Theory of Spin Susceptibility in Frustrated Layered Antiferromagnets

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The self-consistent treatment of real and imaginary renormalizations in the dynamic spin susceptibility \(\chi(q,\omega)\) for the frustrated Heisenberg model reproduces for cuprates at low doping: a spin spectrum \(\omega_{q}\), a saddle point for \(q \approx (\pi/2, \pi/2)\), nearly constant \(q\)-integrated susceptibility \(\chi_{2D}(\omega)\) for \(\omega \lesssim 150\) meV and a scaling law for \(\chi_{2D}(\omega)\). Frustation increase (optimally doped case) leads to a stripe scenario with an \(\omega_{q}\)-saddle point at \(q \approx (\pi; \pi/2)\) and \(\chi_{2D}(\omega)\) peak at \(\omega \approx 30\) meV. The obtained \(\chi(q,\omega)\) describes neutron scattering results and leads to well-known temperature transport anomalies in doped cuprates.

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The imaginary part \(M''(q, \omega)\) is an odd function of \(\omega\). In the simplest approach we put \(M''(q, \omega) = -\omega\gamma\), where the damping \(\gamma\) is taken to be independent on \(q\) and \(\omega\). We take the real part \(M'\) as \(M' \sim |\sin(q_{x})\sin(q_{y})|^{3}\) and introduce a renormalized spectrum \(\tilde{\omega}_{q}^{2} = \omega_{q}^{2} + (\lambda |\sin(q_{x})\sin(q_{y})|)^{3}\). The choice of \(M'\) functional form is dictated by the condition that \(M'\) represents the square harmonic different from those involved in the functional form of \(\omega^{2}(q)\). Though the \(\lambda\)-renormalization is zero along the lines \(\Gamma - X\) and \(X - M\) \((\Gamma = (0, 0), X = (0, \pi), M = (\pi, \pi))\) and mainly modifies the top of the spectrum, it changes the spin gap \(\Delta_{X} = \tilde{\omega}_{q}\) due to self-consistency of calculations. So the dynamic spin susceptibility

\[
\chi(q, \omega) = \frac{-F_{q}}{\omega^{2} - \tilde{\omega}_{q}^{2} + i\omega\gamma}.
\]

contains two parameters \(\gamma\) and \(\lambda\).

We relate the dielectric limit to the case of extremely small frustration \(p = 0.04\). In the inset of Fig.1 the spectrum \(\tilde{\omega}(q)\) is presented in this limit for \(T = 0.1, \gamma = 0.025\) and \(\lambda = -1.0\) \((T \sim 100K\) for \(I \sim 100 meV\)). The spectrum is almost linear on \(\tilde{q} = |q - Q|\) up to \(\tilde{\omega}_{0} \sim 1.5\). It can be found that for fixed \(q\) there is a well-defined \(\chi(q, \omega)\) peak on \(\omega\) which is related to the spectrum \(\tilde{\omega}(q)\). More exactly, the maximum of \(\chi(q, \omega)\) on \(\omega\) corresponds to the frequency close to \(\tilde{\omega}(q)\), but always a bit smaller (due to damping \(\gamma\)). For \(I = 1.2 meV\) a spin-wave velocity \(hc \approx 900 meV \cdot Å\) is close to the value given in [11]. As it is seen from the inset of Fig.1, in accordance with the experiments [13], the dispersion \(\tilde{\omega}(q)\) is anisotropic around the magnetic zone boundary and has a saddle point close to \(q = Q/2\) \((\tilde{\omega}(q = (0, \pi) > \tilde{\omega}(q = (\pi/2, \pi/2)))\). Note that in contrast to our treatment one needs to adopt a ferromagnetic second-neighbor exchange \(I_{2}\) with \(p \leq -0.1\) for the explanation of such an anisotropy in the framework of the linear spin-wave theory [13].

In Fig.1 \(\chi_{2D}(\omega)\) is given for \(p = 0.04, \gamma = 0.25T\) in two cases: \(T = 0.1, \lambda = -1.0\) and \(T = 0.3, \lambda = 2.01/3\). The \(\lambda\)-values are chosen from the condition that the resulting spin gap should be approximately linear on \(T\) : \(\Delta_{M}(T = 0.1) = 0.048, \Delta_{M}(T = 0.3) = 0.134\). Below we show analytically that in the low-frustration limit this linearity is the necessary condition for the scaling law. The qualitative coincidence of calculated function with the experiment [11, 12] is seen \(- \chi_{2D}(\omega)\) is nearly constant in a large \(\omega\) interval and increases for \(\omega > 150 meV\).

