Fluctuation-induced non-Fermi-liquid behavior near a quantum phase transition in itinerant electron systems

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The signature for a non-Fermi-liquid behavior near a quantum phase transition has been observed in thermal and transport properties of many metallic systems at low temperatures. In the present work we consider specific examples of an itinerant ferromagnet as well as an antiferromagnet in the limit of vanishing transition temperature. The temperature variation of spin susceptibility, electrical resistivity, specific heat, and NMR relaxation rates at low temperatures is calculated in the limit of infinite exchange enhancement within the framework of a self-consistent spin fluctuation theory. The resulting non-Fermi-liquid behavior is due to the presence of the low-lying critically damped spin fluctuations in these systems. The theory presented here gives the leading low-temperature behavior, as it turns out that the fluctuation correlation term is always smaller than the mean fluctuation field term in three as well as in two space dimensions. A comparison with illustrative experimental results of these properties in some typical systems has been done. Finally, we make some remarks on the effect of disorder in these systems. [S0163-1829(98)08703-7]

I. INTRODUCTION

The description of the electronic contribution to the low-temperature behavior of metals in terms of Fermi liquids has been highly successful.[1] The low-lying excitations of the Fermi liquid manifest themselves in various thermodynamic and transport properties, such as the specific heat varying as $C_v=\gamma T$, a temperature-independent (Pauli) spin susceptibility $\chi=2\mu_B N(\epsilon_F)$, where $N(\epsilon_F)$ is the density of states at the Fermi energy, a temperature-dependent electrical resistivity varying as $\Delta\rho\sim AT^2$, and a linearly temperature-dependent NMR relaxation rate $T_1^{-1}\sim T$ (Korringa). The values of coefficients such as γ and A, however, are material dependent. For some transition metals these are about one order of magnitude larger than in normal metals and in some compounds containing a large concentration of rare-earth or actinide elements such as Ce, Yb, or U these values are about 1000 times larger, particularly the value of γ and the zero-temperature susceptibility.[2]

The normal Fermi-liquid behavior as mentioned above is understood within the Landau phenomenological theory, where the effect of an interaction in a Fermi system is expressed in terms of a few parameters that renormalize the physical quantities with respect to their free-Fermi-gas values. For example, the modifications in specific heat, spin susceptibility, and isothermal compressibility are given by $C_v/C_v^0=m^*/m=1+(F_1^s/3)$, $\chi/\chi^0=(m^*/m)/(1+F_0^a)$, and $\kappa_s/\kappa_s^0=(m^*/m)/(1+F_0^s)$, respectively. (The superscript 0 denotes the free-Fermi-gas values and other notations are standard.[1]) The basic reason for the success of the Landau theory is the largeness of quasiparticle lifetime near the Fermi surface, i.e., $\tau^{-1}\sim|\epsilon|^2\ll\epsilon$, where $\epsilon=(E-E_F)/E_F$. From these relations it is clear that for certain values of the Landau parameters (i.e., F_0 and F_1), the corresponding quantities become very large, which in turn may indicate the neighborhood of a certain phase transition. For example, $F_0^a\to-1$ implies magnetic instability and $F_0^s\to\infty$ a condensation. In the present work we consider the Fermi system in the vicinity of such a transition and seek an explanation of the non-Fermi-liquid behavior of certain substances in this regime.[3] It seems as though the Fermi-liquid theory gives an indication of the incoming electronic phase transition as the coupling constant changes, but it does not consider the effect of incipient fluctuations in a self-consistent manner.

There are many examples of electronic phase transitions where the coupling constant tunes the transition. These are known as the quantum phase transition. For example, $1-UN(\epsilon_F)>0$ gives instability towards ferromagnetism, $1-U\chi(Q)>0$ gives antiferromagnetic instability corresponding to a wave vector Q, and $n^{1/3}a_H>0.26$ describes the metal-insulator transition due to Coulomb correlation as suggested by Mott. These are essentially zero-temperature transitions; however, in general, $T_c\ll T_F$, where T_F is the Fermi temperature of the system. In contrast, the classical phase transition occurs at finite temperature and is described by the balance in the energy needed (loss) to create disorder with a gain in entropy due to disorder such that the free energy $F=U-TS$ is reduced. One more difference is that the statics and dynamics become correlated in quantum phase transition.[4,5] This is principally due to the noncommutativity of various terms in the Hamiltonian. For example, consider the Hubbard model

$$H=\sum_k \epsilon_k n_k+U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{1}$$

for correlated electrons. Here the kinetic energy and the U terms do not commute. (Otherwise the model will be trivial to solve.) Technically, this means that one should introduce ''time'' and the Feynman time ordering in the functional integral for the partition function. The order-parameter field becomes ''time dependent.'' The time variable thus acts as an extra dimension. This leads to a change in the critical behavior.[4] At first glance it seems that the critical behavior would be the same as that of a $(D+1)$-dimensional classical

system. However, detailed analysis shows that the critical behavior (or the upper critical dimension) depends on the dispersion and damping of the order-parameter fluctuations. The reason is that the spin susceptibility for a ferromagnet above T_c is given by[6]

$$\chi(q,\omega^+)\approx \frac{N(\epsilon_F)}{[1-UN(\epsilon_F)]+\delta q^2-\dfrac{i\pi\gamma\omega}{2q}}. \tag{2}$$

For the free-electron gas $\gamma=1/2$ and $\delta=1/12$. At T_c, $1-UN(\epsilon_F)\to 0$ and therefore $\omega\approx q^3$ gives the order-parameter dispersion. In the case of antiferromagnetism, the staggered spin susceptibility is given by[7]

$$\chi(Q+q,\omega^+)\approx \frac{\chi^0(Q)}{1-U\chi^0(Q)+\delta q^2-i\gamma\omega}. \tag{3}$$

In this case, $\omega\approx q^2$ at the critical point. A dynamical exponent z is introduced, which reflects the change in the static critical behavior. In particular the scaling dimension of the quartic interaction is given by $\epsilon=4-(d+z)$ with $z=3$ for ferromagnets and $z=2$ for antiferromagnets.[4] In field theory $z=1$ since ω and q are linearly related and have the same scaling form. At present the application of the renormalization group to quantum critical phenomena, in particular the correlation of the static and dynamic behavior, is a subject of intense activity. We refer the reader to Refs. 4, 5, 8, and 9 for detailed discussion. To summarize, the vicinity to the phase transition point and the fermionic nature of a correlated electronic system undergoing a phase transition change the nature of the phase transition itself as well as the Fermi-liquid behavior expected in this system. The reason for this behavior is the smallness of the transition temperature T_c compared to the Fermi temperature T_F. This aspect is revealed more clearly as $T_c\to 0$.

