Strong-coupling theory of heavy-fermion criticality

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We present a theory of the scaling behavior of the thermodynamic, transport, and dynamical properties of a three-dimensional metal at an antiferromagnetic (AFM) critical point. We show how the critical spin fluctuations at the AFM wave vector $q = Q$ induce energy fluctuations at small q, giving rise to a diverging quasiparticle effective mass over the whole Fermi surface. The coupling of the fermionic and bosonic degrees of freedom leads to a self-consistent relation for the effective mass, which has a strong coupling solution in addition to the well-known weak-coupling spin-density-wave solution. We use the recently introduced concept of critical quasiparticles, employing a scale-dependent effective mass ratio m^*/m and quasiparticle weight factor Z. We adopt a scale-dependent vertex correction that boosts the coupling of fermions and spin fluctuations. The ensuing spin fluctuation spectrum obeys ω/T scaling. Our results are in good agreement with experimental data on the heavy-fermion compounds $YbRh_2Si_2$ and $CeCu_{6-x}Au_x$ for 3D and 2D spin fluctuations, respectively.

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I. INTRODUCTION

Quantum phase transitions in metallic compounds have attracted considerable interest over the last two decades. These systems exhibit deviations from the standard Fermi liquid model. This "non-Fermi liquid" behavior is a consequence of the interaction of the fermionic (Landau) quasiparticles with bosonic critical fluctuations. Early theories [1,2] of quantum critical behavior, formulated in the framework of a Ginzburg-Landau-Wilson action of the order parameter field ϕ, found that the effective dimension of the corresponding ϕ^4-field theory is increased to $d_{\text{eff}} = d + z$ where d, z are the spatial dimension of the fluctuations and the dynamical critical exponent, respectively. In many cases of interest d_{eff} is above the upper critical dimension, so that the fluctuations are effectively noninteracting and the theory is of the Gaussian type (for a review see Ref. [3]). While this theory is well founded in the case of nonmetallic systems, for metallic systems the question arises whether the fermionic degrees of freedom may be easily integrated out. In this paper, we show that it is often not possible to reduce the description to that of Hertz and Millis [1,2]. Rather, the interplay of fermionic and bosonic degrees of freedom generates critical behavior of the fermionic quasiparticles, acting back on the spectrum of bosonic fluctuations. Then, a strong-coupling regime with respect to the fermion-boson coupling may be reached.

Experimentally well-studied candidate systems we shall focus on are the heavy-fermion compounds $CeCu_{6-x}Au_x$ (CCA) for which, guided by experiment, we consider quasi-two-dimensional antiferromagnetic (AFM) spin fluctuations at the quantum critical point (QCP) $x = 0.1$ [4] and $YbRh_2Si_2$ (YRS), for which we assume AFM fluctuations of three-dimensional character at the magnetic field-tuned quantum critical point $H = H_c$ at temperatures T less than 0.3 K, crossing over to three-dimensional ferromagnetic fluctuations at higher T [5].

An issue that has hampered progress in developing a strong-coupling theory of criticality that involves AFM fluctuations has been that they transfer a large momentum of the order of the ordering wave vector $\mathbf{q} = \mathbf{Q}$. As a consequence, the self-energy in one-loop order becomes highly anisotropic, being critical only at so-called "hot spots" on the Fermi surface that are connected by $\mathbf{Q}$. However, scattering by two AFM fluctuations, which may be viewed as a spin exchange-energy fluctuation [6], may transfer a small total momentum and thus connect cold regions of the Fermi surface. This is because the intermediate fermion state is far from the Fermi surface and thus off-shell. We argue here that the one-loop order process of such energy fluctuations is dominant in providing a renormalization of the fermionic quasiparticle effective mass that is approximately uniform over the Fermi surface. Thus, we consider here the simplest case, in which the fermion self-energy is only weakly momentum dependent. A different way by which the effect of the critical AFM fluctuations may be distributed all over the Fermi surface is by means of impurity scattering [7,8].

However, a problem with multiple fluctuation exchange is that each additional fluctuation propagator gives rise to an additional energy integration and will thus contribute a small phase space factor, anywhere from ω^2 to ω, depending on the critical momentum dependence. As we will show below, such factors may be offset by inverse powers of the Fermi-liquid renormalization factor $Z^{-n} \gg 1$, provided the quasiparticle weight factor Z tends to zero, as the excitation energy ω or the temperature T tends to zero. As discussed in previous work by two of us [7,8], even if $Z \to 0$ in the limit $(\omega,T) \to 0$ the quasiparticle picture may still be applicable at nonzero ω,T, since the quasiparticle width Γ gets renormalized by a factor of Z, which helps to keep it smaller than the excitation energy ω, a necessary condition for the existence of a quasiparticle peak in the single-electron spectral function.