Now we treat the scaling condition which leads to a strong limitation of \(\gamma(T)\) dependence. Fig.2 represents the scaling functions \(f(\omega/T)\). Solid lines \(b\) and \(c\) correspond to temperatures \(T = 0.1\) and \(T = 0.3\) respectively and are calculated for the same parameters, as in Fig.1 (that is, in particular, for \(\gamma = 0.25T\)). The dash-dotted line \(a\) is the best fit for experimental scaling in \(La_{1.96}Sr_{0.04}CuO_{4}\) [4] \(f_{ex}(\omega/T) = (2/\pi) \arctan(0.43(\omega/T) + 10.5(\omega/T)^{3})\). It is approximately a step function on \((\omega/T)\) smeared through \(\delta = \Delta(\omega/T) \sim 0.25\). The calculated curves have close value of \(\delta\). Note that the value of \(\delta\) strictly restricts the \(\gamma(T)\) dependence.

For example, thin curve \(d\) in Fig.2 corresponds to \(T = 0.3, \lambda = 2.01/3\) and \(\gamma = 0.3 > 0.25T = 0.075\). As a result curve \(d\) strongly deviates from curves \(a\) \((f_{ex})\) and \(c\) \((f_{ex}(T = 0.3, \gamma = 0.25T)\) and it has \(\delta \gg 0.25\).

The analogous picture for the frustration \(p = 0.1\) is shown in the inset of Fig.2 for \(\gamma = T\) and \(\lambda = 0\). We relate this case to strongly underdoped Y-cuprates [14]. The calculated scaling functions are given for the temperatures \(T = 0.1, 0.2, 0.4\) by the solid curves \(f, g, h\)
resolved doping. Calculated data are presented for $\chi$ and scaling is ruled by a linear law strongly restricts $\chi$ above calculations we have taken $f(T) = \arctan, the scaling function $\Phi = \arctan(\omega/T) − \delta T/\lambda$ (5) is described by a switched’ arctan law and contains a microscopic information on $\Delta_M$ and $\chi$. The switching by $\Theta$-function takes place at $\omega = \Delta_M$.

In contrast to numerous experimental fittings by simple arctan, the scaling function $f(\omega/T)$ is described by switched’ arctan law and contains a microscopic information on $\Delta_M$ and $\gamma$. The switching by $\Theta$-function takes place at $\omega = \Delta_M$.

In Fig.2 $f$ is represented for $\alpha = 0.25, \beta = 0.5$ by dotted line $e$ and it coincides with $f_T = 0.25$. The scaling function $f(\omega/T)$ with slightly different parameters $\alpha = 0.25, \beta = 0.43$ is almost indistinguishable from $f_{\omega}(\omega/T)$ [13]. Let us remind, that in above calculations we have taken $\gamma = T$ and such $\lambda(T)$ that the self-consistent calculations led to $\Delta \sim T$.

So in the dielectric limit (small $p$) the model leads to an adequate description of experimental results. The scaling law strongly restricts $\gamma(T)$ dependence.

Now we turn to the case $p = 0.28$ which corresponds to $\Delta_M \approx \Delta_X = \omega_0 = 0.28$. We relate this case to the optimal doping. Calculated data are presented for $T = 0.025$ and 0.05 with $\alpha = 0.38 + 0.8T$ (in contrast to low frustration limit here $\gamma$ does not tend to zero at $T \to 0$) and $\lambda = 10^{-1/3}$. For $T = 0.025$ and 0.05 the gaps are $\Delta_M = 0.197, \Delta_X = 0.179$ and $\Delta_M = 0.228, \Delta_X = 0.210$.

