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Memorandum

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Ground State of a 2D Antiferromagnet on a Square Lattice

The 2D antiferromagnetic ground state on a squared lattice was extensively studied theoretically (see Refs.[1]-[4]). It was found that the Heisenberg model

$$\mathcal{H}_{2D} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

with $J > 0$ can be mapped onto a quantum nonlinear sigma model (QNLσM). This model can be solved in the long wave limit. The generic phase diagram is shown in Fig.1. It is consistent with the Mermin-Wagner theorem [5] in the sense that there is no *true* long-range order at any finite temperature T.

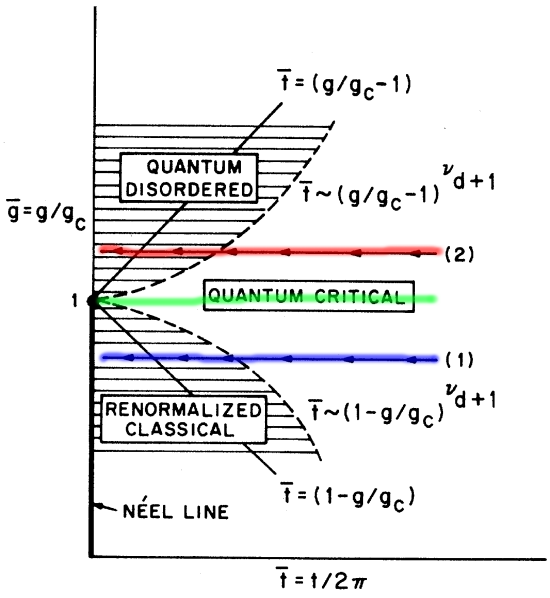

Figure 1: Crossover diagram of the QNLσM at $d = 2$ (see Ref.[1]), $\bar{t} \propto T$.

However, the QNLσM prediction is that for $T = 0$ and $\bar{g} < 1$, where $\bar{g} \propto 1/\rho_S$, with ρ_S the spin stiffness[1] there is a Néel state, *i.e.* true long range order. Moreover, the $T > 0$ state ($\bar{g} < 1$,

[1]The spin stiffness, ρ_S, is defined as $E(\theta) = E(\theta = 0) + 1/2\rho_S\theta^2$, where θ is a small rotation angle. For a classical Heisenberg model in 2D $\rho_S = JS^2$ [6]

called renormalized classical state) shows an exponential growing correlation length ξ_{RC} (see Eq.(3); blue line in Figs.1&2).

The temperature dependence of ξ at the quantum critical point ($\bar{g} = 1$) is following a $1/T$ behavior (see Eq.(2); green line in Figs.1&2).

Above the quantum critical point $\bar{g} > 1$, ξ is finite and pretty much temperature independent at low enough temperature (see Eq.(4); red line in Figs.1&2).

Correlation Length ξ in the Different Regimes

Correlation length ξ for the quantum critical point $\bar{g} = g/g_c = 1$:

$$\xi_{\bar{g}=1} \approx \frac{\hbar c}{k_{\mathrm{B}} T}, \tag{2}$$

whith c the renormalized spin wave velovity.
Correlation length ξ in the renormalized classical regime $\bar{g} < 1$ [2]:

$$\xi_{\mathrm{RC}} \simeq 0.5 \cdot a \cdot \exp(1/x) \cdot \left[1 - x/2 + O(x^2)\right], \tag{3}$$

with $x = k_{\mathrm{B}} T/(1.13J)$, and a the lattice constant.
Correlation length ξ in the quantum disordered regime $\bar{g} > 1$:

$$\xi_{\mathrm{QD}} \approx a \frac{c_1}{\Delta + k_{\mathrm{B}} T \exp(-4\Delta/(k_{\mathrm{B}} T))} \tag{4}$$

where c_1 is a constant and Δ is the gap in the excitation spectrum forming in the quatum disordered regime.

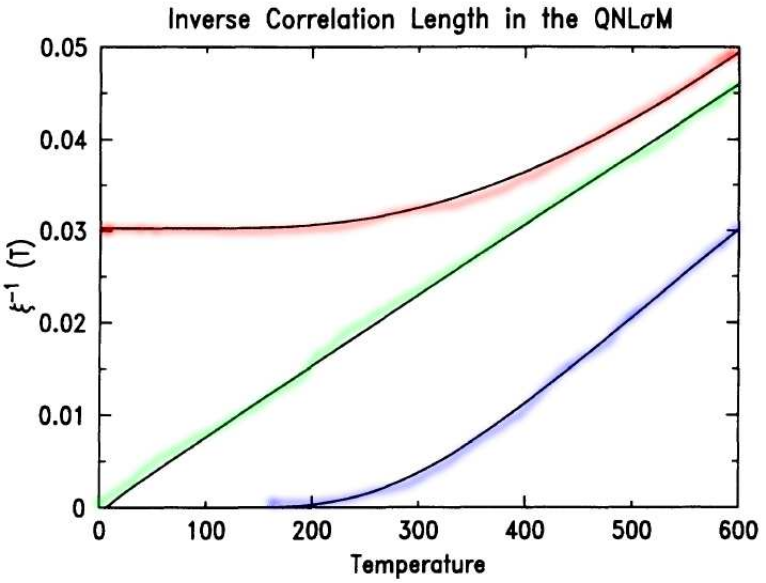

Figure 2: Inverse correlation length $1/\xi$ (units in Å) versus T for the QNLσM. Parameters as for LSCO.

From the μSR point of view, systems with $1/\xi < 0.02 - 0.03$ 1/Å can show spontaneous precession signals in zero field if the system doesn't show much dynamics.

