Magnetic Quantum Critical Point in YBa$_2$Cu$_3$O$_{7-\delta}$?

Resolving the Correlation Length Controversy

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A mode coupling calculation which previously explained the Mott gap collapse induced in cuprates by electron doping is applied to the analogous problem of hole doping. A plateau in the $\tilde{q}$-space susceptibility is found to inhibit the rate of susceptibility divergence as $T \to 0$. This effect could reconcile neutron and NMR measurements of the correlation length in this regime, and clarify the issue of proximity to a quantum critical point.

There is currently a controversy as to the magnetic correlation length $\xi$ in hole-doped cuprates, with neutron scattering [1] finding a T-independent value while NMR studies [2,3] suggest that $\xi$ increases as T decreases. While the numerical values are not greatly dissimilar, the temperature dependence is important, since a weakly-diverging $\xi$ -- even if ultimately cut off by superconductivity -- could provide evidence for proximity to a quantum phase transition (QPT), as has been suggested to occur slightly above optimal doping [4]. Here, a resolution of this problem is suggested, which is consistent with the theoretical model of the QPT.

Recent evidence for a QPT in electron-doped cuprates [5,6] has generated a lot of theoretical interest [7–10]. It is found that at a critical electron doping, there is a QPT where (a) the Mott gap collapses, (b) the $T=0$ Néel transition terminates, and (c) the Fermi surface crosses over from small pockets to a large barrel. The simplest mean field theory [7] can reproduce the transition, if a Kanamori-like [11] doping dependence of the Hubbard $U$ is assumed. The results have been confirmed by a number of calculations [8–10] which incorporate interactions with spin waves, the main difference being that the mean-field gap and Neel transition become a pseudogap and crossover temperature $T^*$. [Secondary interactions can generate a finite Neel temperature $T_N << T^*$.] Extension of the model to the hole-doping case is problematic. The model predicts a nearly electron-hole symmetric QPT, with pseudogap collapse. In fact, the observed pseudogap does follow the predicted doping dependence [8], terminating in a QPT [4] which is approximately electron-hole symmetric. This symmetry can be seen in the phase diagrams [12] of electron-doped Nd$_{2-x}$Ce$_x$CuO$_{4+\delta}$ (NCCO) and hole-doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO). Signatures of strong local magnetic couplings disappear near the dopings of optimal superconducting $T_c$; the corresponding dopings are comparable, and the $T_c$ values themselves do not greatly differ. Near optimal doping the normal-state resistivity is linear in temperature [13], suggestive of a QPT. Moreover, it was recently suggested [14] that this QPT involves a crossover to the large Fermi surface.

Within the SCR approach, the zero-temperature antiferromagnetic (AFM) transition is controlled by a renormalized Stoner criterion [8], $U\chi_{Q0} = \eta$, with $U$ the Hubbard $U$, $\eta > 1$ a quantum correction, and $\chi_{Q0} = \chi_0(Q, \omega = 0)$ the bare magnetic susceptibility at $Q = (\pi, \pi)$,

\[
\chi_{Q0} = \frac{\sum \frac{f(E_\tilde{k}) - f(E_{\tilde{k}+\tilde{Q}})}{E_\tilde{k} - E_{\tilde{k}+\tilde{Q}}}}{2},
\]

where $f$ is the Fermi function, and $E$ the electronic dispersion, taken to be of tight-binding form

\[
E_{\tilde{k}} = -2t(c_x + c_y) - 4t'c_xc_y,
\]

with $c_i = \cos k_ia$ and $a$ is the lattice constant. At finite temperatures, there is a Mott-like pseudogap in the density of states, which first appears at a temperature close to the RPA Néel temperature (for $U^* = U/\eta$) -- in particular, the pseudogap collapses to $T = 0$ at the zero temperature Néel transition. While the doping at which this QPT occurs depends sensitively on $|t'|$, the QPT falls at approximately the same doping for both electron and hole doping.

It is here suggested that the striking differences between electron and hole doped cuprates can be understood from the Stoner criterion, specifically, the doping dependence of $\chi_{Q0}$ for $q$ near $Q$, Fig. 1. For hole doping, the susceptibility has the form of a (diamond-shaped) plateau centered on $Q$; for electron-doping the plateau width has shrunk nearly to zero. Briefly, as $T$ decreases, the Stoner enhancement raises only very near $q = Q$ for electron-doped systems; as the peak height diverges the width (inverse correlation length) shrinks to zero, and the area under the curve remains small, leading to a strong transition, $\xi$ diverging exponentially in $1/T$. For hole-doping, the Stoner enhancement is spread over the full...
plateau. This has two effects: first, the susceptibility width is pinned at the plateau width, and is insensitive to the $\xi$ divergence; second, the large area over which the susceptibility is growing can lead to a sum-rule saturation and a very sluggish divergence, $\xi \sim 1/\sqrt{T}$. The detailed calculations below confirm this scenario, and show that the $\xi$ measured from NMR has the expected $T$-dependence. Thus, the SCR model both explains the seemingly contradictory neutron and NMR data, and simultaneously explains the electron-hole asymmetry.

