Scaling of the Magnetic Response in Doped Antiferromagnets

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A theory of the anomalous ω/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, for both 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 thus 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 $La_{2-x}Sr_xCuO_4$ (LSCO) at low doping $x = 0.04$ [2] that $\mathbf{q}$-integrated spin susceptibility $\chi''_L(\omega)$ follows a simple universal behavior in terms of the scaling variable ω/T. Similar scaling has been observed also in $La_{2-x}Ba_xCuO_4$ [3], in $YBaCu_3O_{6+x}$ (YBCO) with $x = 0.5, 0.6$ [1,4], 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 ω and T as $\chi''_L(\omega, T) = I(\omega)f(\omega/T)$, where $I(\omega) = \chi''_L(\omega, T = 0)$. The scaling function should approach $f(x \to \infty) = 1$ and the simplest form invoked in the analysis is $f(x) \sim (2/\pi)\tan^{-1}(Ax)$. 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 $\mathbf{q}$-dependent $\chi''(\mathbf{q}, \omega)$, saturates at low ω and T. The largest response is at the AFM wave vector $\mathbf{Q} = (\pi, \pi)$ and, as a consequence of the scaling, the peak in $\chi''(\mathbf{Q}, \omega)$ 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 ω/T scaling of $\chi''_L(\omega)$ at $\omega \to 0$ [7].

That such a scaling is inconsistent with the concept of usual Fermi liquid 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 $\chi(\mathbf{q}, \omega)$ [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 two-dimensional 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 ω/T scaling of the magnetic response can be understood as a consequence of a few simple ingredients which appear to be valid for doped AFM in the normal state: (i) the collective mode is strongly overdamped, whereby the damping is nearly ω and T independent at low ω, and (ii) there is no long-range spin order at low T, so that static spin correlations saturate with a finite ξ. 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 $\chi_{\mathbf{q}}(\omega) = -\langle\langle S^z_{\mathbf{q}}; S^z_{\mathbf{q}}\rangle\rangle_\omega$ can be expressed in the form

$$\chi_{\mathbf{q}}(\omega) = \frac{-\eta_{\mathbf{q}}}{\omega^2 + \omega M_{\mathbf{q}}(\omega) - \omega^2_{\mathbf{q}}}, \tag{1}$$

suitable for the analysis of the magnetic response, as manifest in underdoped AFM [14]. $\omega_{\mathbf{q}}$ represents the frequency of a collective mode provided that the mode damping is small, i.e., $\gamma_{\mathbf{q}} \sim M''_{\mathbf{q}}(\omega_{\mathbf{q}}) < \omega_{\mathbf{q}}$. For $\gamma_{\mathbf{q}} > \omega_{\mathbf{q}}$ the mode is overdamped. The advantage of the form (1) is that it can fulfill basic sum rules even for an approximate $M''_{\mathbf{q}}$. Thermodynamic quantities entering Eq. (1) can be expressed as $\eta_{\mathbf{q}} = -i\langle[S^z_{-\mathbf{q}}, \dot{S}^z_{\mathbf{q}}]\rangle$, $\omega^2_{\mathbf{q}} = \eta_{\mathbf{q}}/\chi^0_{\mathbf{q}}$, where $\chi^0_{\mathbf{q}} = \chi_{\mathbf{q}}(\omega = 0)$ is the static susceptibility.

$\eta_{\mathbf{q}}$ is closely related to the spin stiffness and can be expressed in terms of the static correlation functions, and is expected to be weakly $\mathbf{q}$ dependent for $\mathbf{q} \sim \mathbf{Q}$. Static $\chi^0_{\mathbf{q}}$ (or $\omega_{\mathbf{q}}$) remains to be determined, even for known $M_{\mathbf{q}}(\omega)$. Instead of directly evaluating $\chi^0_{\mathbf{q}}$, being quite a sensitive quantity, we rather fix it by the sum rule

$$\frac{1}{\pi}\int_0^\infty d\omega \coth\frac{\omega}{2T}\chi''_{\mathbf{q}}(\omega) = \langle S^z_{-\mathbf{q}} S^z_{\mathbf{q}}\rangle = C_{\mathbf{q}}, \qquad (3)$$

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

Let us define now our central assumptions. First we assume that static correlations follow the standard Lorentzian form, i.e., $C_{\mathbf{q}} = C/(\kappa^2 + \tilde{q}^2)$ [2], where $\tilde{\mathbf{q}} = \mathbf{q} - \mathbf{Q}$, although our results are not very sensitive to the explicit form of $C_{\mathbf{q}}$ (at fixed κ). κ is taken as a T-independent constant, at least on approaching low T. Such an assumption for κ 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 ξ 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 ω, $\tilde{\mathbf{q}}$, and T. 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,

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

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 ω, 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 γ, 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 analyzed 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. In the cases discussed here, $T_{fs} \sim 0.1t$ 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. (1).