A careful identification of the effects of the quasiparticle critical behavior on the bosonic (AFM) propagator is at heart of our theory. This includes the determination of critical vertex corrections of various types. The interplay of spin fluctuations and fermonic excitations has also been considered by Abanov and Chubukov [9,10] and Abanov, Chubukov, and Schmalian [11], and a renormalization group treatment has been given by Metlitski and Sachdev [12]. However, these authors did not consider the quasiparticle renormalization in the strong-coupling regime.

The quantum critical point in heavy-fermion compounds has often been associated with a breakdown of the Kondo effect and therefore a breakdown of the picture of heavy quasiparticles [13–15]. In this approach, it is assumed that at the critical point the energy scales of the Kondo effect and the exchange interaction between the localized f spins (in the absence of the Kondo effect) are approximately equal. Some of these scenarios have been developed enough to allow comparison with experimentally observed critical exponents, in particular for $CeCu_{5.9}Au_{0.1}$ and for $YbRh_2Si_2$ [16,17]. However, experimentally the quasiparticle mass does not appear to be drastically reduced (by orders of magnitude) when the QCP is approached, as would be expected if the Kondo effect were to be suppressed. We argue here that in the cases we consider, the Kondo effect, or more precisely the heavy-quasiparticle picture, remains intact. However, the quasiparticles experience an AFM spin-exchange interaction responsible for the ordering of their spins in the AFM state. In other words, we propose that the ordered state is an itinerant heavy-quasiparticle SDW state, at least in the neighborhood of the critical point. The resulting small ordered magnetic moment is in agreement with observation. Roughly speaking, the ordered moments provide a magnetic field acting on the Kondo ions. As long as the f-electron Zeeman splitting caused by this field is small compared to the Kondo temperature, the Kondo effect is only weakly suppressed.

In this report, we present a semi-phenomenological theory of the scaling behavior near an AFM QCP. As discussed above, we show how spin-exchange energy fluctuations may lead to a momentum-independent critical quasiparticle self-energy. The feedback of the critical quasiparticle properties (the Z factor) into the spin and energy fluctuation spectrum leads to a self-consistent equation for the quasiparticle self-energy and effective mass $m^*/m \propto Z^{-1}$. This allows a strong-coupling solution in the form of a fractional power law $Z(\omega) \propto \omega^\eta$. The value of η for different circumstances will be discussed in Sec. IV. In Sec. V, we show that the dynamical structure factor satisfies ω/T scaling within the quantum critical region of the phase diagram. The free energy obeys scaling characterized by fractional power laws; this is described in Sec. VI. In Sec. VII, we present an alternative derivation of our results in the framework of the spin-fermion model. Comparison of our theory with experimental data is discussed in Sec. VIII and we summarize our findings in Sec. IX.

The above scenario depends sensitively on the detailed nature of spin fluctuations in a given system. For example, 3D AFM fluctuations do not lead to true critical behavior; i.e., a Gaussian fluctuation theory is applicable, [1,2] provided the effective mass enhancement by critical fluctuations is not too large. We argue below that in CCA there is a wide region of 2D antiferromagnetic fluctuations, which gives rise to a substantial enhancement of the effective mass and may drive the system into a strong-coupling regime of 2D or 3D antiferromagnetic fluctuations. In YRS, on the other hand, ferromagnetic fluctuations in the temperature regime $0.3\ \text{K} \lesssim T \lesssim 20\ \text{K}$ lead to a substantial enhancement of the effective mass when the system crosses over into a 3D antiferromagnetic fluctuation regime below 0.3 K.

