Pseudogaps in Nested Antiferromagnets

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We analyze the fluctuation corrections to magnetic ordering in the case of a 3D antiferromagnet with flat Fermi surfaces, as physically realized in the case of chromium, and find that they are insufficient to produce a quantum critical point. This implies that the critical point observed in vanadium doped chromium is due to a loss of nesting. We also derive the fermion self-energy in the paramagnetic phase and find that a pseudogap exists, though its magnitude is significantly reduced as compared to the spectral gap in the ordered state in the limit where the latter is small in comparison to the Fermi energy.

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a normal 3D antiferromagnet is the temperature dependence of the expansion coefficients. Because of this, spin fluctuations become relatively less important as the temperature is lowered, and thus fluctuation effects are less singular.

To see this, we approximate \(< M^2 >\), the fluctuating staggered moment, by its classical value \((\omega \ll T)\)

\[
< M^2 > = \frac{T}{2} \int \frac{d^3 q}{(2\pi)^3} \chi(q, 0) = \frac{Tq_c\chi_0}{4\pi^2 Ng\xi^2} \tag{5}
\]

The latter equality assumes that \(T = T_N\). If \(q_c\), the classical cut-off, is assumed to satisfy the condition \(\Gamma(q_c) = T\), then one can show that the classical value is approximately equal to the true quantum mechanical value for \(< M^2 >\). Here, \(\Gamma\) is the frequency half width of the dynamic susceptibility, which, at \(T = T_N\) is \(q_c = \sqrt{\alpha T}/\xi\).

Using this, \(< M^2 >\) reduces to

\[
< M^2 > = \frac{T^4\sqrt{\alpha}\chi_0}{4\pi^2 Ng\xi^2} \tag{6}
\]

where \(\alpha' = \alpha T\) and \(\xi' = \xi T\) are temperature independent constants. Recognizing that \(b' = bT^2\) is also a temperature independent constant, \(\chi^{-1}(0, 0)\) reduces to

\[
\chi^{-1}(0, 0) = \ln \frac{T}{T_{MF}} + \frac{b'\sqrt{\alpha}T^2\chi_0^2}{4\pi^2 N^2 g^2\xi^2} \tag{7}
\]

That is, the correction to \(T_{MF}\) goes as \(T^2\ln T\), which is less singular than the \(T^{3/2}\) correction for an ordinary 3D antiferromagnet. Our result agrees with earlier results of Hasegawa, though our derivation is more straightforward.

Since \(T_N\) can never be driven to zero for a perfectly flat Fermi surface (due to the logarithmic divergence of \(\chi_0\)), then one might think that the quantum critical point is probably not controlled by fluctuations. Rather, loss of nesting is the likely cause of the quantum critical point. This is consistent with band theory results, which find an increasing mismatch of the electron and hole octahedral surfaces as the hole doping is increased. Such warping corrections will cause the fluctuation corrections to cross over to the standard 3D antiferromagnetic result near the critical point.

Having addressed the question of fluctuations, we now turn to the question of the pseudogap. Postulating a pseudogap in the case of nesting is quite natural given the quasi-1D nature of the fermion dispersion. On the other hand, as we have seen above, despite this quasi-1D behavior, the spin fluctuation spectrum is still 3D-like, and this raises questions about how strong the pseudogap effect will be. To address this, we derive the fermionic self-energy to lowest order. We note that this is given by a convolution of an effective interaction \(V\) with the fermion Greens function, where

\[
V = g + g^2\chi + g^2\chi/(1 + g\chi_0) \simeq (3g/2)\chi/\chi_0 \tag{8}
\]

with the first term the bare interaction, the second one from summing a ladder series, and the third from summing a bubble series. The most singular part of the fermionic self-energy comes from the classical fluctuations, and can be approximated as

\[
\Sigma = \frac{3T}{2N} \int \frac{d^3 q}{(2\pi)^3} \frac{1}{A + \xi^2 q^2} \frac{1}{\omega - \epsilon_{k+q} + q} \tag{9}
\]

where \(\epsilon\) is the fermionic dispersion and \(A = \ln \frac{T}{T_{MF}} + \ln q_0 < M^2 >\). In the flat case, \(\epsilon_{k+q} = -\epsilon_k - vq_||\), where \(v\) is the Fermi velocity and \(q_0\) is normal to the flat surface. \(\Sigma\) now becomes

\[
\Sigma = \frac{3T}{8\pi N\xi^2} \int \frac{dq_||}{2\pi} \ln \left(\frac{A + \xi^2 q_||^2 + \alpha T}{\omega + \epsilon_k + vq_||}\right) \frac{1}{\xi/v} \tag{10}
\]

