Quantum Criticality in Quasi-Two Dimensional Itinerant Antiferromagnets

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Abstract

Quasi-two dimensional itinerant fermions in the Anti-Ferro-Magnetic (AFM) quantum-critical region of their phase diagram, such as in the Fe-based superconductors or in some of the heavy-fermion compounds, exhibit a resistivity varying linearly with temperature and a contribution to specific heat or thermopower proportional to $T \ln T$. It is shown here that a generic model of itinerant AFM can be canonically transformed such that its critical fluctuations around the AFM-vector $Q$ can be obtained from the fluctuations in the long wave-length limit of a dissipative quantum XY model. The fluctuations of the dissipative quantum XY model in 2D have been evaluated recently and in a large regime of parameters, they are determined, not by renormalized spin-fluctuations but by topological excitations. In this regime, the fluctuations are separable in their spatial and temporal dependence and have a dynamical critical exponent $z = \infty$. The time dependence gives $\omega/T$-scaling at criticality. The observed resistivity and entropy then follow directly. Several predictions to test the theory are also given.

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The problem of AFM quantum-critical fluctuations in itinerant fermions has been studied extensively by simple extensions of the theory of classical critical fluctuations. This idea has been proven by S-S. Lee to be uncontrolled in two dimensions. (The theory is controlled for AFM fluctuations in 3D; the measured fluctuation spectra and the properties calculated from it agree well with the experiments also.) Lee has also proposed methods for expansion about 3 dimensions for a problem with a 1 dimensional fermi-surface, as well as a different expansion about a line in the spatial dimension - Fermi surface dimension plane. Other procedures have also been proposed, each yielding different results. While these methods (at least to linear order in the expansion parameter) appear controlled, they do not give the observed singular-Fermi-liquid properties. All these are theories of criticality due to renormalized spin-waves. Other semi-phenomenological ideas, with varying degrees of justification have also been proposed. Imaginative ideas, from our cousins in the string theory family, have also been advanced. At least so far, there is no sense of a symmetry breaking in such theories, which appears invariably in experiments astride the region of singular Fermi-liquid properties.

The linear in $T$ resistivity and the $T \log T$ specific heat and thermopower in the AFM quantum-critical region in 2D are reminiscent of the properties in the similar region in hole-doped cuprate superconductors. Such properties were shown to follow if the quantum-critical fluctuations are scale-invariant in their time-dependence but nearly local in their spatial dependence. The direct measurement of such fluctuations is very difficult but at least in one case in a 2D AFM, such fluctuations have shown up directly by inelastic neutron scattering measurements. They are also directly observed at long wave-lengths in hole-doped cuprates by Raman scattering and deduced by inversion of the angle-resolved photoemission measurements at shorter wave-length. The quantum critical point associated with the singular Fermi-liquid properties in the hole-doped cuprates is obviously not of the AFM order, which goes to 0 at dopings far from the regime of such anomalous metallic properties. A quite different order parameter, which does not break translational symmetry, was predicted for which there is direct experimental evidence in many different kinds of experiments. The fluctuations of such an order parameter can be mapped to a dissipative quantum XY model with four-fold anisotropy.

In the classical limit, the XY model does not have a phase transition in the general class theories with critical fluctuations of the renormalized spin-wave type. Instead, proliferation
of vortices determine the critical fluctuations. Recently, a solution to the dissipative quantum XY model [24] has been found and checked by quantum Monte-Carlo calculations [30]. In this model, \textit{over a range of parameters}, there is a quantum transition whose fluctuations are determined (primarily) by proliferation of topological excitations of a different kind, termed “warps”, which are instantons of monopoles surrounded by anti-monopoles (or vice-versa) with net-charge zero. In that regime, the absorptive part of the fluctuations at the critical point $\chi''(q, \omega)$ are separable in $q$ and $\omega$, with a dynamical critical exponent $z \to \infty$ and with $\omega/T$ scaling at the critical point. Fermions acquire a marginal self-energy through coupling to such fluctuations which leads to a resistivity proportional to $T$ and a contribution to specific heat proportional to $T \log T$.