To calculate various physical properties, we take specific examples of ferromagnetic and antiferromagnetic transitions in an itinerant electron system in two as well as three dimensions in the limit of vanishing transition temperature near the transition temperature. These two examples represent two different types of quantum critical behavior. The basic reason is that in the ferromagnet the order parameter is a conserved quantity, while in the antiferromagnet it is not. This difference is reflected in the dispersion of their respective order parameter fluctuations as shown in Eqs. (2) and (3). The microscopic calculation is done within the self-consistent spin fluctuation theory developed earlier by Ramakrishnan and one of us[10–13] among many others.[14–16] For details of the spin fluctuation theory we refer the reader to the monograph by Moriya.[17] A brief review is given in Ref. 18. We first briefly review the spin fluctuation theory and then write expressions for spin susceptibility, resistivity, specific heat, and nuclear magnetic relaxation rate. Similar expressions for staggered susceptibility and other quantities in antiferromagnets are also written. These quantities are then calculated in the limit of large exchange enhancement [i.e., in the limit of $\chi_P\chi(T=0)^{-1}\equiv\alpha(0)\to 0$]. Though $T_c=0$, fluctuation effects are observable well above T_c. The temperature dependence need not be Fermi-liquid-like because of the low-lying fluctuation (bosonic) degrees of freedom.

II. SPIN FLUCTUATION THEORY

The basic motivation for constructing the spin fluctuation theory is the largeness of the susceptibility (Stoner) enhancement factor $1/\alpha(0)$. In such a case a highly paramagnetic system at low temperature can be considered to be in the vicinity of a magnetic transition. The temperature variation of various physical quantities is therefore governed by transverse and longitudinal spin fluctuations. Even though the order parameter vanishes above the transition, the effect of fluctuations is observable well above the transition. There are many equivalent formulations of this idea available.[17,18] We briefly summarize our approach and then compile results on some physical properties.

Consider the Landau expansion for the free energy $F(M,T)$ in powers of the order parameter M, viz.,

$$F(M,T)=F(0,T)+\frac{1}{2}A(T)M^2+\frac{1}{4}BM^4-HM, \tag{4}$$

where H is the field conjugate to M. The temperature dependence of various quantities in this theory arises due to $A(T)$ and B. For example, the spin susceptibility for the paramagnetic phase is given by

$$\chi^{-1}(T)=A(T). \tag{5}$$

[$A(T)$ and $\alpha(T)$ have qualitatively the same temperature dependence and differ only by some numerical factors, e.g., $A(T)=\alpha(T)/2N(\epsilon_F)$ for ferromagnets, which we ignore and identify $A(T)$ with $\alpha(T)$ now onward.] Similarly, the magnetization in the ordered phase is

$$M^2(T)=-\frac{\alpha(T)}{B} \tag{6}$$

and the equation of state is given by

$$\frac{H}{M}=\alpha(T)+BM^2. \tag{7}$$

The expansion coefficients $\alpha(T)$ and B have been calculated in various approximation schemes. In the Ginzburg-Landau theory for classical phase transition, $\alpha(T)$ is taken as $T-T_c$ and B as independent of temperature. This leads to the Curie-Weiss law for the susceptibility and the well-known mean-field critical exponents. In the mean-field theory of itinerant ferromagnets

$$\alpha_{MF}(T)=1-UN(\epsilon_F) \tag{8}$$

and B is again a constant. In this case the temperature dependence of physical quantities near T_c comes from that of the integral over the density of states through a Sommerfeld expansion. It is weak, of the order of T^2/T_F^2, and therefore it does not give a Curie-Weiss form for the spin susceptibility. This issue is tackled in the spin fluctuation theory, where $\alpha(T)$ is given by,[11,12]

$$\alpha_{SF}(T)=\alpha(0)+u_4(2D^T+3D^L). \tag{9}$$

Here $\alpha(0)$ is the susceptibility enhancement factor at $T=0$. This includes the mean-field part $\alpha_{MF}(T)$ and the zero-temperature part of the fluctuation self-energy whose finite-temperature part comprises the second term. Here D^T and D^L

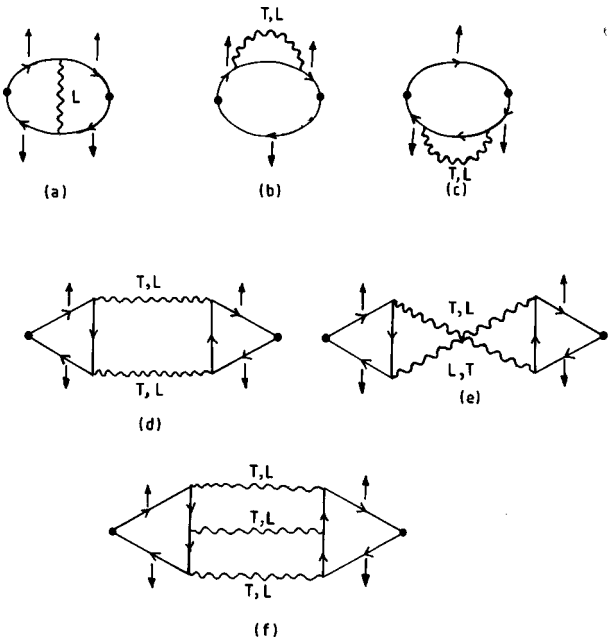

FIG. 1. Self-energy diagrams for the spin fluctuation propagator.

are transverse and longitudinal spin fluctuation amplitudes obtained by the internal frequency summation in the diagrams shown in Figs. 1(a)–1(c). The main contribution to the temperature variation of various physical quantities is governed by these amplitudes. The factor u_4 in the second term is a dimensionless short-range four-fluctuation coupling constant obtained after integration over fast fermionic degree of freedom.

