Freezing of spin dynamics and $\omega/T$ scaling in underdoped cuprates

Igor Sega$^1$ and Peter Prelovšek$^{1,2}$

$^1$ Jožef Stefan Institute, Ljubljana, Slovenia
$^2$ Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia

E-mail: igor.sega@ijs.si

Abstract. The memory function approach to spin dynamics in doped antiferromagnetic insulator combined with the assumption of temperature independent static spin correlations and constant collective mode damping leads to $\omega/T$ scaling in a broad range. The theory involving a nonuniversal scaling parameter is used to analyze recent inelastic neutron scattering results for underdoped cuprates. Adopting modified damping function also the emerging central peak in low-doped cuprates at low temperatures can be explained within the same framework.

1. Introduction

It is by now experimentally well established that magnetic static and dynamical properties of high-$T_c$ cuprates are quite anomalous. Early inelastic neutron scattering (INS) experiments on low-doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [1, 2] revealed that local, i.e., $q$-integrated dynamic spin response in the normal state (NS) exhibits anomalous $\omega/T$ scaling, not reflected in instantaneous spin-spin correlation length $\xi_T$ which shows no significant $T$-dependence below room temperature. Subsequently similar behaviour has been found in a number of other compounds, i.e., in underdoped YBaCu$_3$O$_{6.5}$ (YBCO) and in Zn-doped YBCO [2]. More recent INS experiments on heavily underdoped (UD) cuprates, including Li-doped LSCO [3], YBCO [4, 5, 6, 7], and Pr$_{1-x}$LaCe$_x$CuO$_{4-\delta}$ (PLCCO) [8], confirm the universal features of anomalous NS spin dynamics so that $\omega/T$ scaling is found in a broad range both in $q$-integrated susceptibility $\chi''_L(\omega)$ [3, 5, 7] and in $\chi''_Q(\omega)$ at the commensurate AFM $q = Q = (\pi, \pi)$ [3, 5, 8].

Typically, $\chi''_Q(\omega)$ is a Lorentzian with the characteristic relaxation rate scaling as $\Gamma = \alpha T$, but with a nonuniversal $\alpha$ [3, 5, 8]. Similarly, $\chi''_L(\omega, T) = \chi''_L(\omega, 0)f(\omega/T)$ has been used [2, 8, 6], with $f(x) = 2/\pi \arctan[A_1x + A_2x^3]$ and material dependent $A_{1,2}$. It has been also observed that at low $T < T_g$ some intensity is gradually transferred into a central peak (CP) [3, 4] whereas the inelastic response saturates. This freezing mechanism appears to be entirely dynamical in origin since $\xi_T$ as well as the integrated intensity are unaffected by the crossover.

The present authors introduced a theory of spin dynamics in doped AFM [9] which describes the scaling behavior as a dynamical phenomenon based on two experimental observations: a) $\xi_T$ is (almost) independent of $T$, and b) the system is metallic with finite spin collective-mode damping. Then the system close to AFM naturally exhibits $\omega/T$ scaling in a wide energy range, with saturation at low-enough $T$.

Our starting point in the analysis of recent INS experiments is the dynamical spin susceptibility [9]
\[ \chi_q(\omega) = \frac{-\eta_q}{\omega^2 + \omega M_q(\omega) - \omega_q^2}, \tag{1} \]

where the spin stiffness \( \eta_q \sim 2J (\sim 240 \text{ meV}) \) is only weakly \( q \)-dependent (\( J \) is the exchange coupling), \( \omega_q = (\eta_q/\chi_q^0)^{1/2} \) is an effective collective mode frequency, \( \chi_q^0 = \chi_q(\omega = 0) \) is the static susceptibility and \( M_q \) is (the complex) memory function containing information on collective mode damping \( \gamma_q = M_q''(\omega) \). In the NS of cuprates low-frequency collective modes at \( q \sim Q \) are generally overdamped so that \( \gamma_q > \omega_q \). UD cuprates close to the AFM phase have low charge-carrier concentration but pronounced spin fluctuations whose dynamics is quite generally governed by the sum rule

\[ \int_0^{\infty} \frac{d\omega}{\pi} \chi_q''(\omega) \coth \frac{\omega}{2T} = C_q, \tag{2} \]

where \( C_q \) is strongly peaked at \( Q \) with a characteristic width \( \kappa_T = 1/\xi_T \). Moreover, the total sum rule is for a system with local magnetic moments (spin 1/2) given by \( (1/N) \sum_q C_q = (1 - c_h)/4 \), where \( c_h \) is an effective (hole) doping.