The observation of similar singular Fermi-liquid properties in the AFM quantum-critical region suggests an investigation to see if AFM fluctuations are also described by a similar model. A generic model of itinerant fermions, which has an incommensurate transverse antiferromagnetic quantum critical point, is shown here to transform canonically to a model with a superconductive quantum-critical point. The quantum critical fluctuations of the 2D-superconducting model are described by a dissipative quantum XY model. The fluctuations of the AFM model near the AFM wave-vector $Q$ can then be obtained from the known fluctuations of the XY model in the long wave-length limit. The same is true for the longitudinal incommensurate fluctuations. It is axiomatic that the exchange of the same fluctuations which determine the normal state anomalies above $T_c$ also are responsible for Cooper pairing below $T_c$.

**Canonical Transformation:** Consider the following Hamiltonian for fermions

$$H = \sum_{<ij>, \sigma = \uparrow, \downarrow} t_{ij} a_{i, \sigma}^\dagger a_{j, \sigma} + H.C. + U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) + I_z (S_i^z)^2 - \mu n_i + h S_i^z. \quad (1)$$

$<ij>$ sums over nearest neighbors on a bi-partite two dimensional lattice. $U > 0$ so that for large enough $U/t$, a Mott insulating state is expected with AFM correlations or commensurate order at half-filling when the chemical potential $\mu = 0$. Beyond some deviation from half-filling a metallic state is expected, with AFM correlations at low enough temperatures. These correlations are in general peaked at the incommensurate vectors $Q = (Q_0 + q_0)$ with $Q_0 \cdot R_0 = \pi$, where $R_0$’s are the nearest neighbor vectors and $q_0$ depends on the deviation from half-filling. A single ion anisotropy term with coefficient $I_z > 0$ ensures that the AFM correlations are stronger for planar spin-correlations, i.e. spin in the xy plane, and $I_z < 0$ en-
sures the same for uni-axial correlations, i.e. spins along the z-axis. Only $h = 0$ is considered in this paper but finite $h$ may be useful in further work. No magnetic order is expected for large enough deviation from half-filling. So, there is a quantum critical point as a function of doping. The Hamiltonian of Eq. (1) may be paradigmatic of a general class of models with AFM correlations, but specific details of the Hamiltonian for the actual experimental systems need to be examined to be certain.

The (canonical) transformations [31],

\[
a_i, \uparrow \rightarrow e^{i\phi_i} a_i, \uparrow; \quad a_i, \downarrow \rightarrow a_i, \downarrow e^{iQ_0.R_i+\mu_i} \quad (2)
\]

with

\[
\phi_i = -\frac{1}{2} q_0 \cdot R_i,
\]

transform the Hamiltonian of (1) to

\[
\tilde{H} = -\tilde{U} \sum_i (\tilde{n}_{i\uparrow} - 1/2)(\tilde{n}_{i\downarrow} - 1/2) - \sum_i (\tilde{h} \tilde{S}_i^z + \tilde{\mu} n_i)
\]

\[
+ \sum_{\langle ij\rangle, (\sigma=\pm)} \tilde{t}_{ij} e^{-i\alpha(\phi_i - \phi_j)} \tilde{a}_{i,\sigma}^\dagger \tilde{a}_{j,\sigma} + H.C.
\]

Here $\alpha = \pm$ for $\sigma = \uparrow, \downarrow$, respectively, and

\[
\tilde{t} = t; \quad \tilde{U} = U - 2I_z, \quad \tilde{h} = \mu, \quad \tilde{\mu} = h.
\]

The transformed Hamiltonian is a model with on-site attractive interactions, a Zeeman field related to the deviation of the original model from half-filling and a spin-dependent phase factor $\alpha(\phi_i - \phi_j)$, $\alpha = (\pm 1)$ for $\sigma = (\uparrow, \downarrow)$, in the link $\langle i, j \rangle$ related to the incommensurate vector $q_0$ or the deviation from half-filling. As a result, the Fermi-surface of up and down spins are shifted in opposite directions by $\pm q_0/2$; thus $\alpha(\phi_i - \phi_j)$ is a spin-orbit field. The model has a superconducting ground state for small enough $\tilde{h}$ for $I_z > 0$ and a charge density wave for $I_z < 0$. Corresponding to a quantum critical point in model (1) for $\mu = \mu_c$ with other parameters fixed, there should be a quantum critical point in model (3) for $\tilde{h} = \tilde{h}_c$, as will be clearer below.