The above result has been derived microscopically, within the functional integral scheme on a model of interacting electrons. We consider the Hubbard model as applied to itinerant ferromagnets and for brevity consider only spin degrees of freedom. Applying the Stratanovich-Hubbard functional integral transformation, the partition function can be written as

$$Z=\mathrm{tr}\int\prod_{q,m}\frac{d\xi_{q,m}}{\pi}\exp\left[-\sum_{q,m}|\xi_{q,m}|^2-\int_0^\beta du\left\{\sum_k \epsilon_k n_{k,\sigma,u}-\left(\frac{U}{\beta}\right)^{1/2}\sum_{q,m}[\xi^*_{q,m}S_{q,m}\exp(z_m u)+\mathrm{H.c.}]\right\}\right], \tag{10}$$

where $\xi_{q,m}$ is the spin fluctuation field of wave vector q and frequency z_m $(=2\pi im/\beta)$, ϵ_k is the kinetic energy of the electrons, and U denotes a short-range interatomic repulsion. Integrating over the electronic degrees of freedom, we have the free-energy functional $F(\xi_{q,m})$ for interacting spin fluctuations, that is,

$$Z=\int\prod_{q,m}\frac{d\xi_{q,m}}{\pi}\exp[-\beta F(\xi_{q,m})]. \tag{11}$$

Parameters of this model, e.g., the fluctuation spectrum and fluctuation coupling vertices, are determined by properties of the underlying fermion system. Since these parameters (e.g., the Stoner enhancement factor for ferromagnets or the staggered susceptibility for antiferromagnets) are such that spin fluctuations are low-lying excitations, this transformation is especially helpful for an analysis of temperature-dependent properties of weak itinerant electron ferromagnets and antiferromagnets. The free-energy functional $F(\xi qm)$ then expanded in powers of these fluctuation fields up to a quartic term and a self-consistent mean fluctuation field approximation (quasiharmonic approximation or the self-consistent renormalization scheme of Moriya) can be generated. The mean fluctuation field approximation corresponds to the diagrams in Figs. 1(a)–1(c) and shown in a compact manner in Fig. 2, where the double wiggle represents the dressed propagator $D(\mathbf{q})$. The details are given in earlier papers.[11,12] One can also estimate corrections due to higher-order fluctuation terms. Figures 1(d)–1(f) represent typical higher-order fluctuation correlated terms.

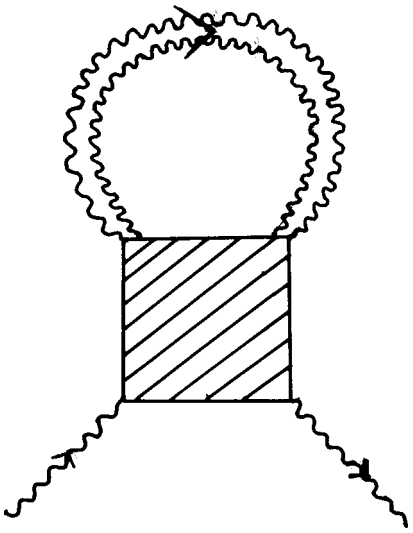

FIG. 2. Self-energy in the mean fluctuation field approximation.

III. PHYSICAL PROPERTIES NEAR THE QUANTUM CRITICAL POINT

A. Spin susceptibility

The self-consistent equation for the temperature dependence of $\alpha(T)$ is given by Eq. (9) which is written explicitly as

$$\alpha(T)=\alpha(0)+\lambda\sum_q\int d\omega\; n(\omega)\mathrm{Im}\chi(q,\omega^+), \tag{12}$$

where λ is related to u_4, $n(\omega)=(e^{\omega/T}-1)^{-1}$ is the Bose distribution function, and

$$\chi(q,\omega^+)=\frac{N(\epsilon_F)}{\alpha(T)+\delta q^2-\imath\dfrac{\pi\omega\gamma}{2q}} \tag{13}$$

is spin susceptibility for the ferromagnetic case. (ω and T are written in units of ϵ_F and q in units of k_F. We have set $\hbar=1$ and $k_B=1$.) Performing the frequency integral,

$$\alpha(T)=\alpha(0)+\frac{\lambda}{\pi}\sum_q q\left\{\ln(y)-\frac{1}{2y}-\psi(y)\right\}, \tag{14}$$

where

$$y=\frac{q}{\pi^2\gamma T}[\alpha(T)+\delta q^2]. \tag{15}$$

An interpolation formula for

$$\phi(y)\equiv\left\{\ln(y)-\frac{1}{2y}-\psi(y)\right\}\simeq\frac{1}{2y+12y^2}, \tag{16}$$

which is valid for small as well as large y, is useful in calculating the momentum integral. For three dimensions,

$$\alpha(T)=\alpha(0)+\frac{\lambda}{2\pi^3}\int\frac{q^3dq}{2y+12y^2}. \tag{17}$$

A finite $\alpha(0)$ introduces two regions of temperatures.[11] For $T<\alpha(0)$ one gets the standard paramagnon theory results and for $\alpha(0)<T<1$ one gets the classical Curie-Weiss susceptibility

$$\chi=\chi_P/\alpha(T)\simeq\mu_B^2/[a\alpha(0)+T], \tag{18}$$

which is similar to the susceptibility of a collection of classical spins. This feature is revealed more clearly if we set $\alpha(0)=0$ in the expression for $\chi(T)$ and solve the equation self-consistently. In this case the paramagnon regime $[T\leqslant\alpha(0)]$ shrinks to zero and a classical behavior is expected down to $T=0$. One is then essentially calculating the susceptibility of a ferromagnet with $T_c=0$. Since $\alpha(0)$ is taken to be zero and there is only one region of temperature $T<1$. In this case, typically $y\leqslant 1$, the limiting form is obtained using the form $\phi(y)\approx(1/2y)$ (valid for $y\ll 1$). We then find that

$$\alpha(T)=\frac{T}{\delta}\left[q_T-\left(\frac{\alpha(T)}{\delta}\right)^{1/2}\arctan\left(q_T\frac{\delta}{\alpha(T)}\right)^{1/2}\right], \tag{19}$$

where q_T is a thermal cutoff such that $y_{q_T}\approx 1$. For the form of y given by Eq. (15), the estimate of the cutoff is $q_T^3\approx T\gamma/\delta$ or $q_T\approx T^{1/3}$. The dominating contribution to $\alpha(T)$ comes from the first term, which is given by $T^{4/3}$. However, since δ is small, the thermal cutoff q_T is high, $\approx q_c$ (the spin fluctuation energy rises only slowly with q). Thus $\alpha(T)$ rises nearly linearly with T. This is the classical spin fluctuation behavior, first pointed out for itinerant ferromagnets by Murata and Doniach.[14] Note that we have assumed $T<1$, i.e., the system is degenerate. Even so, since the characteristic fluctuation energy $\alpha(0)$ is zero, the system behaves classically with regard to spin fluctuations. An estimate of the size of the second term is obtained by setting $\alpha(T)\approx T^{4/3}$. We then find it to be of order $T^{1/3}$ relative to the first term. Since $T^{1/3}$ is not very small, it is essential to do a self-consistent calculation, particularly in the classical regime that is of interest in the present calculation.

