Scaling of the magnetic response in doped antiferromagnets

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A theory of the anomalous $\omega/T$ scaling of the dynamic magnetic response in cuprates at low doping is presented. It is based on the memory function representation of the dynamical spin susceptibility in a doped antiferromagnet where the damping of the collective mode is constant and large, whereas the equal-time spin correlations saturate at low $T$. Exact diagonalization results within the $t$-$J$ model are shown to support assumptions. Consequences, both for the scaling function and the normalization amplitude, are well in agreement with neutron scattering results.

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Magnetic properties of cuprates, as they evolve by doping the reference antiferromagnetic (AFM) insulator and lead to a high-$T_c$ superconductor, have been so far a subject of intensive experimental and theoretical investigations. One of the puzzles awaiting proper theoretical explanation is the scaling behavior of the magnetic response observed in cuprates, mostly in the regime of low doping [1]. It has been first found by the inelastic neutron scattering experiments in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) at low doping $x=0.04$ [2] that momentum-integrated spin susceptibility $\chi_L^{M}(\omega)$ follows a universal behavior in terms of the scaling variable $\omega/T$. Similar scaling has been observed also in La$_{2-x}$Ba$_x$CuO$_4$ [3], in YBaCu$_3$O$_{6+\delta}$ (YBCO) with $x=0.5, 0.6$ [4], and even more pronounced in Zn-substituted YBCO [5].

In particular, experiments on cuprates at low doping indicate that one can represent results for the local susceptibility in a broad range of $\omega$ and $T$ as $\chi_L^{M}(\omega, T) = I(\omega)f(\omega/T)$ where $I(\omega) = \chi_0^{M}(\omega, T = 0)$. The scaling function should approach $f(x \rightarrow \infty) = 1$ and the simplest form invoked in the analysis is $f(x) \sim (2/\pi \tan^{-1}(A x))$. It seems, however, that the function is not universal for all cases, i.e., $A \sim 1.0 - 2.2$ varies between YBCO results [4,5] and LSCO, whereby in the latter case corrections to the simplest form reveal an even better agreement [2]. At the same time it is found that the inverse AFM correlation length $\kappa = 1/\xi$, as extracted from the $q$-dependent $\chi''(q, \omega)$, saturates at low $\omega$ and $T$. The largest response is at the AFM wavevector $Q = (\pi, \pi)$ and as a consequence of the scaling the peak in $\chi''(Q, \omega)$ should move downward with decreasing $T$, this being in fact established in YBCO [6]. It should be noted that also NMR relaxation experiments test and confirm the $\omega/T$ scaling of $\chi_L'(\omega)$ at $\omega \rightarrow 0$ [7].

Such a $\omega/T$ scaling is inconsistent with the concept of usual Fermi liquid. This has been recognized quite early and the concept of the 'marginal' Fermi liquid has been introduced [8] to explain scaling of the magnetic response as well as of other anomalous electronic properties. One appealing explanation still considered is the vicinity of the quantum critical point [9]. However, the latter should in general require also a critical variation of $\kappa(\omega, T)$, as indeed observed in LSCO near the optimum doping [10]. A random-phase-approximation treatment of $\chi(q, \omega)$ [11] yields a relaxation rate $\Gamma \propto 1/\xi^2$, and the scaling form could be reproduced provided that the correlation length is critical, i.e., $\xi \propto T^{-1/2}$, which is not consistent with experiments [1,2]. On the other hand, numerical investigations of the twodimensional $t$-$J$ model confirm the scaling of $\chi'_L(\omega)$ [12], although results are restricted to rather high $T$ as compared to experiments.

In the following we will argue that the anomalous $\omega/T$ scaling of the magnetic response can be understood as a consequence of few simple ingredients which appear to be valid for doped AFM in the normal state: a) the collective mode is strongly overdamped, whereby the damping is nearly $\omega$- and $T$- independent at low $\omega$, and b) there is no long-range spin order at low $T$, so that static spin correlations saturate with a finite $\xi$. It will be shown that these prerequisites are sufficient to reproduce several experimental findings for $\chi_L(\omega)$.