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 $T = 0.15t > T_{fs}$. 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 $\tilde{q} > \kappa$.

Figure 1 confirms that it is meaningful to extract $\gamma_{\mathbf{q}} = M''_{\mathbf{q}}(\omega = 0)$, which we present in Fig. 2 for $\mathbf{q} = \mathbf{Q}$ and various doping $c_h = N_h/N \leq 0.15$ as a function of T. As expected, our results in an undoped system are consistent with vanishing $\gamma_{\mathbf{Q}}(T \to 0)$, whereas for $c_h > 0$ they lead to a finite extrapolated value $\gamma_{\mathbf{Q}}(T \to 0)$. Note that the slopes of $d\gamma_{\mathbf{Q}}(T)/dT$ in Fig. 2 are quite similar for all presented c_h. This can be interpreted as a signature that the damping is a sum of the spin-exchange contribution and the fermionic contribution [14]. Only the spin-exchange term is active in an undoped system and apparently it adds to the fermionic damping, the latter dominating the $T \to 0$ behavior in a doped system. It should be also noted that the characteristic (saturation) scale for the dominant spin-exchange damping is $T \sim J$ which is far above the T investigated in experiments. Hence, for the T window of interest, our results confirm that in a doped system the simplification of constant γ is sensible. On the other hand, it is evident from Fig. 2 that γ increases with doping, becoming very large $\gamma \sim t$ on approaching the "optimum" doping $c_h \sim 0.15$.

Let us consider the consequences of proposed simplifications. The dynamical susceptibility now takes the

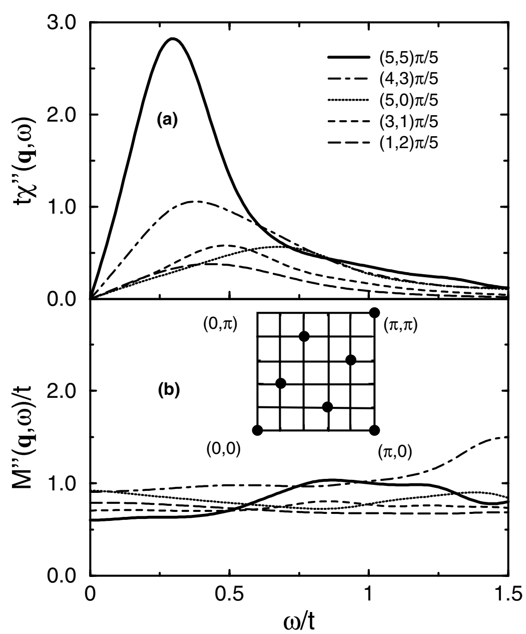

FIG. 1. (a) Spin susceptibility $\chi''_{\mathbf{q}}(\omega)$ within the t-J model for doping $c_h = 2/20$ and $T = 0.15t$, for different $\mathbf{q}$; (b) damping function $M''_{\mathbf{q}}(\omega)$ for the same parameters. The inset shows nonequivalent $\mathbf{q}$ for the lattice of $N = 20$.

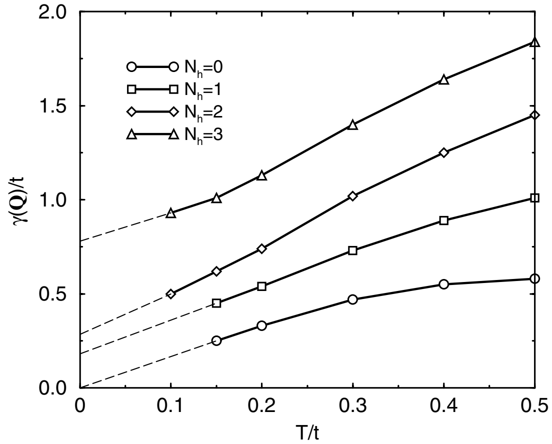

FIG. 2. Low-frequency damping $\gamma_{\mathbf{Q}}$ as a function of T for various doping $c_h = N_h/N$.