Fig.3 shows the $Q$-peaks, i.e. $\chi(\mathbf{q}, \omega)$, for $T = 0.025$ and $T = 0.05$. They are also in good agreement with the experiment [12]. In the inset of Fig.3 the calculated spectrum $\omega(\mathbf{q})$ has the following new features: the saddle points close to $\mathbf{q} = (\pi/2, \pi/2, \pi)$ and $\omega(\mathbf{q})$ changes weakly along $X - M$ direction. That is why $\chi(\mathbf{q}, \omega)$ has a peak at $\omega \approx 2 \Delta_M$. This is explicitly seen in the another inset of Fig.3 which gives $\chi(\mathbf{q}, \omega)$ (solid line) and $\chi(\mathbf{q}, \omega)/(2n_{Bose} + 1)$ (dashed line) for $T = 0.05$. These curves qualitatively correspond to the experimental ones [12] for optimally doped cuprates. It is clear that the shown behavior of $\omega(\mathbf{q})$ and $\chi(\mathbf{q}, \omega)$ is a result of a stripe scenario if we remind that the increase of $p$ drives the system to a state which is close to a coherent superposition of two semiclassical stripe phases with $\Delta_X = 0$. It can be shown that $c_0 = (S_0^z S^-_0)$ is qualitatively different for small and large frustrations. For $p \leq 0.1$ the structure factor $c_0$ has an extremely narrow peak at $\mathbf{q} = \mathbf{Q}$. For $p = 0.28$ the structure factor has peaks at $\mathbf{q} = \mathbf{Q}$ and at $\mathbf{q} = \mathbf{X}$. With $p$ increase the peaks at $\mathbf{X}$ points increase and the $\mathbf{M}$-peak disappears.

We capture this physics taking a spin-only model. But this model is too simple to reflect a well-known low-energy incommensurate magnetic excitations at wave vectors close to $\mathbf{Q}$ at optimal doping. It is obvious that one needs to introduce explicitly the spin-hole scattering to describe this feature.

To check the applicability of the obtained spin susceptibility $\chi(\mathbf{q}, \omega)$ for the kinetics of the optimally doped HTSC we calculate the in-plane resistivity $\rho(T)$ and the Hall coefficient $R_H(T)$ in the framework of the spinfermion model with the Hamiltonian

$$
\hat{H} = \hat{H}_0 + \hat{H}_F
$$

$$
\hat{H}_0 = \sum_{k, \sigma} \varepsilon_k a_k^\dagger a_k + J \sum_{k, q, \gamma_1, \gamma_2} a_k^\dagger S_{\gamma_1}^\dagger a_{\gamma_2}^\dagger a_{\gamma_2} a_{\gamma_1}
$$

The hole spectrum $\varepsilon_k$ is obtained from the calculation of
the lower spin-polaron band in a six pole approximation \cite{17} and is shown in the inset of Fig.4. It is well known that scattering by the spin-fluctuations with momenta $\mathbf{Q}$ leads to a strongly $T$-dependent anisotropy. To take it into account the equation of motion for the non-equilibrium density matrix $\hat{\rho}(\mathbf{q}, \omega)$ \cite{17} is solved by seven-moment approach $\hat{F} = \sum_{l=1,2,7} \eta_l \hat{F}_l$, $\hat{F}_l = \sum_{\mathbf{k}} F_l(\mathbf{k}) a^\dagger_{\mathbf{k}l} a_{\mathbf{k}l}$. The moments $F_l(\mathbf{k})$ are taken to be polynomials in velocity components $v_k = \partial \varepsilon_k / \hbar \partial \mathbf{k}$ and their derivatives: $F_l^\mathbf{v}(\mathbf{k}) = \{ v_{k_x}^\mathbf{v}, (v_{k_x}^\mathbf{v})^2, v_{k_y}^\mathbf{v}, v_{k_x}^\mathbf{v} v_{k_y}^\mathbf{v}, (v_{k_y}^\mathbf{v})^2, \partial v_{k_x}^\mathbf{v} / \partial y, \partial v_{k_y}^\mathbf{v} / \partial x \}$. The detailed expressions for $\rho(T)$ and $R_H(T)$ are given in \cite{13}. The susceptibility $\chi(\mathbf{q}, \omega)$ \cite{3} is involved in scattering integrals. To clarify the importance of the form \cite{3}, we also present the results for widely used so-called overdamped susceptibility $\chi_{ovd}(\mathbf{q}, \omega)$ (when $\omega^2$ term in the denominator of \cite{3} is omitted) \cite{14, 20}.