Within the memory function approach [13] the dynamical spin susceptibility $\chi_q(\omega) = -\langle S_q^z S_q^z \rangle / \omega$ can be expressed in the form

$$\chi_q(\omega) = \frac{-\eta_q}{\omega^2 + \omega M_q(\omega) - \omega_q^2} \quad (1)$$

suitable for the analysis of the magnetic response, as manifest in underdoped AFM [14]. $\omega_q$ represents the frequency of a collective mode provided that the mode damping is small, i.e., $\gamma_q \sim M_q'(\omega_q) < \omega_q$. For $\gamma_q > \omega_q$ the mode is overdamped. The advantage of the form (1) is that it can fulfill basic sum rules even for an approximate $M_q''$. Thermodynamic quantities entering Eq. (1) can be expressed as

$$\eta_q = -\langle |S_q^z| S_q^z \rangle , \quad \omega_q^2 = \eta_q / \chi_0^2 \quad (2)$$

where $\chi_0^0 = \chi_q(\omega = 0)$ is the static susceptibility.

$\eta_q$ is closely related to the spin stiffness and can be expressed in terms of the static correlation functions, and is expected to be weakly $q$-dependent for $q \sim Q$. Static $\chi_0^0$ (or $\omega_q$) remains to be determined, even for known $M_q(\omega)$. Instead of directly evaluating $\chi_q^0$, being quite a sensitive quantity, we rather fix it by the sum rule

$$\frac{1}{\pi} \int_0^{\infty} dw \cot \omega \frac{\Gamma_q'(\omega)}{2T} = \langle S_q^z S_q^z \rangle = C_q \quad (3)$$

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given in terms of equal time correlations, which are expected to be less $T$-dependent. $C_\mathbf{q}$ are bound by a local constraint $(1/N) \sum_\mathbf{q} C_\mathbf{q} = (1 - \epsilon) / 4$, where $c_h$ is an effective hole doping.

Let us define now our central assumptions. We first take that static correlations follow the standard Lorentzian form, i.e., $C_\mathbf{q} = C / (\omega^2 + q^2)$ [2], where $\mathbf{q} = \mathbf{q} - \mathbf{Q}$, although our results are not very sensitive to the explicit form of $C_\mathbf{q}$ (at fixed $\kappa$). $\kappa$ is taken as a $T$-independent constant, at least on approaching low $T$. Such an assumption for $\kappa$ is consistent with the neutron scattering data for weakly doped LSCO [2] and YBCO [4,5], as well as with results for the $t$-$J$ model at finite doping [15]. It furthermore indicates that the system remains paramagnetic with finite AFM $\xi$ down to the lowest $T$, as well as the absence of any ordered ground state.

Less plausible is the second assumption that the damping is also constant, $M_\mathbf{q}''(\omega)$ $\sim$ $\gamma$, i.e., (roughly) independent of $\omega$, $\mathbf{q}$ and $T$, or at least not critically dependent on these variables. We can give several arguments in favor of this simple choice. Recently the present authors [14] studied the spin dynamics within the $t$-$J$ model,

$$H = - \sum_{i,j,s} t_{ij} \hat{c}^\dagger_{i \sigma} \hat{c}_{j \sigma} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j),$$

with the nearest neighbor $t_{ij} = t$ and next-nearest-neighbor hopping $t_{ij} = t'$. It has been shown that the dominant contribution to the damping $M_\mathbf{q}''(\omega)$ in a doped system comes from the decay of spin fluctuations into fermionic electron-hole excitations [14]. If the fermionic excitations in a doped system behave as in a Fermi liquid, and the Fermi surface crosses the AFM zone boundary, the damping in the normal state is essentially constant at low $\omega$, and also weakly dependent on $T$ and $\mathbf{q} \sim \mathbf{Q}$. This is clearly very different from an undoped AFM where one expects vanishing $M_\mathbf{q}''(\omega_\mathbf{q})$ for $\mathbf{q} \to \mathbf{Q}$ and $T \to 0$ [16].