**Relation of Spin-Correlations to Superconducting Correlations:** With the canonical transformations, the spin-raising/lowering operator in $H$ are related to the Cooper pair
creation/annihilation operator in $\tilde{H}$, and $S^z_i$ is related to the density operator,

$$S^+_i \rightarrow e^{iQ \cdot R_i} \Psi^+_i, \quad S^-_i \rightarrow e^{-iQ \cdot R_i} \Psi^-_i; \quad S^z_i \rightarrow \tilde{n}_i - 1$$

Define the response functions for two operators $A$ and $B$ for a Hamiltonian $H$ by

$$\chi^H_{(AB)}(i, j; t - t') = -i\theta(t - t') \langle [A_i(t), B_j(t')] \rangle_H$$

Consider $I_z < 0$ so that the incommensurate longitudinal fluctuations of the order parameter, i.e. $\chi^H(x_i, S^z_i)(Q + q, \omega)$ are important. They map to incommensurate charge density fluctuations at the same momenta. Such fluctuations are described by the fluctuations of an XY model [32]. This follows from the fact that an incommensurate wave of charge (or $z$-component of magnetization) has in general an order parameter $A \sin(Q \cdot R_i + \phi)$, where $A$ is the amplitude. Any spatially uniform value of $\phi$ has the same energy, just as the phase-variable in a superfluid. Spatial variations in $\phi$ cost an energy $\propto \rho_s \parallel |\nabla_\parallel \phi|^2 + \rho_s \perp |\nabla_\perp \phi|^2$, where $\nabla_\parallel, \perp$ refer to variations parallel and perpendicular to $Q$. The edge dislocations in the incommensurate wave in 2D correspond to vortices in 2D superfluids. In complete analogy, the longitudinal incommensurate AFM fluctuations are also modeled by an XY model. For such fluctuations, the mapping made above is in fact unnecessary. It is generally hard to find two-dimensional charge density fluctuations because the charge-coupling between layers even in materials like $TaSe_2$ is large and so the special properties of the 2D-XY model are not invoked [32] for them. But in some Antiferromagnets, there is clear evidence [1, 19] for two-dimensional fluctuations in the quantum-critical regime.

Consider $I_z > 0$ so that the important fluctuations are transverse. These are the relevant fluctuations for the Fe-based compounds and for some heavy Fermions. The transverse spin-response function in the model of Eq. (1) is identical to the Cooper pair response function for the model of Eq. (3):

$$\chi^H_{(S^+ S^-)}(Q + q, \omega) = \chi^H_{(\Psi^+ \Psi)}(q, \omega).$$

The transverse AFM correlation at small $q$ around $Q$ in model (1) may therefore be obtained from the superconducting correlations at $q$ in model (3).

The Zeeman and spin-orbit fields in model (3) make the Fermi-sphere for one spin bigger than the other and they are displaced with respect to each other by $2q_0$. The spin-orbit as
well as the Zeeman field is taken into account in the one-particle spectra by the condition of equal chemical potential, by introducing spin-dependent Fermi-vectors

\[ \mathbf{p}_F = \mathbf{p}_F^0 + (\delta \mathbf{p}_F) \sigma_3; \quad \delta \mathbf{p}_F \equiv q_0 \sigma_3 + \frac{g \mu_B \tilde{h}}{v_F} \]

for \( q_0 / p_F^0 \ll 1 \). Time-reversal symmetry is preserved by the shift \( q_0 \sigma_3 \) while it is broken by the shift proportional to \( \tilde{h} \).

A uniform Zeeman field depresses superconductivity. The depression of the usual BCS superconductivity with Cooper pairs of 0 total momentum is due to the displacement in momentum of the up and down Fermi-surfaces so that the infra-red logarithmic singularity for any attractive interaction is cut-off due to the mass term \( g \mu_B \tilde{h} \). In the weak-coupling approximation for attractions over an energy-range \( \omega_c \), there is no transition down to \( T \to 0 \) if

\[ g \mu_B |\tilde{h}| \gtrsim \omega_c e^{-1/\lambda}, \]

where \( \lambda \) is the weak-coupling constant. We assume that the critical point exists more generally. Correspondingly, a AFM critical point exists for the model \( \Pi \).