The approximate electron-hole symmetry of the hot-spot regime leads to a corresponding symmetry of the QPTs.

Figure 1 shows the bare susceptibility as a function of $q$ both in and out of the hot spot regime. At each doping in the hot spot regime, there is a plateau in $q$-space centered at $\bar{Q}$, where $Re(\chi(q))$ is nearly constant, Fig. 1a. This plateau is highly asymmetric between electron and hole doping: the width of this plateau $q_c$ shrinks to zero at $x_C$, Fig. 1c, but actually has its largest value at $x_H$. The $q$-plateau half-width $q_c$ is the point where the $Q + \bar{q}_c$-shifted-FS no longer overlaps the original FS. For displacements along the [110] direction, $q_c$ is found from

$$\sin \frac{q_c x}{2} = \frac{1}{\tau} \sqrt{\frac{\tau^2 - \mu}{4t}},$$

with $\tau = 2t'/t$, while along the [100] direction, $q_c = 2\sin^{-1}(-\mu/2t)$. The plateau is a Fermi surface caliper: Eq. 3 represents the distance in $\bar{q}$-space between the nodal point and the zone diagonal. The cutoffs are plotted in Fig. 2. The experimental data [19,1] will be discussed below.

For doping off of the plateaus, either for $x > x_H$, Fig. 1b, or $x < x_C$, Fig. 1c, there are two independent QPTs. First, the magnetization vector changes from commensurate ($\bar{q} = \bar{Q}$) or weakly incommensurate on the plateau to strongly incommensurate off of the plateau, due to Kohn anomalies [20,21]. However, while this involves a transition between two different forms of magnetic order, there is a second transition. Due to the rapid falloff of the magnitude of $\chi_0$, there is a Slater-type transition to a nonmagnetic state. It is this latter transition which matches experimental observations for the cuprate QPTs. The falloff is so sudden that the strongly incommensurate susceptibilities have not yet been seen.

The susceptibility plateau is controlled by hot spot physics, where a hot spot is defined as a point on the Fermi surface (FS) which is separated from another FS point by exactly the antiferromagnetic vector $\bar{Q}$. For any $t' \neq 0$, the hot spots exist in a finite range of doping about half filling; the critical dopings which terminate the hot spot regime are called $x_C$ (electron doping) and $x_H$ (hole doping) – the latter coinciding with the van Hove singularity (VHS). Between these two dopings, the susceptibility is large [16–18], but outside this doping range the susceptibility falls rapidly, so for a wide range of couplings, $U$, the Stoner criterion will hold when hot spots are present, but will fail when the hot spots disappear.

\[\text{FIG. 1. (a) Susceptibility } \chi_0q \text{ for several hole dopings in the hot spot regime, at the mean-field Néel temperature } T_N. \text{ From lowest to highest curve, dopings } x \text{ [and } T_N] \text{ are 0 [4700], 0.05 [2200], 0.078 [1520], 0.109 [961], 0.127 [701], 0.147 [475], 0.160 [369], 0.175 [278], 0.188 [222], 0.214 [133], 0.225 [105], 0.236 [70], 0.241 [55], and 0.246 [40K]. (b) Susceptibility } \chi_0q \text{ for several hole dopings } x \geq x_H \text{ near } \bar{Q}, \text{ at } T = 10K. \text{ From bottom to top (at } \bar{Q}): x = 0.300, 0.286, 0.274, 0.261, 0.253, 0.250, 0.247, \text{ and 0.246. (c) Susceptibility } \chi_0q \text{ for several electron dopings near the } C \text{-point: for dashed lines from bottom to top: } x \text{ [ } T_N = -0.147 [1661], -0.171 [1304], \text{ and } -0.196 [853K]. \text{ Solid lines, from top to bottom: } x = -0.213 \text{ [C-point, } T_N = 199K], \text{ and, beyond C-point, } T = 100K, x = -0.223, -0.246, -0.269, \text{ and } -0.293.\]

\[\text{FIG. 2. Widths of susceptibility plateaus near } \bar{Q}, \text{ as a function of chemical potential } \mu. \text{ Data from Ref [19] (circles).}\]

Figure 2 compares the theoretical plateau widths near the $H$-point with the measured [19,1] plateau widths in YBa$_2$Cu$_3$O$_{7-\delta}$ in the normal state, along the [110]-direction. [Note that the broad feature analyzed in Ref. [19] is distinct from the resonance peak.] For low
doping ($\mu > -0.28eV$) the widths are only weakly $\omega$-dependent, and are measured in the low-$\omega$ limit. For higher doping there is a spin gap at the lowest frequencies, but since this may be a sign of a competing instability, the magnetic linewidth can be estimated at the lowest frequencies above the gap. Particularly at high doping, the agreement with the calculated plateau width is quite good: i.e., neutron scattering is measuring the plateau width, which is not indicative of the correlation length. The ‘deviations’ near half filling ($\mu = -0.2eV$) are in fact the expected SCR behavior, with the system developing long-range Néel order, $\xi \sim 1/(\Delta q) \to \infty$. In turn, the large values of $q_c$ can explain why $T_N \to 0$ at such a low hole-doping: the dotted line in Fig. 2 shows the criterion $\xi/a = 100$, which is the threshold for a finite Neel temperature in the electron-doped cuprates [22].