In order to support the simplification of constant $\gamma$, we present in the following numerical results for the $t$-$J$ model, obtained via the finite-$T$ Lanczos method (FTLM) [12] for a system of $N = 20$ sites on a square lattice with periodic boundary conditions. The model is analysed for the parameter $J / t = 0.3$ as appropriate for cuprates (note also the relevant value $t \sim 400$ meV), and within the regime of low hole doping, $c_h = N_h / N \leq 0.15$. Note that results within the FTLM have macroscopic relevance for high enough $T$, while at $T < T_{fs}$ they become influenced by finite-size effects. As a criterion for $T_{fs}$ we use the thermodynamic sum $Z(T) = \text{Tr} \exp(-H / E_0 / T)$ and the requirement $Z(T_{fs}) = Z^* \gg 1$ [12]. In the cases discussed here $T_{fs} \sim 0.1 t$ at intermediate doping, i.e., $T_{fs} \sim 400$ K in terms of cuprate parameters [12]. Within the FTLM we calculate directly $\chi_\mathbf{q}''(\omega)$. Since $\eta_\mathbf{q}$ and $\omega_\mathbf{q}$ are given as frequency moments of $\chi_\mathbf{q}''(\omega)$, it is then easy to extract also the damping function $M_\mathbf{q}''(\omega)$ via Eq. (4).

In Fig. 1 we present results both for $\chi_\mathbf{q}''(\omega)$ and for $M_\mathbf{q}''(\omega)$, for fixed doping $c_h = 2 / 20$ and $T = 0.15 t > T_{fs}$. In the analysis a smoothing $\epsilon = 0.07 t$ is used for convenience. One can conclude that in the presented case we are clearly dealing with overdamped spin dynamics for all presented $\mathbf{q}$. In spite of widely different $\chi_\mathbf{q}''(\omega)$ the damping function $M_\mathbf{q}''(\omega)$ is nearly constant in a broad range of $\omega < t$ and almost independent of $\mathbf{q}$. For this particular $c_h$ we estimate $\kappa = 0.7$ so that the span of $\mathbf{q}$ goes beyond $\hat{q} > \kappa$.
Let us consider the consequences of proposed simplifications taking both $\gamma$ and $\eta$ as constants. The dynamical susceptibility now takes the resonance form

$$\chi''_q(\omega) = \frac{\eta \gamma \omega}{(\omega^2 - \omega_q^2)^2 + \gamma^2 \omega^2}, \quad (5)$$

which we have to investigate together with the sum rule, Eq.(3). At given $q$ there are several regimes with respect to the values of $T$, $\gamma$ and $\omega_q$. Most evident is the situation for $\gamma, T < \omega_q$ with an underdamped mode with a frequency $\omega_q \sim \eta/(2C_q) = \alpha(q^2 + \kappa^2)$ where $\alpha = \eta/2C$. In such a case both $\chi''_q(\omega)$ as well as the local susceptibility $\chi''_0(\omega) = (1/N) \sum_q \chi''_q(\omega)$ show more or less (depending on $\gamma$) pronounced gap for $\omega < \omega_q \sim \alpha q^2$. This regime clearly does not exhibit the desired $\omega/T$ scaling. On the other hand, even in a weakly doped AFM at low $T$ with $\kappa \ll 1$ one should enter such an underdamped regime for the collective mode with $\tilde{q} \gg \kappa$. Still, in this case for $\omega_q \gg \gamma$ one would expect that the dispersion becomes that of AFM paramagnons with $\omega_q \propto \tilde{q}$. This indicates that a Lorentzian form for $C_q$ presumably is not appropriate for such a regime and should be modified for $\tilde{q} \gg \kappa$.