We have calculated $\alpha(T)$ and other properties in two dimensions also. For this we consider the same approximate form of the spin susceptibility or the fluctuation propagator as in three dimensions and the effect of dimensionality is considered only through the phase space in the momentum integration. The assumption regarding the form of the susceptibility function in two dimensions is in doubt. It is well known[19] that the Lindhardt function from which this functional form has been derived has a different analytic form in two dimensions. As far as the low-momentum behavior is concerned, the assumption is closer to reality if δ is considered to be far smaller than its value in three dimensions. For the sake of comparison, we assume the same value of δ in three as well as in two dimensions. Following the same procedure as in three dimensions, we find in two dimensions a logarithmic temperature dependence

$$\alpha(T)=\frac{T}{2\delta}\ln\left(\frac{\delta q_c^2}{\alpha(T)}\right). \tag{20}$$

Because of the Bose factor $1/[\exp(\omega/T)-1]$, the number of thermal (classical) fluctuations becomes smaller and smaller as $T\to 0$ (i.e., as the T_c approaches). This reduces the phase space for the fluctuation correlations. In the renormalization-group analysis of Hertz[4] and others[5] this requires the introduction of a suitably scaled ''energy'' variable as a degree of freedom in addition to the three momentum variables. In effect, the dimensionality increases and the behavior becomes mean-field-like. We see this explicitly in our procedure of calculating the fluctuation correlation correction perturbatively. The terms involving two or more internal thermal spin fluctuations are shown in Fig. 2. These have been calculated in detail earlier.[11] It turns out that apart from a numerical factor, the two internal thermal spin fluctuation term has the same temperature dependence as the mean fluctuation field term. However, the three internal thermal spin fluctuation term is approximately equal to $T^2\ln[1/3\alpha(T)]$ in three-dimensional (3D) ferromagnets. We see that this term is of the order of $T\ln T$ relative to the simplest nonvanishing contribution. The perturbation expansion therefore converges.

For a finite-T_c ferromagnet the mean fluctuation field theory is valid outside the critical regime. As the critical regime approaches higher-order fluctuation correlations become comparable to the mean fluctuation term. In the present case, in contrast, the mean fluctuation field term gives the leading critical behavior. The reason is the following. Suppose for $\alpha(0)=0$, $\alpha(T)\sim T^{\lambda}$. Then the quantum region $T\ll\alpha(T)$ means $T^{1-\lambda}\ll 1$ and it occurs only if $\lambda\leqslant 1$. This is not possible and so one always has the other classical (Curie-Weiss) region. Here the fluctuation correlation term is of the form $T^2\ln[1/\alpha(T)]\sim T^2\ln(1/T)^{\lambda}\ll T^{\lambda}$. If $\lambda\sim 1$, the correlation term never becomes more important than the mean fluctuation field term.

In the case of antiferromagnets, the formalism is identical. One replaces the Pauli susceptibility with the staggered susceptibility for a noninteracting electron system $\chi_0(\mathbf{Q})$; for brevity, we retain the same notation for the enhancement factor, which is defined in the present case as $\alpha(0)=\chi_0(\mathbf{Q})/\chi(\mathbf{Q})$. The expansion of the dynamic staggered susceptibility $\chi_0(\mathbf{Q}+\mathbf{q},\omega)$ for small $\mathbf{q}$ and small ω around the static staggered susceptibility is also written in the form[7]

$$\chi(\mathbf{Q}+\mathbf{q},\omega^+)=\frac{\chi^0(\mathbf{Q})}{\alpha(T)+\delta q^2-\imath\gamma\omega}. \tag{21}$$

Making similar transformations as for the ferromagnetic case, we get

$$\alpha(T)=\alpha(0)+\frac{\lambda}{2}\sum_q \frac{1}{2z+12z^2}, \tag{22}$$

where

$$z=\frac{\alpha(T)+\delta q^2}{2\pi\gamma T}. \tag{23}$$

Thus, for 3D antiferromagnets,

$$\alpha(T)=\alpha(0)+\frac{\lambda}{2\pi}\int \frac{q^2dq}{2z+12z^2}. \tag{24}$$

The result turns out to be identical to the ferromagnetic case once we consider only $z<1$, where the corresponding momentum cutoff turns out to be $T^{1/2}$,

$$\alpha(T)=\frac{T}{\delta}\left[q_c-\sqrt{\frac{\alpha(T)}{\delta}}\arctan\left(\sqrt{\frac{\delta}{\alpha(T)}}q_c\right)\right], \tag{25}$$

and in two dimensions there is again a logarithmic behavior

$$\alpha(T)=\frac{T}{2\delta}\ln\left(\frac{\delta q_c^2}{\alpha(T)}\right). \tag{26}$$

B. Resistivity

The electrical resistivity for pure transition and rare earth metals is usually calculated within a two-band model,[20] where the ''conducting'' electrons come from an s band while the d electrons contribute to magnetism. The d band is assumed to be narrow and the d electrons are assumed to be heavy. The conducting s electrons scatter from the spin fluctuations corresponding to d electrons. The temperature-dependent part of the resistivity due to this mechanism for a $3D$ ferromagnet is given by[21–23]

$$\rho(T)\propto\frac{1}{T}\int q^3dq\int \mathrm{Im}\chi(q,\omega^+)\omega n(\omega)[1+n(\omega)]d\omega. \tag{27}$$