II. CRITICAL QUASIPARTICLES

Our starting point is a heavy Fermi liquid as in an Anderson lattice model of correlated f electrons (on-site interaction U) hybridizing with conduction electrons. The energy scale of the heavy-fermion band is given by the "coherence temperature" T_{coh}, which is well above the temperature regime for which "non-Fermi liquid" behavior is observed near a QCP. On top of the heavy-fermion quasiparticle renormalization, the critical fluctuations cause a further renormalization on which we focus here. The single-particle Green's functions may be decomposed into a quasiparticle term and an incoherent contribution, $G(\mathbf{k},\omega) = ZG^{qp} + G^{\text{inc}}$, where the quasiparticle weight factor Z determines the quasiparticle effective mass m^* and is defined by $Z^{-1} = 1 - \partial \text{Re}\Sigma(\omega)/\partial\omega = m^*/m$. Here, $\Sigma(\omega)$ is the electron self-energy, whose real and imaginary parts determine the quasiparticle properties. The quasiparticle Green's function is given by $G^{qp}(\mathbf{k},\omega) = [\omega - E_k - i\Gamma]^{-1}$, with $E_k = (m/m^*)v_F(k - k_F)$, where v_F is the Fermi velocity of the heavy-fermion band and the quasiparticle width is $\Gamma = Z\,\text{Im}\Sigma(E_k)$.

The condition for the quasiparticle picture to be valid is $\Gamma < |E_k|$, which is satisfied in the Fermi-liquid regime, ($\Gamma = cE_k^2 \ll |E_k|$ in the limit $E_k \to 0$). Here, we argue that this quasiparticle stability condition may be satisfied even in non-Fermi-liquid situations. We extend the usual quasiparticle picture by recognizing that the parameter $Z = m/m^*$, as defined above, depends on the energy scale, $Z = Z(\omega)$. Since the (retarded) self-energy is an analytic function in the upper-half ω plane, the real and imaginary parts of any nonanalytic term (in the lower half plane) are locally connected. Even in a true non-Fermi-liquid phase with $\Sigma(\omega) \propto -i(i|\omega|)^{1-\eta}$, $\eta < 1$ so that $\text{Im}\Sigma(\omega) \propto \text{Re}\Sigma(\omega) \propto |\omega|^{1-\eta}$ and $Z \propto (|E_k|)^\eta$, one finds $\Gamma/|E_k| = \tan(\frac{\pi}{2}\eta) < 1$ for $0 < \eta < 1/2$. In this case, although $Z = 0$ at the Fermi surface, the spectral function for nonzero excitation energy may be peaked sharply enough to separate a quasiparticle contribution from the incoherent part. In Fig. 1, we show the spectral function $\text{Im}\,G(\mathbf{k},\omega)$ for various choices of this "non-Fermi-liquid exponent" η, demonstrating that there is still a well-defined quasiparticle peak.

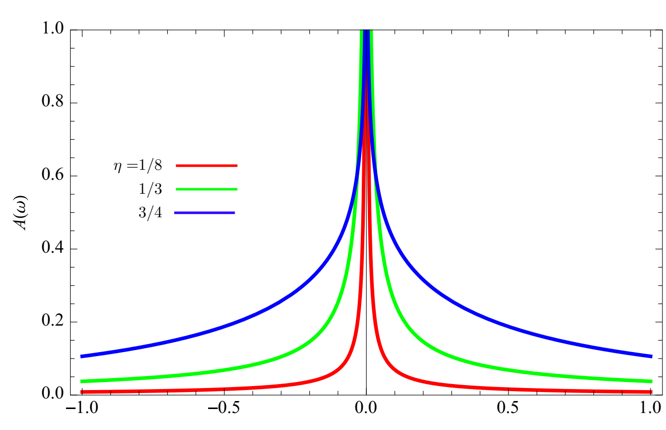

FIG. 1. (Color online) Non-Fermi-liquid spectral function, for self-energy $\Sigma(\omega) \propto -i(i|\omega|)^{1-\eta}$, with $\eta = 1/8, 1/3, 3/4$ (red, green, blue, resp.).

III. CRITICAL FLUCTUATION SPECTRUM

We assume that in the paramagnetic phase of a metal close to an antiferromagnetic quantum critical point, the self-energy for the single-particle Green's function is determined by the interaction with magnetic fluctuations. We take the imaginary part of the renormalized retarded dynamical spin susceptibility for wave vectors near the AFM ordering wave vector $\mathbf{Q}$ to be of the form

$$\mathrm{Im}\chi(\mathbf{q},\omega) = \frac{N_0\left(\omega\lambda_Q^2/v_F Q\right)}{\left(r+\mathbf{q}^2\xi_0^2\right)^2+\left(\omega\lambda_Q^2/v_F Q\right)^2}, \qquad (1)$$