Near the phase transitions of model \( \Pi \), we may, using techniques such as the Hubbard-Stratonovich transformation, write it in terms of a Hamiltonian for its collective fluctuations \( H_{coll} \), for the Fermions \( H_F \) and for the interaction between the fermions and the collective fluctuations \( H_{int} \).

\[ H = H_F + H_{coll} + H_{int}. \]

The model for collective critical fluctuations in a superconductor may be expressed in terms of the pair-field operators \( \Psi \), which are products of a pair of time-reversed fermions. In 2D, the amplitude fluctuations are irrelevant and the phase fluctuations determine the critical properties. The critical fluctuations are then those for an XY model for a field \( \Psi(r, \tau) \equiv |\Psi| e^{i \theta(r, \tau)} \), with \( |\Psi| \) weakly enough varying that it may be kept fixed. Then the action for \( H_{coll} \) is expressed in terms of the phase \( \theta_i(\tau) \) on a lattice of sites \( R_i \)

\[ S_{coll} = \int_0^\beta d\tau \sum_i \frac{K_T}{2} \left( \frac{d \theta_i(\tau)}{d\tau} \right)^2 - K \sum_j \cos (\theta_i(\tau) - \theta_j(\tau)) - h_4 \cos 4 \theta_i(\tau) + S_{diss}. \]

\( j(i) \) are neighbors of \( i \). The relationship of the parameters in \( 12 \) and \( \Pi \) is very hard to derive microscopically, except for weak-coupling or for strong coupling, \( |U|/t << 1 \), or \( >> 1 \),
respectively. In general terms, $K$ is related to the superfluid density which decreases as the Zeeman field $\tilde{h}$ increases, and $K_\tau$ to the inverse compressibility. $h_4$ reflects the anisotropy of the kinetic energy parameter $t_{ij}$. The relations are not necessary for studying the critical properties. $S_{\text{diss}}$ is the dissipative term in the action. In the solution of the problem of quantum-criticality of the XY model, the nature of dissipation has been chosen to be that of the Caldeira-Leggett form [33], which is due to the decay of collective current $\mathbf{J}$ to incoherent fermion current. It is simpler to write $S_{\text{diss}}$ in Fourier transform space. Using $\mathbf{J} = \nabla \theta$, the dissipation term for small $\mathbf{q}$ is,

$$S_{\text{diss}} = \sum_{\mathbf{q}, \omega} i \alpha |\omega| q^2 |\theta(q, \omega)|^2,$$

where $\alpha$ is then proportional to inverse of the normal state resistance [35] as will be discussed more below. For the AFM quantum-critical problem, the form of dissipation chosen, is due to the decay of collective transverse AFM fluctuations to the incoherent $S = 1$ particle-hole fluctuations:

$$i \tilde{\alpha} |\omega| (S^+ S^-)(\mathbf{Q} + \mathbf{q}, \omega).$$

(14)

The transformations on (13) lead to this dissipation for the AFM problem or vice-versa. To see this, we note that the current operator $J_{ij} = (\Psi_i^+ \Psi_j - \Psi_j^+ \Psi_i)$ transforms to the imaginary part of the operator $S_i^+ S_j^-$. On Fourier transformation and taking $|\mathbf{Q} + \mathbf{q}|^2 \approx |\mathbf{Q}|^2$, which may be replaced by a constant, leads to (13).

The dissipative quantum 2D-XY model has a rich phase diagram [30, 36]. For large $K_\tau$ compared to $\alpha$, the transition at $T \to 0$ is of the 3D-XY class, the dynamical critical exponent $z$ being 1. For $K_\tau$ small compared to $\alpha$, the phase diagram is given in Fig. (2) of Ref.(30) and Fig. (1) of Ref. (36). The disordered phase has a transition with Kosterlitz-Thouless criticality for $K$ large compared to $\alpha$ to a quasi-ordered phase in which the temporal correlations do not change from those of the disordered phase and are $\propto \tau^{-2}$. This in turn has a transition to an ordered phase with increase in $\alpha$ with critical corelations $\propto \tau^{-1}$. There is also a direct transition from the disordered phase to the ordered phase for larger $\alpha$ compared to $K$. The ordered phase, irrespective of the route at which it is arrived at has a finite order parameter in the limit of large spatial size and has the low frequency excitations of the 3D-XY phase.
We focus here on the quantum critical response at the disordered to the ordered phase transition line in the $K - \alpha$ plane, as it seems the most relevant to the experiments noted earlier. This transition occurs along a line in the $p_c(K, \alpha) = K_c(\alpha_c)$ plane. Given the relationship and the results in Ref. (30, 24), the correlation function $\chi_{H}^{S+S_{-}}(r, \tau)$ for the AFM is obtained from $\chi_{H}^{S+S_{-}} \propto e^{i\theta(r, \tau)}e^{-i\theta(0,0)}$ for the XY model.