The integral over \(q_||\) gives \((\xi^2\chi_0^2 = \alpha T)\)

\[
\Sigma = \frac{3T}{8\pi N\xi^2} \int \frac{dq_||}{2\pi} \ln \left(\frac{A + \xi^2 q_||^2 + \alpha T}{\omega + \epsilon_k + vq_||}\right) \frac{1}{\xi/v} \tag{11}
\]

The \(q_0\) integral is convergent, and the cut-off can be taken to infinity. The result is

\[
Re\Sigma = \frac{3T}{8\pi N\xi^2} \ln \left(\frac{A + (\xi/v)^2(\omega + \epsilon_k)^2 + \alpha T}{A + (\xi/v)^2(\omega + \epsilon_k)^2}\right) \tag{12}
\]

\[
Im\Sigma = \frac{3T}{16\pi N vq_0^2} \ln \left(\frac{A + (\xi/v)^2(\omega + \epsilon_k)^2 + \alpha T}{A + (\xi/v)^2(\omega + \epsilon_k)^2}\right) \tag{13}
\]

To understand these expressions further, we assume that \(T = T_N\) (\(A=0\)) where the pseudogap effect should be most pronounced. This yields

\[
Re\Sigma = \frac{\Delta^2}{2.7T_N} \left(\frac{\pi}{2} \text{sgn}(\omega + \epsilon_k) - \tan^{-1} \frac{\omega + \epsilon_k}{2.7T_N}\right) \tag{14}
\]

\[
Im\Sigma = \frac{\Delta^2}{5.4T_N} \ln(1 + \frac{2.7T_N}{\omega + \epsilon_k}) \tag{15}
\]

where a typical energy scale \(\Delta\) is defined as

\[
\Delta^2 = 8.1T_N/(8\pi N\xi^2) \tag{16}
\]

These were obtained by noting that for the flat case, \(\alpha' = \pi/8\) and \(\xi' = v\sqrt{\xi(3)/(16\pi^2)}\), where \(\xi(3) = 1.202\). We note that \(2.7T_N\) is the natural frequency scale of the problem, and that \(\Delta\) has units of energy.

The fermion spectral function is given as

\[
A(k, \omega) = \frac{1}{\pi} \frac{Im\Sigma}{(\omega - \epsilon_k - Re\Sigma)^2 + (Im\Sigma)^2} \tag{17}
\]

In Fig. 1, we show the spectral function at the Fermi surface for two cases, \(\Delta = 2.7T_N\) and \(0.27T_N\). In the first
These conditions, \( \Re \). As (high frequency expansion) imply that \( T \) since (strong coupling limit), the spectral gap is approximately equal to \( \Delta \). In the second case (more appropriate for chromium as will be seen below), the spectral gap is significantly smaller than \( \Delta \). In Fig. 2, we plot the spectral gap obtained from half the spectral peak to peak separation in Fig. 1 versus \( \Delta \). For large \( \Delta \) (comparable to \( T_N \)), the spectral gap scales with \( \Delta \), whereas for small \( \Delta \), the spectral gap scales quadratically with \( \Delta \).

To understand these results analytically, we note that the pole of the fermion Greens function on the Fermi surface is given by the condition \( \omega - \Re \Sigma(\omega) = 0 \). Let us first assume this pole energy is of order \( 2.7T_N \). Then under these conditions, \( \Re \Sigma \) in Eq. 12 can be approximated as (high frequency expansion)

\[
\Re \Sigma_{\text{high}} = \frac{\Delta^2}{\omega}
\]  

This expression is identical to the BCS expression for the self-energy, and the pole can easily be seen to occur at an energy \( \Delta \). That is, there is a spectral gap equal to \( \Delta \), and this explains the behavior for large \( \Delta \) in Fig. 2. By noting that the density of states for the flat case, \( N \), is \( 1/(2\pi v a^2) \), then

\[
\Delta = 6.2T_N^2a/v
\]  

Since \( v/a \sim E_F \) (\( a \) is the lattice constant), this would imply that \( T_N \) must be of order the Fermi energy, \( E_F \), for this high frequency approximation to be valid. This is not satisfied for chromium, since \( T_N \ll E_F \) in that case.