Is anything known experimentally about the temperature dependence of ξ? Of course any real system like La_2CuO_4 or $Sr_2CuO_2Cl_2$ has some additional coupling terms in the spin Hamiltonian which will eventually drive the system 3D and hence a phase transition at finite temperature will take place. The transition temperature can be estimated from the self-consistent equation

$$J' \left[\frac{\xi_{2D}(T_{\rm N})}{a}\right]^2 \simeq k_{\rm B} T_{\rm N} \tag{5}$$

where J' is the exchange coupling between neighboring CuO_2 planes with $J'/J \simeq 2 \cdot 10^{-5}$. Since J'/J is small, it has been argued that $\xi(T)$ can be sufficiently accurate measured in the paramagnetic phase of these systems. This has been extensively studied by INS Refs.[7]-[9] and by NMR/NQR Refs.[10]-[13]. **All these measurements consistently find that La_2CuO_4 is found in the parameter space of the renormalized classical regime, *i.e.* $\bar{g} < 1$.** Fig.3 shows data for $La_{2-x}Sr_xCuO_4$ measured by INS. First focus on the $x = 0$ data. They indeed are well described by $\xi_{\rm RC}$ Eq.(3). The parameters found from these measurements are consistent with the one found by NMR/NQR.

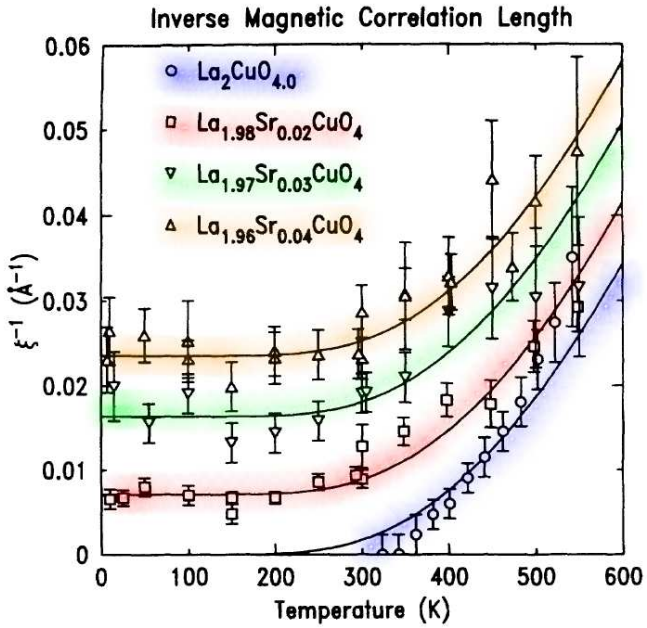

Figure 3: Measured values of $1/\xi$ versus T (INS [8]).

Now, if the system is going to be doped, the character of $\xi(T)$ is changed as can be seen in Fig.3. The $x > 0$ data look somewhat similar than $1/\xi_{\rm QD}(T)$ (see Fig.2), however one needs to be careful here. Doping is adding an additional dimension to the phase diagram of Fig.1. I haven't found any quantitative analysis dealing with this problem. However, Keimer *et al.* ([8], Fig.3) found experimentally that

$$\begin{aligned} \xi^{-1}(x,T) &= \xi^{-1}(x,0) + \xi^{-1}(0,T) \\ \xi^{-1}(x,0) &= a/\sqrt{x}. \end{aligned} \tag{6}$$

Gooding and Mailhot [15] modelled this the following way: it is assumed that at low enough temperature the doped holes localize. This is also what is seen in μSR where a spin freezing is observed. The quasi localized hole will fluctuate in order to restore the symmetry of the pure system. This is leading to a long-range coupling between the magnetic system and the charge impurity.

Random perturbations to the ordered quantum antiferromagnetic ground state

One questions which needs to be answered is the following: How robust is $\mathcal{H}_{2D}$ in respect to any kind of random perturbations, especially keeping in mind the hole doping? Murthy discussed this case in Ref.[16], based on the following Hamiltonian:

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \underbrace{\sum_{\langle ij \rangle} K_{ij} \mathbf{S}_i \cdot \mathbf{S}_j}_{(*)} + \underbrace{\sum_i \mathbf{h}_i \cdot \mathbf{S}_i}_{(\triangle)} \tag{7}$$

with

$$\begin{aligned} \overline{K}_{ij} &= 0,\ \overline{K_{ij} K_{kl}} = \sigma_J^2 \delta_{ik} \delta_{jl} \\ \overline{h}_i^{\alpha} &= 0,\ \overline{h_i^{\alpha} h_j^{\beta}} = \sigma_h^2 \delta_{ij} \delta_{\alpha\beta}. \end{aligned}$$

The term $(*)$ is a short range random coupling, whereas the $(\triangle)$ originates from a long range random coupling. He showed that $(*)$ is leading to a mere renormalization of J and hence the phase diagram of Fig.1 is still valid. However, $(\triangle)$ in 2D is always a relevant perturbation and hence will kill long-range order ($T = 0$). Of course this term is thus also strongly influencing $\xi(T)$. Since the charge localization model of Gooding is predicting a long range perturbation of the magnetic state, this could mimic a term like $(\triangle)$.

Think about our LSCO superlattice (SL) results, this could at least qualitatively explain the very weak magnetic state for the [3LSCO+6LCO] and [3LSCO+9LCO] samples. When changing the SL stacking, not only the dimensionality is affected but also the charge level in the LCO layers.

In order to optimize this kind of SL studies the metallic LSCO layer should be switched to optimally doped LSCO ($LSCO_{opt}$). Since the chemical potential difference between $LSCO_{opt}$ and LCO is very small or even absent, charge transfer effects should be minimal, only leaving Sr interdiffusion as a source of doping.

References

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