$$\chi_{S+S_{-}}^{H}(r, \tau) = \chi_0 \frac{1}{\tau}e^{-\sqrt{\tau/\xi}} \ln \left(\frac{r_c}{\tau}\right)e^{-r/\xi}e^{iQ \cdot r}, \quad (15)$$

$$\xi_\tau = \tau_c e^{\sqrt{p_c-p}}; \quad \xi_r/r_c \approx \ln(\xi_\tau/\tau_c). \quad (16)$$

Here $\tau$ is the imaginary time, periodic in $1/(2\pi k_B T)$, which has a lower cut-off $i\tau_c \approx (KK_\tau)^{-1/2}$. There are several remarkable features in these results. The correlation function is separable in space and time; the spatial correlation length diverges only logarithmically with the temporal correlation showing, i.e., the correlations have an effective dynamical exponent $z \to \infty$; the temporal correlation at the critical point $p \to p_c$ is $1/\tau$, which gives an absorptive part as a function of $\omega$ and $T \propto \tanh(\omega/2T)$, with an upper cut-off of order $\omega_c = (-i\tau_c)^{-1}$. This simple scaling, with no anomalous dimensions, persists over an exponentially large range in the $(T, (p - p_c))$ plane.

It is hard to analytically Fourier transform to get the $\omega, T$ dependence away from criticality. If one changes the exponential of the square root in (15) to a simple exponential, the representation for the absorptive part of the correlation function in $\omega$ and $q$ is

$$Im \chi(\omega, q) \approx -\chi_0 \tanh \left(\frac{\omega}{(2k_B T)^2 + (\xi_\omega)^2}\right) F_c(\omega/\omega_c) \frac{q_0}{|Q + q_0|^2 + \xi_r^2}, \quad (17)$$

$$\xi_\omega = \omega_c e^{-\sqrt{p_c-p}}. \quad (18)$$

$F_c(\omega/\omega_c)$ is a cut-off function, $F_c(0) = 1, \lim(\omega \gg \omega_c)F_c(\omega/\omega_c) = 0$.

**Experimental Consequences:** The results obtained in this paper are for a very simple model of itinerant Anti-ferromagnetism. In heavy fermions, as well as in the Fe-based compounds, the multi-band nature of the problem and the diverse nature of the renormalization for the different orbitals with different interactions is essential for a complete description. One may ask however if universal features may govern the phenomena so that the present treatment gives some essential results. The most direct test of the applicability of the theory is of-course a measurement of $\chi(\omega, q)$.

There is only one measurement of the fluctuation spectrum at several $(q, \omega, T)$ near an AFM quantum-critical point in a quasi-2D system - CeCu$_6-x$Au$_x$. Within the limited
accuracy of the data, taken by the essential but difficult technique of inelastic neutron
scattering, the results are consistent with Eq. \([17][20]\), although they have also been fitted
to a different form earlier \([19]\).

Earlier, one relied on the assumed non-singular nature of the spatial correlations to predict
that the single-particle self-energy of the fermions, due to the interaction term \(H_{\text{int}}\) is

\[
\Sigma(k, \omega) = g^2 \chi_0 N(0) \left( \omega \ln \left( \frac{\omega_c}{x} \right) - i \frac{\pi}{2} x \right),
\]

for \(x \approx \max(|\omega|, T) \lesssim \omega_c\). \(N(0)\) is the density of states near the Fermi-energy and \(g\) is the
coupling energy in \(H_{\text{int}}\). For \(x \gtrsim \omega_c\), the imaginary part goes to a constant. The Monte-
Carlo calculations have now found that the spatial correlation length also diverges, albeit
\(z = \infty\). It is easy to show using the large \(z\) and the separability in \(q\) and \(\omega\) of the fluctuations
that the result for the self-energy does not change from that given by \([19]\).

