method on systems with $N = 16-20$ [14]. In Fig. 3 we present the corresponding integrated spectra $I_C(\omega) = \int_0^\omega C(\omega')d\omega'$ for fixed doping in the optimal regime $c_h = 3/16$, for various $T \leq t$. We establish several remarkable features: (i) for $T \leq J$ spectra $I_C(\omega)$ are essentially independent of T, at least for available $T > T^*$, (ii) at the same time the slope of $I_C(\omega < 2t)$ is nearly constant, i.e., $C(\omega) \sim C_0$ in a wide ω range, C_0 being weakly J dependent (tested for $J/t = 0.2, 0.6$), and (iii) even for higher $T > J$ the differences, e.g., in the slope C_0 and in the sum rule $I_C(\infty)$, appear as less essential [note that for $T \gg t$ we know exactly $I_C(\infty) = t^2 c_h(1 - c_h)$ [14]]. We reproduce the same characteristic behavior also for $c_h = 4/16$ (confirming $C_0 \propto c_h$). On the other hand, $c_h = 2/18$ seems to represent a crossover to the underdoped regime, where in contrast (e.g., for $c_h = 1/20$) we find a pronounced T and ω dependence of $C(\omega)$ at $T \leq J$. This qualitative change can again be attributed to a pseudogap appearing at larger T in underdoped systems [1].

Restricting our discussion to the intermediate doping, we note that $C(\omega) \sim C_0$ implies a nonanalytic behavior of $\sigma(\omega \to 0)$, starting with a finite slope at $\omega = 0$. This has been already evident in our previous results [14]. Moreover, with $C(\omega) = C_0$ we can claim a simple universal form for $\omega < 2t$:

$$\sigma(\omega) = C_0\frac{1 - e^{-\beta\omega}}{\omega}. \quad (10)$$

It is rather surprising that this form can be well fitted (for $\omega, T \ll t$) with a Drude-type form with a MFL

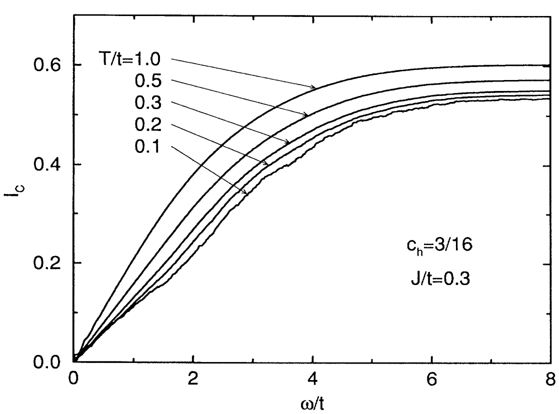

FIG. 3. Integrated current correlation spectra $I_C(\omega)$ for $c_h = 3/16$ and various T.

effective relaxation rate $\tau^{-1} = 2\pi\lambda(\omega + \eta T)$ [7] with specific $\lambda \sim 0.09$ and $\eta \sim 2.7$ [14]. The form Eq. (10) for $\sigma(\omega)$ trivially reproduces the remarkable linear law $\rho \propto T$ in cuprates [1], as well as the non-Drude falloff at $\omega > T$. A quantitative comparison of our $\sigma(\omega)$ with experimental results [2,3] has been already established in Ref. [14], including the MFL form for τ. It is evident that the expression (10) is universal, containing only C_0 as a parameter (the MFL ansatz contains at least one more) and should be retested in more detail with experiments. More generally, for larger ω one should replace C_0 with a universal $C(\omega)$, which could be, however, sensitive to a particular model, as could be also $S(\omega)$.

It should be mentioned that $C(\omega) \sim C_0$ has been derived for a single hole conductivity within the retraceable path approximation [17], with a restricted validity for $T > t$ (or possibly $T > J$). We find this behavior only for the intermediate doping, hence new arguments are needed. We can follow the analysis analogous to $\bar{S}(\omega)$, Eq. (6), expressing $C(\omega)$ in terms of eigenstates. As before, the T independence of $C(\omega > T)$ seems plausible. The fact that $C(\omega < 2t) \sim C_0$ requires, however, that the current relaxation is very fast, i.e., determined only by the incoherent hopping and the interhole collisions. The spin fluctuation scale J does not enter directly, i.e., even for $T \ll J$ the spin system only serves as a random bath for charge degrees of freedom (holons). This conclusion remains valid as long as there is no characteristic frequency $\omega_c < T$ (e.g., the pseudogap) in the system.

The above arguments, for both $S_L(\omega)$ and $C(\omega)$, require a large density (degeneracy) of the low-lying many-body states, apparently being a crucial feature for the most challenging intermediate-doping regime. To quantify this statement we calculate the entropy density $s = S/N$, using again the finite-T diagonalization method, which is less space and time consuming for static quantities [13]. In Fig. 4 we present results obtained for $N = 18$ at various c_h. Here c_h varies continuously, since we have to employ a grand canonical distribution. Our data agree with the high-T expansion results by Putikka (unpublished). The main lesson from Fig. 4 is that optimal cases with $c_h \sim 0.1-0.3$ are characterized by the largest entropy s at low $T < J$, e.g., $s > 0.2$/site for $T \sim 0.2J$, being almost one-half of $s(T = \infty)$ for the AFM. This implies a very large degeneracy of low-lying states, which could be attributed to the spin subsystem, frustrated by the hole motion.

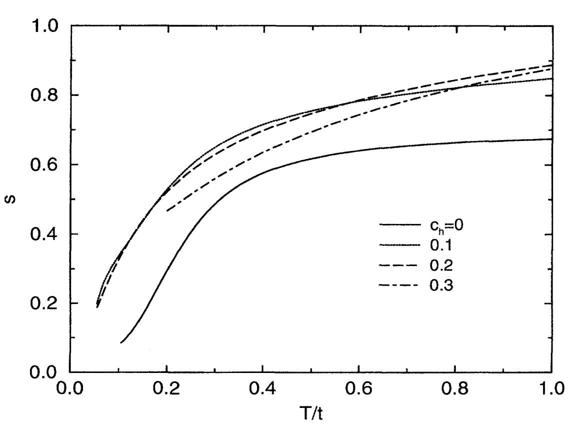

FIG. 4. Entropy density s (in units of k_B) vs T for various dopings c_h.

In conclusion, our results for the t-J model seem to indicate that the anomalous, but universal, dynamics in the intermediate-doping regime of correlated systems is a consequence of the extreme degeneracy and the collapse of low-lying quantum states (introduced by doping the magnetic insulator), which lead to a diffusivelike charge and spin response where T represents the only relevant energy (frequency) scale. On the other hand, our results do not exclude the possible onset of coherence (related to pseudogaps and superconductivity) at lower $T < T^*$.

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