While the formalism so far is very general, we now introduce approximations specific to UD cuprates [9]. INS experiments listed above indicate that within the NS the effective \( q \) width of \( \chi_q''(\omega) \), i.e., dynamical \( \kappa(\omega) \), is only weakly \( T \)- and \( \omega \)-dependent, even on entering the regime with the CP response [4]. Within further analysis we assume the commensurate AFM response at \( Q \) and the double-Lorentzian form \( C_q = C/[q^2 + \kappa^2] \) although qualitative results at low \( \omega \) do not depend on a particular form of \( C_q \).

2. Paramagnetic metal:

We also assume that the damping \( \gamma_q(\omega) \) is dominated by particle-hole excitations being only weakly \( q \) and \( \omega \) dependent. Hence \( \gamma_q(\omega) \sim \gamma \) with \( \gamma \) a phenomenological parameter. The assumption of constant \( \gamma \) in Eq. (1) then leads to

\[ \chi_q''(\omega) \sim \chi_q^0 \frac{\omega \Gamma_q}{\omega^2 + \Gamma_q^2}, \quad \Gamma_q = \frac{\eta}{\gamma \chi_q^0}, \tag{3} \]

Note that recent INS data are fully consistent with this form which has been used to extract \( \Gamma_q(T) \) [5].

We next exploit the sum rule, Eq.(2), to determine \( \Gamma_q \). As shown elsewhere [9, 10] \( \Gamma_q \) is mainly determined by the parameter

\[ \zeta = \pi \gamma C_q/(2\eta), \tag{4} \]

subject to \( T \ll \gamma \) which is experimentally relevant. The results are presented in Fig. 1 for a range of \( \zeta = 1 - 8 \). While \( \Gamma_q(0) = \Gamma_q^0 \sim \gamma \exp(-2\zeta) \) [9, 10], for \( T > \Gamma_q^0 \) the variation is nearly linear.
UD YBCO with $\zeta = 1.8$ and $\gamma = 60$ meV (lines).

Figure 2. Temperature evolution of $\chi_{Q}''(\omega, T)$ for UD YBCO with $x = 0.45$ [7] (symbols) compared with theoretical result, Eq. (3), with $\zeta = 1.8$ and $\gamma = 60$ meV (lines).

Figure 4. Left panel: the temperature dependence of $\kappa^2 \chi_{Q}$ for several $\zeta$ as a function of $T$. Right panel: $T$-dependence of $\chi_{q}$ relative to a Lorentzian $C_{q}$.

Figure 3. Scaling of theoretical normalised $\chi''_{Q}(\omega, T)$ based on $\zeta$ and $\gamma$ as in Fig. (2). For comparison, the scaling function $f(x)$ as frequently used in fits to experiments is also plotted.

$\Gamma_{Q} \sim \alpha T$ being a manifestation of the $\omega/T$ scaling. But $\alpha$ is not universal and depends on $\zeta$ (and weakly on $\gamma$). Then to leading order

$$\Gamma_{Q}(T) \equiv \max\{\frac{\pi T}{2\zeta}, \gamma \exp(-2\zeta)\}, \quad (5)$$

from which $\alpha = \pi/(2\zeta)$ is identified [10]. Note that the above $\Gamma_{Q}$ leads to $\chi''_{L}(\omega)$ consistent with the "marginal Fermi liquid" model introduced by Varma et al. [11]. However, contrary to the usual assumption of proximity to a quantum critical point where $\xi_{T} \propto 1/T$, here $\xi_{T} \propto \text{const}$.