The frequency integral can be performed by first using the identity

$$\frac{1}{T^2}\omega n(\omega)[1+n(\omega)]=\frac{\partial}{\partial T}n(\omega), \tag{28}$$

leading to

$$\rho(T)\approx T\int dq\ q^3\int d\omega\frac{dn(\omega)}{dT}\frac{q\omega}{q^2[\alpha(T)+\delta q^2]^2+\omega^2}$$
$$\approx\int dq\ q^4 y\phi'(y), \tag{29}$$

where $\phi'(y)=d\phi(y)/dy$ and $\phi(y)$ and y are given by Eqs. (16) and (15), respectively. In the limit $y<1$ the momentum integral gives

$$\rho(T)=\frac{T}{2\delta}\left[q_c^2-\frac{\alpha(T)}{\delta}\ln\left(\frac{\alpha(T)+\delta q_c^2}{\alpha(T)}\right)\right]. \tag{30}$$

With $q_c\sim T^{1/3}$ we recover the well-known result $\Delta\rho\sim T^{5/3}$.[22] However, the self-consistenct correction changes the power of temperature. Similarly, for two dimensions,

$$\rho(T)=\frac{T}{\delta}\left[q_c-\sqrt{\frac{\alpha(T)}{\delta}}\arctan\left(\sqrt{\frac{\delta}{\alpha(T)}}q_c\right)\right]. \tag{31}$$

The case of 3D antiferromagnets formalism is similar, except for the power of q in the momentum integral. This is due to the fact that the small momentum expansion is not done around $q=0$ but around $q=Q$, the antiferromagnetic wave vector. The result is[7]

$$\rho(T)\propto\frac{1}{T}\int q^2dq\int \mathrm{Im}\chi(\mathbf{Q}+\mathbf{q},\omega^+)\omega n(\omega)[1+n(\omega)]d\omega. \tag{32}$$

Following the same steps as for the ferromagnetic case, we get

$$\rho(T)\propto T\int q^2dq\frac{1+12z}{2z(1+6z)^2}, \tag{33}$$

where z is given by Eq. (23). The result in the limit of $z<1$ is

$$\rho(T)=\frac{T}{\delta}\left[q_c-\sqrt{\frac{\alpha(T)}{\delta}}\arctan\left(\sqrt{\frac{\delta}{\alpha(T)}}q_c\right)\right]. \tag{34}$$

Similarly, for two dimensions, $\rho(T)=(T/2\delta)\ln[\delta q_c^2/\alpha(T)]$.

C. Specific heat

The spin fluctuation contribution to the free energy within the mean fluctuation field approximation (or quasiharmonic approximation) is given by[13]

$$\Delta\Omega=\frac{3T}{2}\sum_{q,m}\ln\left\{1-U\chi^0_{qm}+\lambda T\sum_{q',m'}D_{q'm'}\right\}, \tag{35}$$

where $D_{q,m}$ is the fluctuation propagator that is related to the inverse dynamical susceptibility and χ^0_{qm} is the free-Fermi-gas (Lindhardt) response function. The argument of the logarithm is related to inverse dynamic susceptibility. Considering only the thermal part of the integral and ignoring the zero-point part, we perform the frequency summation and obtain

$$\Delta\Omega_{thermal}=\frac{3}{\pi}\sum_q\int_0^\infty\frac{d\omega}{e^{\omega/T}-1}\arctan\left\{\frac{\pi\omega/4q}{\alpha(T)+\delta q^2}\right\}. \tag{36}$$

Integrating over frequency, we get

$$\Delta\Omega_{thermal}=3T\sum_q\left[\ln\Gamma(y)-\left(y-\frac{1}{2}\right)\ln(y)+y-\frac{1}{2}\ln(2\pi)\right], \tag{37}$$

where y is given by Eq. (15). Once the free-energy correction is known, the specific-heat correction is given by

$$\frac{\Delta C_v}{k_B} = -T\frac{\partial^2 \Delta\Omega}{\partial T^2}$$

$$= -3T^2 \sum_q \left[\left(\frac{2}{T}\frac{\partial y}{\partial T} + \frac{\partial^2 y}{\partial T^2} \right) \phi(y) + \left(\frac{\partial y}{\partial T} \right)^2 \frac{\partial \phi(y)}{\partial y} \right]$$

$$= 6 \int q^2 dq \left\{ \phi'(y) \left(\frac{q}{\pi^2 \gamma} \frac{\partial \alpha(T)}{\partial T} - y \right)^2 + T\phi(y) \frac{q}{\pi^2 \gamma} \frac{\partial^2 \alpha(T)}{\partial T^2} \right\}. \tag{38}$$

Making the small-y approximation and introducing the appropriate cutoff,

$$\frac{\Delta C_v}{k_B} \approx \frac{1}{2\pi^2} \left[\left(T^2 \frac{\partial^2 \alpha(T)}{\partial T^2} + 2T \frac{\partial \alpha(T)}{\partial T} \right) \int_0^{q_c} dq \frac{q^2}{\alpha(T) + \delta q^2} - T^2 \left(\frac{\partial \alpha(T)}{\partial T} \right)^2 \int_0^{q_c} dq \frac{q^2}{[\alpha(T) + \delta q^2]^2} - \int_0^{q_c} dq\, q^2 \right]$$

$$= -\frac{1}{\delta} \left(T^2 \frac{\partial^2 \alpha(T)}{\partial T^2} + 2T \frac{\partial \alpha(T)}{\partial T} \right) \times \left[q_c - \sqrt{\frac{\alpha(T)}{\delta}} \arctan\left(\sqrt{\frac{\delta}{\alpha(T)}} q_c \right) \right] + \frac{T^2}{2\delta} \left(\frac{\partial \alpha(T)}{\partial T} \right)^2 \left[\frac{1}{\sqrt{\alpha(T)\delta}} \arctan\left(\sqrt{\frac{\delta}{\alpha(T)}} q_c \right) - \frac{q_c}{\alpha(T) + \delta q_c^2} \right] + \frac{q_c^3}{3}. \tag{39}$$

The last result is obtained after the momentum integration. Approximately, the terms can be arranged as

$$C_V \approx \frac{1}{2\pi^2} \left[q_c^3 + T^2 \left(\frac{\partial \alpha(T)}{\partial T} \right)^2 \frac{1}{\sqrt{\alpha(T)}} - \left(T^2 \frac{\partial^2 \alpha(T)}{\partial T^2} + 2T \frac{\partial \alpha(T)}{\partial T} \right) q_c \right]. \tag{40}$$

The first term gives the classical result (for constant cutoff), the second dominant term gives leading temperature correction, and the last term is about two orders of magnitude smaller in the temperature range of interest. Similarly, in two dimensions,

$$C_V = -\frac{1}{2\delta} \left(T^2 \frac{\partial^2 \alpha(T)}{\partial T^2} + 2T \frac{\partial \alpha(T)}{\partial T} \right) \ln\left(\frac{\delta q_c^2}{\alpha(T)} \right) + \frac{T^2}{2\delta \alpha(T)} \times \left(\frac{\partial \alpha(T)}{\partial T} \right)^2 \left(1 + \frac{\alpha(T)}{\delta q_c^2} \right)^{-1} + \frac{q_c^2}{2}. \tag{41}$$

The calculation for antiferromagnets is identical except that y is replaced by z in Eq. (40) and the final equation in terms of $\alpha(T)$ turns out to be identical except that the temperature dependence of $\alpha(T)$ is different in an antiferromagnet.