![Graph](image)

**FIG. 3.** (a) Normalized susceptibility as the QPT is approached, for $x = 0.1, T = 100K$. From broadest to narrowest, the susceptibility denominator is $\delta_0 = 1, 0.51, 0.27, 0.145, 0.023, 0.011, 0.0048, 0.0011,$ and 0.00027. (b) Peak width $\Delta q$ vs normalized correlation length $\xi = 1/\sqrt{\delta_0}$.

The relation between linewidth $\Delta q$ and correlation length $\xi$ can be readily demonstrated. In a self-consistent renormalization (SCR) calculation [8,15], the RPA susceptibility is renormalized to $\chi_Q = \chi_{0Q}/\delta$, with $\delta = 1 - U\chi_{0Q} + \lambda$, and $\lambda$ is a fluctuation-induced correction which keeps $\delta > 0$ for $T > 0$. For $\vec{q} = \vec{Q} + \vec{q}'$ close to $\vec{Q}$,

$$\delta \propto \xi^{-2} + q'^2. \quad (4)$$

Thus if Eq. 4 holds over a wide $q$-range, the peak width is a measure of the magnetic correlation length. In the presence of the susceptibility plateau, this is no longer the case, Fig. 3. Figure 3a shows the SCR susceptibility (normalized to its peak value) at a typical hole doping, for several values of $\delta_0 = \delta(q' = 0)$. In Fig. 3b, the resulting half-width $\Delta q$ is plotted as a function of a normalized $\xi = 1/\sqrt{\delta_0}$. It can be seen that for an extended range of $\xi$ the linewidth is unrelated to $\xi$ and measures the plateau width, as expected from Fig. 2. In the present calculation, the magnetization becomes incommensurate, causing $\Delta q$ to start decreasing again and $\to 0$ as $\xi \to \infty$. However, this is due to a giant amplification of fine structure on the plateau close to the ordering transition; in reality such fine structure may be washed out by fluctuations.

The presence of the susceptibility plateau can affect the $T$-dependence of $\xi$. In two-dimensions, fluctuations prevent a finite temperature Neel transition, but in the renormalized classical regime the susceptibility is expected to diverge exponentially as $T \to 0$, leading to a similar divergence of $\xi$. However, the susceptibility must satisfy a sum rule, and if the peak width stops decreasing (due to the plateau), this sum rule can be saturated, leading to a weaker temperature dependence for $\xi$. The fluctuation-dissipation theorem can be written as [15,23]

$$\langle M^2 \rangle = - \int \frac{d\omega}{\pi} n(\omega) \int \frac{d^2q}{(2\pi)^2} \frac{c_x + c_y}{2} Im \chi(\vec{q}, \omega) \quad (5)$$

where $\langle M^2 \rangle$ is the mean square local amplitude of nearest neighbor spin fluctuations and $n$ is the Bose function. The integral can be separated into a part over the plateau and a background term from regions far from [24] $\vec{Q} = (\pi, \pi)$, and approximately evaluated as $A/T - B = q_c^2/\delta_0$ where $q_c$ is the plateau width, or

$$\xi^2 = \frac{a}{T} - b, \quad (6)$$

which holds at low temperatures, $T \ll a/b$. Figure 4 plots Eq. 6 for the NMR derived coherence lengths [3] for optimally doped $T_c = 90K$, and underdoped $T_c = 66K$ YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO). It can be seen that both curves follow Eq. 6 at low $T$. Hence, the plateaus explain the weak divergence of the correlation length in hole doped cuprates. (Note that if there were no plateaus, $q_c \to 0$, there would be no constraint on $\xi$ – the width would decrease as the peak height increased – and the exponential divergence would be recovered, as in the electron-doped cuprates.) Finally, since $a$ is proportional to the square of the staggered magnetization, the decrease of the $a$ coefficient with doping may signal the proximity of the system to a magnetic QPT.
Thus the present model can explain the high-T properties of the pseudogap in the hole-doped cuprates. At lower temperatures the hole-doped cuprates are also susceptible to a number of competing instabilities, most notably superconductivity, but also including stripe physics. Certainly, the broad $q$-plateau is conducive to incommensurate modulations, Fig. 3. While these competing orders will complicate detailed calculations, they are unlikely to significantly modify the picture of the Mott gap collapse presented here.

In conclusion, the broad $q$-plateaus near the H-point can reconcile the neutron scattering and NMR measurements of the correlation length – NMR should see a divergence, albeit weak $\xi \sim T^{-1/2}$, as $T \to 0$. The neutron linewidth measurement should not see such a divergence, but the divergence should be reflected in neutron measurements as a $1/T$ growth of the peak intensity. A resolution of the correlation length problem along these lines would mean that the same Mott gap collapse can explain the QPTs for both electron and hole doped cuprates – indeed the disappearance of hot spots provides a natural phase boundary for QPTs. Superconductivity near an AFM or ferromagnetic QPT has recently been observed in a number of systems [25].

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