Recently a number of INS experiments have been reported where $\chi''_{Q}(\omega)$ can be well described by Eq.3, including linear-in-$T$ behaviour of $\Gamma_{Q}$, where, depending on material $\alpha \sim 0.18 - 0.75$ [3, 5, 8]. All these $\alpha$ require rather large $\zeta$, which implies very low saturation $\Gamma_{Q}^{0}$, whereas INS data for YBCO and LSCO indicate quite substantial $\Gamma_{Q}^{0}$. However, saturation of $\Gamma_{Q}$, setting in for $T < T_{g}$, is accompanied by simultaneous appearance of the CP which absorbs the ‘missing’ sum rule.

In Fig. 2 INS measurements by Hinkov et al. [6, 7] on UD YBCO with $x = 0.45$ [7] are presented together with theoretical curves were the only relevant parameter is $\zeta = 1.8$, while in Fig. 3 theoretical scaling function $\chi''_{Q}(\omega, T)/\chi''_{Q}(\omega, 0)$ for the same $\zeta$ (and $\gamma$) is plotted. The overall agreement between theory and experiment (Fig. 2) is quite satisfactory. The agreement is less satisfactory for $\omega = 32.5$ meV and should be attributed to the breakdown of scaling since $\omega_{Q} > \gamma/2$, as also evident in Fig. 3. Note that the ad hoc ansatz for $f(x)$ commonly used (with $A_{2} = 0$) can be easily obtained assuming a Lorentzian dependence of $\chi_{Q}^{0}$ on $q$. A simple
calculation yields \(\arctan(A_1\omega/T)\) with \(A_1 \sim 1/\alpha\), provided that \(\kappa \ll 1\) but \(\kappa^2\chi^0_Q \sim \text{const}\) (see Fig. 4).

3. CP response:
The advantage of the memory-function formalism is that the emergence of the CP at \(T < T_g\) in the spin response can be as well treated within the same framework. One has to assume that unlike in a paramagnet the mode damping \(\gamma_q\) is not constant but may acquire an additional low frequency contribution. In particular we can take \(\tilde{M}_q \sim i\gamma - \delta^2/(\omega + i\lambda)\), with \(T\)-dependent \(\delta\) and \(\lambda\), which leads to \(\chi''_q(\omega)\) of the form used also to analyse experimental INS data for YBCO with \(x = 0.35\) [4, 14].

For \(\lambda \to 0\) but \(\delta^2/\lambda \gg \gamma\) the modified \(\tilde{M}_q\) leads to two distinct energy scales and hence to two contributions to spin dynamics, i.e., the CP part \(\chi''_q(\omega)\) and the regular contribution \(\chi''_q(\omega)\),

\[
\chi''_q(\omega) \sim \frac{\chi^0_0(q)}{\kappa_q \sim \chi^{\alpha}(q) + \chi^{\beta}(q)}
\]

valid for \(\omega < \lambda \) and \(\lambda < \omega \ll \gamma\), respectively. Thus, below \(T_g\) new scales are set by \(\gamma = \Omega^2_q/\gamma\) and \(\Gamma = (\eta/\delta^2)\lambda/\chi^0_q\), with \(\chi^0_0 = \eta/\Omega^2_q\) and \(\Omega^2_q = \omega^2 + \delta^2\). If one assumes that \(\delta\) saturates at low \(T\), as is manifest by saturation of \(\Gamma_r\) [5], \(\Gamma \propto \lambda/\chi^0\) becomes the smallest energy scale, resulting in a quasielastic peak of width \(\Gamma_c\). The saturation of \(\Gamma_r\), although at present unclear physically, is responsible for the transfer of spectral weight, since \(C^r_q \sim C_q - \pi T/(\gamma\Gamma_r)\) [10], which is again consistent with experiment on \(x = 0.35\) YBCO [5].

4. Conclusions
The approach presented gives a consistent explanation of the \(\omega/T\) scaling both in \(\chi''^0_q(\omega)\) as well as in \(\chi''_L(\omega)\). It is based on two well established experimental facts: the overdamped nature of the response and the saturation of \(\kappa_T\) at low \(\omega\) and \(T\). The appearance of the CP for \(T < T_g\) is easily incorporated into the formalism via the (almost) singular \(\omega\)- and \(T\)-dependent damping \(\tilde{M}_q(\omega)\). However, the question as to the origin of CP remains to be settled.

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