D. Nuclear spin relaxation rate

The nuclear spin relaxation rate in metals is given by the Korringa relation[24]

$$\frac{1}{T_1 T} \approx \left(\frac{\Delta H}{H} \right)^2, \tag{42}$$

which essentially tells that $1/T_1$ is proportional to the square of the static spin susceptibility of metals, which in turn is independent of temperature for most normal metals. However, it was pointed out by Moriya[25] long ago that this relation is modified in the presence of electron correlations. The nuclear spin lattice relaxation rate in metals is given by

$$\frac{1}{T_1 T} \sim \sum_q \frac{\mathrm{Im}\chi^{-+}(q, \omega_0^+)}{\omega_0}, \tag{43}$$

where ω_0 is the nuclear magnetic resonance frequency, which is taken to be very small ($\to 0$) in the problem of nuclear spin relaxation rate. Substituting the expression for $\chi^{-+}(q, \omega_0^+)$ and taking the limit, we have

$$\frac{1}{T_1 T} \sim \sum_q \frac{1}{q[\alpha(T) + \delta q^2]^2} \tag{44}$$

for a ferromagnet in three dimensions. After the momentum integration, the result is $(T_1 T)^{-1} \sim \alpha(T)^{-1}$. For a normal Fermi liquid $\alpha(T)$ is constant, but in the present case it varies as $T^{4/3}$. This leads to a non-Fermi-liquid behavior again. A similar calculation is done for antiferromagnets.

E. Effect of disorder

The effect of disorder can be included in the above-mentioned formalism by modifying the propagators and vertices in diagrams for the spin fluctuation self-energy. This has been done in our earlier papers.[26,27] In the presence of disorder the electron moves randomly, getting scattered from impurities repeatedly. This introduces a finite mean free path for the electron and a finite lifetime τ in the electron propagator, which also modifies the free-particle–hole propagator (diffuson), the free-particle–particle propagator (cooperon), and the electron-spin fluctuation vertex. The correction to $\alpha(T)$ to leading order is given by,

$$\alpha(T) = \alpha_{SF}(T) - \alpha_d(T), \tag{45}$$

where $\alpha_d(T)$ is the correction due to diffusive modes. It is given to the leading order in $1/\epsilon_F \tau$ as

$$\alpha_d(T) \sim (1 - \sqrt{2\pi\tau T})/(\epsilon_F \tau)^2 \tag{46}$$

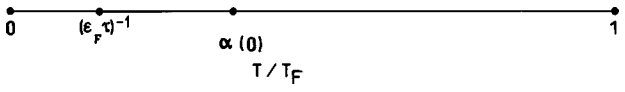

FIG. 3. Schematic diagram of the various temperature scales involved in the disordered material.

TABLE I. Summary of the temperature dependence of various thermal and transport properties near a quantum phase transition point. For each property results are displayed in three rows. The first row gives the non-self-consistent calculation scheme. For ferromagnets the upper cutoff for q is $T^{1/3}$, while for antiferromagnets it is $T^{1/2}$. The second row gives the self-consistent calculation scheme results. The upper cutoff for q has been taken to be 1. The range of temperatures in which these exponents have been calculated is $T=10^{-3}$–10^{-2}. The third row gives the classical spin fluctuation results, i.e., the first row with q_T as a constant.

	Fermi liquid	Ferromagnets (3D)	Antiferromagnets (3D)	Ferromagnets (2D)	Antiferromagnets (2D)
$[\chi(T)]^{-1}$	const	$T^{4/3}$ $T^{1.20}$ T	$T^{3/2}$ $T^{1.44}$ T	$T\ \ln T$ $T^{0.87}$ T	$T\ \ln T$ T T
$\rho(T)$	T^2	$T^{5/3}$ $T^{1.56}$ T	$T^{3/2}$ $T^{1.45}$ T	$T^{4/3}$ $T^{1.24}$ T	$T\ \ln T$ T T
$C_v(T)$	T	T $T^{0.74}$ const	$T^{3/2}$ $T^{0.99}$ const	$T^{2/3}$ $T^{0.52}$ const	T $T^{0.86}$ const
$(T_1T)^{-1}$	const	$T^{-4/3}$ $T^{-1.284}$ T^{-1}	$T^{-3/4}$ $T^{-0.72}$ $T^{-1/2}$	$(T\ \ln T)^{-3/2}$ $T^{-1.305}$ $T^{-3/2}$	$(T\ \ln T)^{-1}$ T^{-1} T^{-1}

for $T \ll 1/\tau$ and vanishes otherwise. Clearly, the disorder introduces a new energy scale $(1/\tau)$ in the lowest temperature range, as shown schematically in Fig. 3. In the case of nonvanishing $\alpha(0)$, in the case of ferromagnets in three dimensions, the susceptibility inverse $\alpha(T)$ behaves as $\sim T^{1/2}$ for $T<1/\tau$, as $T^2/\alpha(0)$ for $1/\tau<T<\alpha(0)$, and as $T^{4/3}$ for $\alpha(0)<T<1$. Similarly, the resistivity correction $\Delta\rho(T)$ behaves as $\sim T^{1/2}$ for $T<1/\tau$, as $T^2/\sqrt{\alpha(0)}$ for $1/\tau<T<\alpha(0)$, and as $T^{5/3}$ for $\alpha(0)<T<1$. In the case of a zero-T_c system the quantum fluctuation regime $[T<\alpha(0)]$ vanishes and the other two regimes merge. At the lowest temperature the effect of the diffusive mode seems to give the dominant contribution, i.e., $\alpha(T)\sim T^{1/2}$ and $\Delta\rho(T)\sim T^{1/2}$, but a more detailed analysis is needed.