Both the marginal fermi-liquid energy/temperature dependence and the momentum-
independence in Eq. \([19]\) are important prediction which could be tested in the Fe-based
high temperature superconductors. In such multi-band compounds, the coefficient of pro-
portionality \(g^2 N(0)\) may vary between bands and be ambiguous in regions where the bands
come close together. So, it is best to measure the self-energy different angles across the
various fermi-surfaces for low energies. Note that the results are quite unlike the usual
theory, which has anomalous self-energies only at the ”hot-points”, i.e. those where the
fermi-surface spans \(Q\). The results for the self-energy are much stronger than the linearity
in the temperature dependence of the resistivity, which follows from it. As mentioned above,
the linear in \(T\) resistivity and a \(T \ln T\) contribution to entropy in the quantum fluctuation
regime of quasi-2D antiferromagnets appear to be universally observed. The latter immedi-
ately follows from the marginal fermi-liquid self-energy. An indication that the prediction
about the \(q\)-independence of the self-energy may come true is that the coefficient of propor-
tionality of the \(T \ln T\) contribution to the entropy indicates that the entire fermi-surface is
”hot”. Beside the linearity in \(T\) of the resistivity, the change in resistivity in a magnetic
field of the form \(f(|B|/T)\), as observed \([17]\), is given by the theory because the Hamiltonian
(Energy) changes linearly with \(|H|\) thought he Zeeman term. It also follows from \([15]\) that
the nuclear relaxation rate (for nuclei at which, for reasons of symmetry, the projection of
the fluctuation spectra is not zero) should have a nearly constant contribution as a function
of temperature. Given a relaxation of momentum conservation, due to impurities, the Ra-
man spectra should exhibit a continuum due to (15). Some evidence [34] for this already exists for experiments in the Fe-compounds.

Consistency of Theory: To be assured of the consistency of the theory, it is important to check that the singular quantum-critical fluctuations, Eqs. (15, 17), do not undergo further singular corrections because of the logarithmic renormalization of the single-particle spectra. Since the fermions entered the theory of the collective fluctuations through the dissipation of the collective currents into incoherent fermions currents, Eq. (13), this is the same as inquiring if the damping parameter $\alpha$ of the collective degrees of freedom in the XY model is regular at low energies. If it is singular, the theory is not consistent.

Since, following Caldeira-Leggett, Eqs. (13) are derived by eliminating the coupling of the collective currents to fermion currents, it follows that $|\omega|\alpha = |\omega|Im < jj >_F (q = 0, \omega) = \sigma(\omega)$. $< jj >_F (q = 0, \omega)$ is the fermion current-current correlation in the long wave-length limit, so that $\sigma(\omega)$ is their conductivity. To test the consistency of the theory, we need to look at only the limit $\omega \to 0$, of $\sigma(0) = \rho^{-1}$, where $\rho$ is the resistivity. There are two (additive) leading contributions to $\rho(\omega, T)$ given the derived form of (15), the impurity contribution $\rho_{\text{imp}}$ and the contribution $\propto \max(\omega, T)$. For momentum independent fluctuations, there is no (singular) renormalization of either of these contributions [37]. This follows from the fact that the compressibility is un-renormalized for momentum-independent fluctuations. In any event, the frequency and temperature dependent contribution vanishes as the critical point is approached, as it is loss-less. The theory is consistent. This also leads to the prediction that the quantum-critical point is moved to higher values of the parameter $K$ as the impurity resistivity in the sample is decreased, i.e. $\alpha$ increased.

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Such canonical transformation have been extensively used at half-filling in the past. The transformation introduced here away from half-filling which introduces a spin-orbit field has is new. Some of the references to earlier work are: Matsubara, T., and H. Matsuda, 1956, Prog. Theor. Phys. 16, 569; K. Dichtel, R. J. Jelitto, and H. Koppe, Z. Phys. 246, 248 (1971); Shiba, H., 1972, Prog. Theor. Phys. 48, 2171; Liu, K. S., and M. E. Fisher, 1973, J. Low Temp. Phys. 10, 655; Micnas et al., Phys. Rev. B 37, 9410 (1988); C.M. Varma, Phys. Rev. Lett., 61, 2713 (1988).