resonance form

$$\chi''_{\mathbf{q}}(\omega) = \frac{\eta\gamma\omega}{(\omega^2 - \omega_{\mathbf{q}}^2)^2 + \gamma^2\omega^2}, \qquad (5)$$

which we have to investigate together with the sum rule, Eq. (3). At given $\mathbf{q}$, there are several regimes with respect to the values of T, γ, and $\omega_{\mathbf{q}}$. Most evident is the situation for $\gamma, T \ll \omega_{\mathbf{q}}$ with an underdamped mode with a frequency $\omega_{\mathbf{q}} \sim \eta/(2C_{\mathbf{q}}) = \alpha(\tilde{q}^2 + \kappa^2)$, where $\alpha = \eta/2C$. In such a case, both $\chi''_{\mathbf{Q}}(\omega)$ as well as the local susceptibility $\chi''_L(\omega) = (1/N)\sum_{\mathbf{q}}\chi''_{\mathbf{q}}(\omega)$ show a more or less (depending on γ) pronounced gap for $\omega < \omega_{\mathbf{Q}} \sim \alpha\kappa^2$. This regime clearly does not exhibit the desired ω/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 $\omega_{\mathbf{q}} > \gamma$, one would expect that the dispersion becomes that of AFM paramagnons with $\omega_{\mathbf{q}} \propto \tilde{q}$. This indicates that a Lorentzian form for $C_{\mathbf{q}}$ 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 and 2), however, show that in the normal state the collective mode is *always overdamped* in the vicinity of $\mathbf{q} = \mathbf{Q}$, i.e., $\omega_{\mathbf{Q}} < \gamma$. Now, one gets a simple Lorentzian for low $\omega < \omega_{\mathbf{q}}$:

$$\chi''_{\mathbf{q}}(\omega) \sim \frac{\eta}{\gamma}\frac{\omega}{(\omega^2 + \Gamma_{\mathbf{q}}^2)}, \qquad \Gamma_{\mathbf{q}} = \frac{\omega_{\mathbf{q}}^2}{\gamma}, \qquad (6)$$

and $\Gamma_{\mathbf{q}} < \omega_{\mathbf{q}}$. An overdamped form as in Eq. (6) has been frequently invoked in the analysis of the magnetic response [2,11] in the normal state of cuprates. However, without the knowledge of $\omega_{\mathbf{q}}$, Eq. (6) is not sufficient to analyze the relation with the sum rule, Eq. (3).

Let us first discuss low $T \to 0$. In this case, the left-hand side of Eq. (3) can be explicitly integrated, and for $\omega_{\mathbf{q}} < \gamma$ we get $C_{\mathbf{q}} \sim (2\eta/\pi\gamma)\ln(\gamma/\omega_{\mathbf{q}})$. The relevant quantity is the peak frequency $\omega_p = \Gamma_{\mathbf{Q}}(T \to 0)$. We see that the crucial parameter is

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

which exponentially renormalizes ω_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 $\eta \sim 0.6t$ [14] at low doping, ζ is effectively governed by the ratio γ/κ^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 presented $T = 0$ analysis is the local $\chi''_L(\omega, 0) = I(\omega)$ directly related to the measured "normalization" function [2,5]. In order to evaluate the latter, we first find for each $\tilde{q}$ the appropriate $\omega_{\mathbf{q}}$ satisfying the sum rule (3) and then integrate over $\mathbf{q}$. Results for $I(\omega)$ at various ζ are presented in Fig. 3. For convenience, we fix $\gamma = 0.2t$, 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 ζ is qualitatively similar at high ω while the difference is mainly in the position of ω_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 $x = 0.04$ [2] and Zn-substituted YBCO [5] are quite similar. Both indicate a steep increase of $I(\omega)$ below $\omega = 10$ meV and no sign of saturation even at $\omega = 2$ meV. In terms of our analysis, this means that $\zeta \gg 1$. The comparison of $I(\omega)$ with our results at $\zeta = 8$ reveals very good agreement . The difference seems to appear at larger $\omega > 20$ meV, which could be again due to our Lorentzian form of $C_{\mathbf{q}}$. Namely, taking $C_{\mathbf{q}} \propto 1/\tilde{q}$ for $\tilde{q} \gg \kappa$ would lead to a flat $\chi''_L(\omega) \sim$ const, as in an ordered AFM where only transverse fluctuations (magnons) contribute.