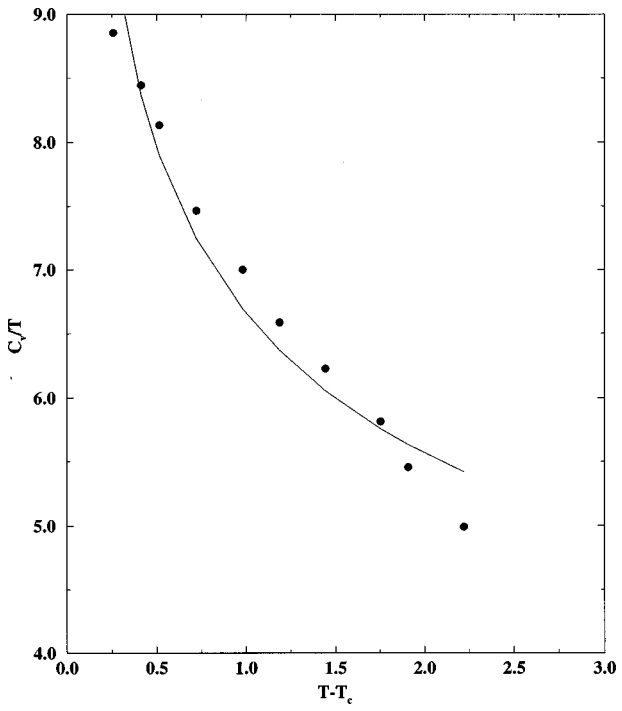

FIG. 4. Plot of C_v/T as a function of $T-T_c$ for Sc_3In. The experimental points (Ref. 30) are represented by circles and the solid line represents the theoretical fit. $\delta=1/12$, $\gamma=1/2$, and $T_F \approx 1000$ K.

F. Summary

Table I summarizes our results. In the first column Fermi-liquid theory results are written and the other columns compile the fluctuation theory results. These results are presented

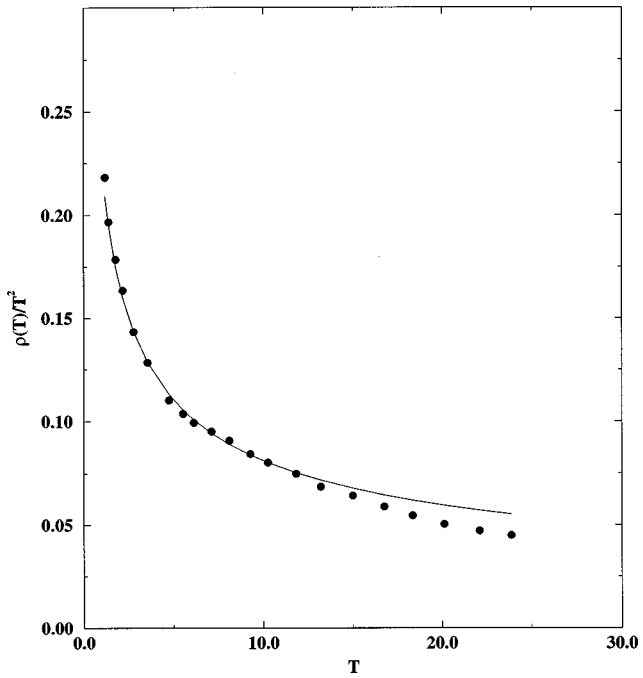

FIG. 5. Plot of $\rho(T)$ as a function of T for MnSi. The experimental points[31] are represented by circles and the solid line represents the theoretical fit. $\delta=1/12$, $\gamma=1/2$, and $T_F \approx 1000$ K.

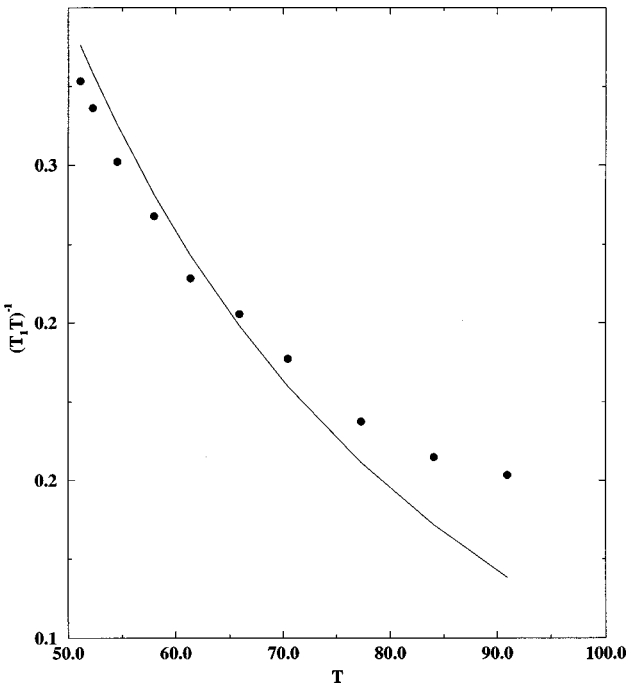

FIG. 6. Plot of $(T_1T)^{-1}$ as a function of T for Ni_3Al. The experimental points (Ref. 32) are represented by circles and the solid line represents the theoretical fit. $\delta=1/12$, $\gamma=1/2$, $T_F\approx1000$ K.

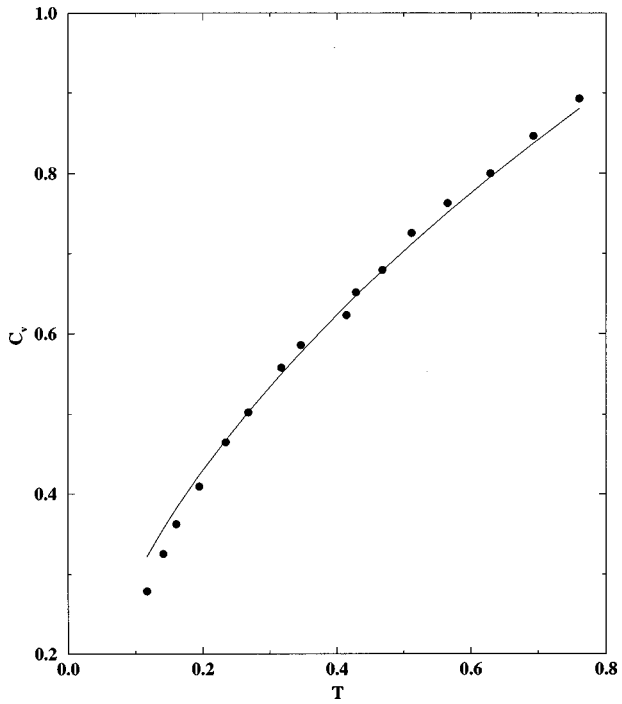

FIG. 7. Plot of C_v as a function of T for $CeCu_{5.7}Au_{0.3}$ at a pressure of 8.2 kbar. The experimental points (Ref. 34) are represented by circles and the solid line represents the theoretical fit. $\delta=1/2\pi$, $\gamma=1$, and $T_F\approx5$ K.