where $\mathbf{q}$ is measured from the ordering wave vector $\mathbf{Q}$. Here, N_0 is the bare density of states at the Fermi surface, v_F is the bare Fermi velocity, and $\xi_0 \simeq k_F^{-1}$ is the microscopic AFM correlation length. The control parameter r is a function of both the tuning field and the temperature. The factor λ_Q is the low-energy vertex for the AFM fluctuation—electron scattering. A microscopic derivation of Ward identities valid at nonzero momentum q, which shows that $\lambda_Q \propto Z^{-1} \propto \omega^{-\eta}$, is available [18]. The singular enhancement of the vertex is present even if only one of the fermions entering the vertex is on-shell. In what follows, we use this result. We expect it to have singular behavior, e.g., $\lambda_Q \sim \omega^{-\phi}$, similar to that of the $\mathbf{q}=0$ vertex for which $\phi=\eta$, the Z-factor exponent, by virtue of a Ward identity. In what follows, we use the results of Ref. [18] and choose $\phi=\eta$ also for λ_Q. In fact, we show in this paper that this choice enables excellent agreement with experiment.

At $T=0$, the control parameter r vanishes at the QCP as a fractional power $r \propto |r_0|^{2\nu}$, where $r_0 \propto (H-H_c)$ or $r_0 \propto (P-P_c)$, for magnetic field or pressure tuning, and ν is the correlation length exponent. In the Appendix, we show that $\nu = 1/(2+z\eta)$ [Eq. (A1)], where z is the dynamical exponent, determined in Sec. V. The non-Fermi-liquid exponent η is self-consistently determined in Sec. IV.

We now define an energy-fluctuation propagator $\chi_E(\boldsymbol{\kappa},\omega)$ by combining two spin fluctuation propagators, in the form

$$\mathrm{Im}\,\chi_E(\boldsymbol{\kappa},\omega) = \sum_{\mathbf{q}_1,\omega_1} G_{k+q_1}G_{k+q_1-\kappa}\mathrm{Im}\chi(\mathbf{q}_1,\omega_1) \times \mathrm{Im}\chi(\mathbf{q}_1-\boldsymbol{\kappa},\omega_1-\omega)[b(\omega_1-\omega)-b(\omega_1)], \qquad (2)$$

where $b(\omega)$ is the Bose function. The Green's functions $G_{k+q_1}, G_{k+q_1-\kappa}$ are off-shell for most values of the momentum $\mathbf{q}_1$ and each may be replaced by $1/\epsilon_F$. Performing the d-dimensional momentum integration by Fourier transform, we get

$$\mathrm{Im}\chi_E(\boldsymbol{\kappa},\omega) \approx N_0^3\lambda_Q^{-2}\left(\frac{\omega\lambda_Q^2}{v_F Q}\right)^{d-1/2}\frac{1}{\left(\frac{\omega\lambda_Q^2}{v_F Q}+\kappa^2\xi_0^2+r\right)^{(d+1)/2}}. \qquad (3)$$

IV. SELF-CONSISTENT DETERMINATION OF QUASIPARTICLE SELF-ENERGY

Now we set up a self-consistent determination of the quasiparticle self-energy via the leading term in a skeleton graph expansion in terms of the boson propagator χ_E. The imaginary part of the self-energy is given by

$$\begin{aligned}\mathrm{Im}\Sigma(k,\omega) &= -\lambda_E^2\int\frac{d\nu_1}{\pi}\sum_{\mathbf{q}}\mathrm{Im}G(\mathbf{k}+\mathbf{q},\omega+\nu_1)\\ &\quad\times \mathrm{Im}\chi_E(\mathbf{q},\nu_1)[b(\nu_1)+f(\omega-\nu_1)]\\ &\approx v_F Q Z^{-2}\left(\omega\lambda_Q^2/v_F Q\right)^{d-1/2}\\ &\propto |\omega|^{d-1/2-\eta(2d+1)}.\end{aligned} \qquad (4)$$

The interaction vertex $\lambda_E = \lambda_Q^2\lambda_v$, where λ_v is $\propto Z^{-1}$, as it arises through a Ward identity connected to energy conservation. We used $\lambda_Q \propto Z^{-1}$, as discussed above, below Eq. (1). The Fermi and Bose functions $f(\omega), b(\omega)$ confine the ν_1 integration at low T to the interval $[0,\omega]$. In Eq. (4), we used the power law $Z(\omega) \propto |\omega|^{\eta}$. The scale-dependent contribution to $\mathrm{Re}\,\Sigma(\omega)$ follows from analyticity as $\mathrm{Re}\,\Sigma(\omega) \propto (\omega/v_F Q)^{d-1/2}Z^{-(2d+1)}$. This leads to the self-consistency relation for $Z(\omega)$

$$\begin{aligned}Z^{-1}(\omega) &= 1-\partial\mathrm{Re}\Sigma(\omega)/\partial\omega\\ &\approx 1+Z^{-2d-1}(\omega/v_F Q)^{d-3/2}.\end{aligned} \qquad (5)$$