The results presented in Fig.4 are obtained for $p = 0.28$, $I = 100 \text{ meV}$ and $J = 200 \text{ meV}$. The plots are the resistivity $\rho(T)$ and the Hall angle cotangent $\cot \Theta_H = \rho_{xx}/R_H B$ (in the inset) obtained for the $\chi(\mathbf{q}, \omega)$ \cite{3} – solid lines and for $\chi_{ovd}(\mathbf{q}, \omega)$ – dashed lines. In accordance with the experiment \cite{21}, the $\rho(T)$ curve exhibits a temperature dependence close to a linear one starting from low $T$ with the value $\rho(400K)/\rho(100K) \approx 5$. It can be shown that $\chi_{ovd}(\mathbf{q}, \omega)$ approximation underestimates the scattering for large $\omega$. As a result at $\rho(T)_{ovd} < \rho(T)$ and, as it is seen from Fig 4, in some temperature regions $\rho(T)_{ovd}$ has a different curvature. The $\cot \Theta_H$ exhibits nearly linear behavior on $T^2$ in a wide temperature range, however, at low temperatures deviation from linearity is obvious. It seems hopeful that the self-consistent spin susceptibility $\chi(\mathbf{q}, \omega)$ allows to describe experimental temperature anomalies of two kinetic coefficients simultaneously.

In summary, we have made a systematic self-consistent study of the spin problem in 2D frustrated Heisenberg antiferromagnet. Key features of the model – temperature dependence of the damping in low frustration limit and the appearance of saddle points of the dispersion $\tilde{\omega}(\mathbf{q})$ close to $\mathbf{q} = (\pi; \pi/2); (\pi/2; \pi)$ in the case of strong frustration increase – allow to relate the results to a wide hole doping interval in cuprates.

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\begin{thebibliography}{99}

\bibitem{1} P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
\bibitem{2} R. J. Birgeneau et al., cond-mat/0604667 (2006).
\bibitem{3} B. Lake et al., Nature 400, 43 (1999).
\bibitem{4} B. Keimer et al., Phys. Rev. B 46, 14034 (1992).
\bibitem{5} P. Prelovsek, I. Sega and J. Bonca, Phys. Rev. Lett. 92, 027002 (2004).
\bibitem{6} I. A. Larionov, Phys. Rev. B 72, 094505 (2005).
\bibitem{7} A. Sherman, and M. Schreiber, Phys. Rev. B 68, 094519 (2003).
\bibitem{8} H. Shimahara, and S. Takada, J. Phys. Soc. Jpn. 60, 2394 (1991).
\bibitem{9} A. F. Barabanov, and V. M. Berezovsky, Phys. Lett. A 186, 175 (1994); JETP 79, 627 (1994); J. Phys. Soc. Jpn. 63 (1994) 3974.
\bibitem{10} A. F. Barabanov, L. A. Maksimov, Phys. Lett. A207, 390 (1995).
\bibitem{11} S. M. Hayden et al., Phys. Rev. Lett. 76, 1344 (1996).
\bibitem{12} S.M. Hayden, G. Aeppli, T.G. Perring, H.A. Mook, F. Dogan, Phys. Rev. B 54, R6905 (1996).
\bibitem{13} R. Colden et al., Phys. Rev. Lett. 86, 5377 (2001).
\bibitem{14} C. Stock et al., Phys. Rev. B 69, 014502 (2004).
\bibitem{15} N. B. Christensen et al., Phys. Rev. Lett. 93, 147002 (2004).
\bibitem{16} H. F. Fong et al., Phys. Rev. B 61, 14773 (2000).
\bibitem{17} A. F. Barabanov et al., JETP 92, 677 (2001).
\bibitem{18} A. M. Belemouk, A. F. Barabanov and L. A. Maksimov, Zh.Eksp.Teor.Fiz. 129, 493 (2006) [JETP 102, 431 (2006)].
\bibitem{19} B. P. Stojev and D. Pines, Phys.Rev. B 55, 8576 (1997).
\bibitem{20} R. Hlubina, and T. M. Rice, Phys. Rev. B 51, 9253 (1995).
\bibitem{21} Y. Ando, S. Komiyay, K. Segawa, S. Ono, Y. Kurita, Phys. Rev. Lett. 93, 267001 (2004).
\end{thebibliography}