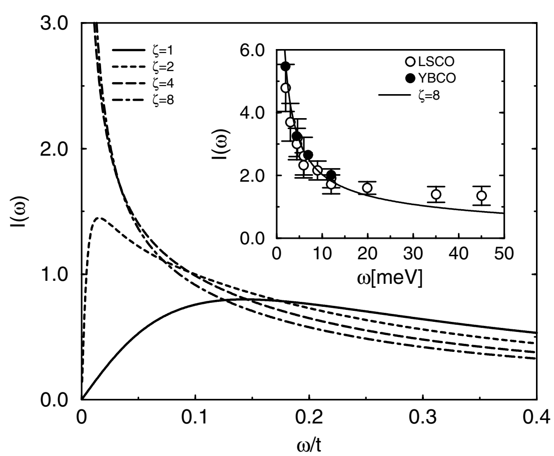

FIG. 3. Local susceptibility $\chi''_L(\omega, T = 0)$ for different ζ. The inset shows the comparison with (intensity scaled) experimental data for normalization function $I(\omega)$ in LSCO [2] and Zn-doped YBCO [5]. The vertical scales are adjusted since the experimental scales are not in absolute units.

We next discuss the behavior at $T > 0$. It is evident that for $T > \omega_p$ the temperature dependence of $\Gamma_{\mathbf{Q}}(T)$ [or $\omega_{\mathbf{Q}}(T)$] becomes crucial. In order to satisfy the sum rule (3), it follows $\Gamma_{\mathbf{Q}}(T) \propto T$ which is the origin of the ω/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 $T \sim \gamma$. We show in Fig. 4 for comparison also the experimental scaling function for Zn-substituted YBCO [5] which generally fits our results very well. It is also evident that at least at lower $T < 0.05t$ our scaling function can be closely represented by $f(x) = (2/\pi)\,\mathrm{atan}(Ax)$ with $A \sim 1.2$.

There is still some dependence of $f(x)$ on parameter ζ. 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 $\zeta \rightarrow 1$, we get $f(x \rightarrow 0) > 0$ and the saturation moves to somewhat higher x.

In conclusion, we presented a theory giving an explanation for the anomalous ω/T scaling behavior in magnetic response of doped AFM. It is based on two key assumptions: (i) the saturation of static spin correlations and of the correlation length ξ at low T, and (ii) on the constant damping γ of the collective mode. Both requirements are intimately related since they are consistent with a paramagnetic liquid, with fermionic excitations dominating low-ω, low-T behavior. This picture is supported by angle-resolved photoemission spectroscopy experiments revealing well pronounced quasiparticle excitations even in a weakly doped LSCO [17].

In the presented picture, the broad validity of the scaling is due to large $\zeta \gg 1$, i.e., the AFM $\mathbf{q} = \mathbf{Q}$ 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. Our scenario for the ω/T scaling differs from a quantum-critical one [9] in spite of a similar behavior of $\Gamma_{\mathbf{Q}} \propto T$, since κ does not scale in the same way. It should be pointed out, however, that $\tilde{\kappa}$ as deduced, e.g., from $\chi^0_{\mathbf{q}}$ or from $\chi''_{\mathbf{q}}(\omega)$ at fixed ω 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 thus 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 [1]. 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 T_1 relaxation results [7] showing the same scaling in LSCO for $T > T_c$ up to $x = 0.15$.

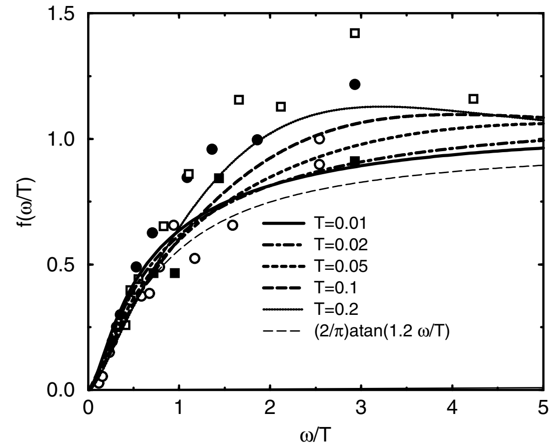

FIG. 4. Scaling function $f(\omega/T)$ for $\zeta = 8$ for different T (in units of t). For comparison, data for Zn-substituted YBCO are also plotted, as measured for different energies ω, taken from Ref. [5].

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