Experiments on cuprates as well as numerical results for the $t$-$J$ model (as apparent in Figs.1,2), however, show that in the normal state the collective mode is always overdamped in the vicinity of $q = Q$, i.e., $\omega_Q < \gamma$. Now, one gets a simple Lorentzian for low $\omega < \omega_Q$,

$$\chi''_q(\omega) \sim \frac{\eta \omega}{\gamma (\omega^2 + \Gamma_q^2)}, \quad \Gamma_q = \frac{\omega_q^2}{\gamma}, \quad (6)$$

and $\Gamma_q \ll \omega_q$. An overdamped form as in Eq.(6) has been frequently invoked in the analysis of the magnetic response \[11\] in the normal state of cuprates. However, without the knowledge of $\omega_q$, Eq.(6) is not sufficient to analyse the relation with the sum rule, Eq.(3).

Let us first discuss low $T \to 0$. In this case the l.h.s. of Eq.(5) can be explicitly integrated, and for $\omega_q < \gamma$ we get $C_q \sim (2\eta/\pi \gamma) \ln(\gamma/\omega_q)$. The relevant quantity is the peak frequency $\omega_p = \Gamma_Q(T \to 0)$. We see that the crucial parameter is

$$\zeta = C\pi \gamma/(2\eta \kappa^2), \quad \omega_p \sim \gamma e^{-2\zeta}, \quad (7)$$

which exponentially renormalizes $\omega_p$. Since $C$ is fixed by the total sum rule, i.e., $C \sim (1 + c_h \pi/(2\ln(\pi/\kappa)) \sim O(1)$ and $\eta \sim 0.6 t$ \[14\] at low doping, $\zeta$ is effectively governed by the ratio $\gamma/\kappa^2$. Our results for the $t$-$J$ model, as presented above as well as the analysis of experiments on cuprates, indicate that generally $\zeta \gg 1$.

A nontrivial quantity which is the consequence of the present $T = 0$ analysis is the local $\chi''_q(\omega, 0) = I(\omega)$ directly related to the measured 'normalization' function \[2, 5\]. In order to evaluate the latter we first find for each $\tilde{q}$ the appropriate $\omega_q$ satisfying the sum rule \[3\] and then integrate over $q$. Results for $I(\omega)$ at various $\zeta$ are presented in Fig. 3. For convenience we fix $\gamma = 0.2 t$, which appears to correspond (see Fig. 2) to low doping $c_h \sim 0.05$, close to doping in cuprates with observed scaling behavior. We note that the range $\zeta = 2 - 8$ presented in Fig. 3 corresponds to $\kappa = 0.35 - 0.19$. We see from Fig. 3 that the behavior for all $\zeta$ is qualitatively similar at high $\omega$ while the difference is mainly in the position of $\omega_p$, where $I(\omega)$ is maximum.

We can make a direct comparison with experiments on cuprates at low doping which reveal a nontrivial $I(\omega)$, as presented in the inset of Fig. 3. We first note that data for LSCO at $\omega = 0.04$ \[2\] and Zn-substituted YBCO \[5\] are quite similar. Both indicate a steep increase of $I(\omega)$ below $\omega \sim 10$ meV and...
no sign of saturation even at \( \omega = 2 \text{ meV} \). In terms of our analysis this means that \( \zeta \gg 1 \). The comparison of \( I(\omega) \) with our results at \( \zeta = 8 \) (any \( \zeta \gg 1 \) would be in fact quite satisfactory) reveals very good agreement. The difference seems to appear at larger \( \omega > 20 \text{ meV} \) which could be again due to our Lorentzian form of \( C_q \). Namely, taking for \( \hat{q} \gg \kappa C_q \propto 1/\hat{q} \) would lead to a flat \( \chi''_L(\omega) \sim \text{const.} \), as in an ordered AFM where only transverse fluctuations - magnons - contribute.