In the other limit, one expands the self-energy for small \( \omega \), obtaining (low frequency expansion)

\[
\Re \Sigma_{\text{low}} = \frac{\Delta^2}{2.7T_N} \left( \frac{\pi}{2} \sgn(\omega) - \frac{\omega}{2.7T_N} \right)
\]  

The pole energy is then given approximately by \( \pi \Delta^2/(2.7T_N) \). Therefore, for the case where \( T_N \ll E_F \), the spectral gap scales as \( T_N^2/E_F^2 \).

Pure chromium exhibits a classic mean field transition as far as specific heat measurements are concerned. This implies that it is in the weak coupling limit, consistent with the small ratio of \( T_N \) to \( E_F \). We can quantify this by using parameters extracted from neutron scattering data. In Ref. 5, the authors use a form for the susceptibility identical to the one employed here

\[
\chi(q;\omega) = \frac{\chi Q}{1 + q^2/k_0^2 - i\omega/\omega_{sf}}
\]  

By comparing to our expressions, we see that \( k_0^2 = A/\xi^2 \) and \( \omega_{sf} = A/\alpha \). Using this, the prefactor outside the parenthesis in Eq. 12 becomes \( 6T^2\kappa_0 a^2/(\pi \omega_{sf}) \) and the quantities dividing \( (\omega + \epsilon_k) \) in the tan\(^{-1}\) functions in Eq. 12 are \( 2.7\sqrt{\omega_{sf}T} \) and \( 2.7\sqrt{\omega_{sf}T + T^2} \) respectively. For Cr-V 5\%, \( \kappa_0 = 0.11A^{-1} \) and \( \omega_{sf} = 88meV \) for \( T=12K \) (\( a = 2.88\AA \)). We plot the resulting self-energy from Eqs. 12 and 13 in Fig. 3. Though the \( \omega \) structure of \( \Sigma \) is reasonable (looking like a damped version of Eq. 18 with a maximum in \( \Re \Sigma \) at 26 meV), the value of \( \Sigma \) itself (nanovolts) is far too small to cause a pseudogap.

Based on this, we expect only weak pseudogap effects, even in the magnetically ordered part of the phase diagram. We note that our derivation of the self-energy assumes that the spin structure factor is quasi-static, a
property of the renormalized classical regime. That is, we would not necessarily expect pseudogap effects in the quantum critical regime. This conclusion is bolstered by our evaluation of quantum corrections to the self-energy, which we do not find to be singular.

On the other hand, in the flat model, $T_{MF}$ never vanishes as a function of doping. It is a loss of nesting which leads to the quantum critical point. Therefore, it is possible that a pseudogap exists for all dopings which satisfy $T_N < T < T_{MF}$. This is illustrated in Fig. 4. Still, we expect that although pseudogap effects are possible near the quantum critical point of vanadium doped chromium, they are likely to be weak. They could perhaps be best searched for by photoemission, which sees the spectral gap quite easily in pure chromium.

This begs the question of what is responsible for the strong temperature dependence of the Hall number observed by Yeh et al. which occurs even for dopings far beyond the quantum critical point. The Hall number is temperature dependent in transition metals such as Cu, which can be attributed to the temperature dependence of the electron-phonon scattering rate. For the vanadium doped chromium case, this would be consistent with the $T^3$ dependence of the resistivity, which points to the prevalence of electron-phonon effects. Moreover, the experimental Hall number is in excess of the uniaxial magnetic band theory value for temperatures above 150 K, again indicating the presence of an inelastic scattering contribution (which could be of magnetic origin as well). Calculation of the $T$ dependence of the Hall number, though, is technically challenging since it involves going beyond the Boltzmann approximation, so we do not consider this further here.

On the other hand, our results do indicate a large pseudogap in the strong coupling limit. We note that there are examples of quantum critical points where Fermi liquid theory is known to break down, and where nesting may be playing an important role, such as in the case of the bilayer ruthenate $Sr_3Ru_2O_7$. Moreover, magnetic incommensurability is seen in most quantum critical heavy fermion systems, such as Au doped $CeCu_2$. It is possible that the results presented here, which were derived for the case where a strong Fermi surface rearrangement takes place at the quantum critical point, are quite relevant for these systems. Based on this, we suggest that pseudogap effects be searched for in heavy fermion quantum critical systems.

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FIG. 4: Illustration of a possible scenario for the pseudogap phase in the V doped Cr system. $T_{MF}$ is the mean field temperature for a flat Fermi surface, $T_N$ the actual transition temperature which is suppressed by loss of nesting (warping of the Fermi surface). The pseudogap, if it exists, should be confined to the region between these two temperatures.
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