in three rows for each property. The first row gives results from a non-self-consistent calculation, for example, when only the first term in Eq. (19) for $\alpha(T)$ is considered, but with a proper momentum cutoff. This behavior is expected in the extreme low-temperature range. These results are in general known, but are presented here in a coherent form. The second row gives these results with the temperature dependence of $\alpha(T)$ taken in account and the integration performed with the functional form for $\phi(y)$ valid for all y but approximated by Eq. (16). The power of temperatures so obtained depends slightly on the temperature regime considered (i.e., whether T is in the range 10^{-3}–10^{-2} or otherwise). The third row gives the classical spin fluctuation results, where the Bose factor $n(\omega)$ is approximated as T/ω (effectively the first row with a constant cutoff). The experimental results are expected to lie between those given in rows 1 and 3.

IV. EXPERIMENTAL RESULTS

In this section we give examples of materials exhibiting non-Fermi-liquid behavior at low temperatures and also compare some results with a theory presented above. The most popular example of a system showing non-Fermi-liquid behavior is, of course, the high-temperature superconductors.[28] It seems, however, that the effective low dimensionality, the specific nature of the density of states, and the structural aspects of the Fermi surface (nesting, etc.) play important roles in this system. We therefore want to consider examples from three-dimensional correlated electronic system in the neighborhood of an electronic phase transition.

The next example is that of phosphorus-doped silicon (Si:P).[29] This material goes through a Mott insulator to metal transition as the doping by P increases. At $n_c\sim3.7\times10^{18}$ atoms/cm^3 of P there is a metallic state. The spin susceptibility of Si:P gets enhanced and becomes strongly temperature dependent as the metal-insulator transition is approached from the metallic side. The T dependence observed does not fit the $1/T$ behavior expected for weakly interacting localized spins either. Moreover, the spin lattice relaxation times in barely metallic Si:P is strongly temperature dependent, $T_1^{-1}\sim T^{-1/2}$, similar to the correction to the zero-T conductivity, $\sigma\sim T^{1/2}$, in this material. There are theories that associate these anomalies to spin fluctuations induced due to incipient localization. There is a subtle interplay of disorder and correlation effects in this material. Only a spin fluctuation kind of theory will not work.

Some transition metal (and also some actinide) intermetallic compounds show a low saturation moment per transition-metal atom and a low magnetic transition temperature T_c compared to conventional ferromagnetic materials such as Fe, Co, and Ni. These compounds are known as weak itinerant electron ferromagnets. The prototype examples are $ZrZn_2$, Ni_3Al, and Sc_3In.[18] Their low-temperature properties have been discussed within spin fluctuation theories for a long time.[17] Here we compare the specific-heat behavior of Sc_3In above T_c with our present calculation (Fig. 4). The experimental curves are due to Ikeda[30] and show a good fit to the theory with $\Delta\rho(T)\sim T$ and $C_v(T)/T\sim(T-T_c)^{-0.25}$.

The example of MnSi is interesting from the perspective of the present work. The material has a transition temperature around 30 K. As the hydrostatic pressure is applied the

T_c decreases continuously and collapses towards absolute zero at $p_c = 14.6$ kbar. This is an example where an approach to a zero-temperature quantum phase transition can be observed as a function of pressure. This has been done by Pfleiderer, McMullan, and Lonzgrich.[31] The deviation of the resistivity curve from the T^2 behavior becomes pronounced as p_c is approached. In Fig. 5 we have compared $\Delta\rho/T^2$ with a power-law temperature dependence, as suggested in our calculation.

We have compared the nuclear spin relaxation rate of ^{27}Al in Ni_3Al as a function of temperature.[32] This material has a transition temperature about 41 K and shows all other characteristic properties of weak itinerant ferromagnet.[33] The low-field data fit to power law $T^{-0.89}$ for $(T_1T)^{-1}$, as shown in Fig. 6.

The heavy fermion material $CeCu_6$ is nonmagnetic. On alloying with Au the lattice expands and an antiferromagnetic order is observed in $CeCu_{6-x}Au_x$ above a critical concentration $x_c \approx 0.1$. The Nèel temperature of the antiferromagnetic heavy-fermion alloy $CeCu_{5.7}Au_{0.3}$ can be continuously tuned to zero with increasing hydrostatic pressure. At the critical pressure the specific heat has been fitted to the $C/T \sim \ln T_0/T$ curve.[34] We analyze the data again and fit the curve to our prediction ($T^{0.58}$ corresponding to the temperature range of interest) in Fig. 7.

V. CONCLUSION

We have calculated the temperature dependence of various physical properties near the quantum phase transition point. The results hold for electronic phase transitions with a finite T_c also. This is clear, as the results from the first row in Table I match some well-known results in the literature. However, they are pronounced and a clear non-Fermi-liquid behavior is obtained when $T_c \to 0$. Our results are perturbative, but as discussed in the text the fluctuation correlation term is always smaller than the mean fluctuation field term. The behavior of these quantities is different in ferromagnets from the antiferromagnetic system. This is a reflection of the fact that the order-parameter fluctuations have a different form of dispersion in these systems. Finally, we made some remarks about the inclusion of the effect of disorder near quantum critical point within the spin fluctuation formalism. The present approach can be applied to other systems also. One only needs an appropriate form of the order-parameter correlation function to calculate various quantities. For example, this approach can be applied to systems with a pseudogap[35] in the excitation spectrum and also with phononlike dispersion as it happens in short coherence length superconductors. For example, in 2D short coherence length superconductors it has been shown through Monte Carlo simulations that the relaxation rate varies as the spin susceptibility[36] $[\alpha(T)]^{-1}$ of the system, which matches our result on 2D antiferromagnets.

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