We next discuss the behavior at \( T > 0 \). It is evident that for \( T > \omega_p \), the temperature dependence of \( \Gamma_Q(T) \) (or \( \omega_Q(T) \)) becomes crucial. In order to satisfy the sum rule it follows \( \Gamma_Q(T) \sim T \) which is the origin of the \( \omega/T \) scaling. In Fig. 4 we present the 'scaling' function \( f(\omega/T) = \chi''_L(\omega,T)/\chi''_L(\omega,0) \) for various \( T \) and chosen \( \zeta = 8 \). Results confirm that indeed \( f(\omega/T) \) is nearly universal in a very broad range of \( T \), i.e., between \( T \sim \omega_p \) and \( T \sim T_f \). We show in Fig. 4 for comparison also experimental scaling function for Zn-substituted YBCO which generally fits our results very well. It is also evident that at least at lower \( T < 0.05 T_f \) our scaling function can be closely represented by \( f(x) = (2/\pi)\text{atan}(Ax) \) with \( A \sim 1.2 \).

There is still some dependence of \( f(x) \) on parameter \( \zeta \). A general tendency is that at larger \( \zeta \gg 1 \) we observe the saturation at somewhat smaller \( \omega/T \sim 1 \), i.e., appropriate \( A \) increases. On the other hand, for decreasing \( \zeta \to 1 \) we get \( f(x \to 0) > 0 \) and the saturation moves to somewhat higher \( x \).

In conclusion, we presented a theory giving an explanation for the anomalous \( \omega/T \) scaling behavior in magnetic response of doped AFM. It is based on two key assumptions: a) the saturation of static spin correlations and of the correlation length \( \xi \) at low \( T \) and, b) on the constant damping \( \gamma \) of the collective mode. While the former is supported by experimental data, the latter follows from numerical analysis on finite clusters within the \( t-J \) model and deserves further theoretical confirmation. However, both requirements are intimately related since they are consistent with a paramagnetic liquid, with fermionic excitations dominating low-\( \omega \), low-\( T \) behavior. This picture is picture is supported by ARPES experiments revealing well pronounced quasiparticle excitations even in a weakly doped LSCO.

In the presented picture the broad validity of the scaling is due to large \( \zeta \gg 1 \), i.e., the AFM \( q = Q \) collective modes are heavily overdamped even at low \( T \). This is consistent both with neutron scattering results in cuprates as well as with available numerical results within the \( t-J \) model. Note, however, that our results should remain equally valid for the case of strong-coupling, i.e., \( U \gg t \) effective single band Hubbard model, which in the low energy sector reduces to the \( t-J \) model with \( J = 4t^2/U \). Our scenario for the \( \omega/T \) scaling differs from a quantum-critical one in spite of a similar behavior of \( \Gamma_Q \sim T \), since \( \kappa \) does not scale in the same way. It should be pointed out, however, that \( \tilde{\kappa} \) as deduced, e.g., from \( \chi''_L \) or from \( \chi''_L(\omega) \) at fixed \( \omega \) is significantly reduced, i.e., \( \tilde{\kappa} < \kappa \) at low \( T \).

There are still some open questions. The theory predicts the existence of the crossover temperature \( T \sim \omega_p \) below which the scaling would cease to exist, and the response would approach \( \chi''_L(\omega, T = 0) \). Such a saturation has so far not been reported for weakly doped LSCO and Zn-substituted YBCO, which do not exhibit other phase instabilities at low \( T \). One should, however, not forget a possible influence of disorder, since the same region of the phase diagram is often associated with the spin glass character. Since our assumptions appear to remain valid also at higher (up to optimum) doping in the normal state, we can speculate on a possible validity of the same scenario in this regime as well, provided that other instabilities are absent (e.g., superconductivity, stripe ordering). The indication for the latter are the NMR relaxation results showing the same scaling in LSCO for \( T > T_c \) up to \( x = 0.15 \).

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