We now explore the consequences of the scale-dependent Z. In general, the ω and T dependence of Z is obtained by substituting $\sqrt{\omega^2+a^2T^2}$ for ω, where a is a constant of order unity. For frequencies less than the temperature, we may replace ω by T. As long as $Z^{-2d-1}(T/v_F Q)^{d-3/2} \ll 1$ for any T, the system will be in the Gaussian fluctuation regime all the way down to the critical point. If, however, the initial value of $Z^{-1}(T)$, when one enters the AFM fluctuation regime, is sufficiently large, such that $Z^{-2d-1}(T/v_F Q)^{d-3/2} \gg 1$, a new regime is accessed, which is of a strong-coupling nature. We find the characteristics of this new regime within the present approximation by solving the self-consistent Eq. (5), to get

$$Z(T) \propto (T/v_F Q)^{\eta}, \qquad (6)$$

where the exponent η is found to be

$$\eta = (2d-3)/4d. \qquad (7)$$

In the case of only AFM fluctuations in a clean system, it is difficult to satisfy the strong-coupling condition of sufficiently large $Z^{-1}(T)$. However, if on the initial approach to the critical point, fluctuations dominate that lead to a growing $Z^{-1}(T)$ with decreasing T, the condition may be met at some point. The precise crossover point is determined by the crossover of these precursor fluctuations to the critical AFM fluctuations and by the condition above that leads to Eq. (6). As discussed in [7,8] impurity scattering helps to enhance the effect of AFM fluctuations on $Z(T)$. In addition, there are clear indications in the data on $YbRh_2Si_2$ of 3D FM fluctuations [19]. In that case, one finds $Z^{-1}(T) \propto \ln(T_0/T)$, so that indeed Z^{-1} grows as $T \to 0$.

V. CRITICAL EXPONENTS AND DYNAMICAL SCALING

The critical behavior of the spin-excitation spectrum as discussed above, see Eq. (1), is given by [employing units

$(v_F Q,\xi_0^{-1})$ for (ω,q)]

$$\mathrm{Im}\chi(\mathbf{q},\omega) \propto \frac{\omega^{1-2\eta}}{[\xi^{-2}+q^2]^2+(\omega^{1-2\eta})^2}, \tag{8}$$

where

$$\xi = r^{-1/2}. \tag{9}$$

By equating the terms q^2 and $\omega^{1-2\eta}$ in the denominator, we find the dynamical critical exponent as

$$z = 2/(1-2\eta) = 4d/3. \tag{10}$$

Thus, in the critical region, the leading temperature dependence of the correlation length is given by $\xi(H_c,T) \sim T^{-1/z}$ and using Eq. (A1), we find the correlation length exponent $\nu = 3/(3+2d)$. The boundary of the critical region—the "critical cone"—in the (H,T) phase diagram is found from $\xi(H,T=0) = \xi(H_c,T)$ as $T \sim |H-H_c|^{z\nu}$.

Then $1/\xi(r_0,T)$ has the form

$$1/\xi(r_0,T) = T^{1/z} g(r_0 T^{-1/\nu z}), \tag{11}$$

where $g(x) \approx 1 + x^\nu$. The (ω,T) dependence of Z may be accounted for with the form $Z(\omega,T) \propto T^\eta \zeta(\omega/T)$, where $\zeta(x) \propto (x^2+a^2)^{\eta/2}$.

Then

$$\mathrm{Im}\chi(\mathbf{q},\omega) \propto T^{-2/z} \frac{(\omega/T\zeta^2)}{[g^2+T^{-2/z}q^2]^2+(\omega/T\zeta^2)^2}, \tag{12}$$

which, with the use of Eq. (8), shows the following general scaling relation:

$$\mathrm{Im}\chi(\mathbf{q},\omega) \propto T^{-2/z}\Phi\left(\frac{\omega}{T},q\xi;r_0 T^{1/z\nu}\right). \tag{13}$$

Inside the critical cone, we may set $r_0 = 0$ so that $g = 1$ and $\xi^{-1} \propto T^{1/z}$. Defining $x = \omega\xi^z = \omega/T$ and $y = q\xi$, we find the scaling form

$$\mathrm{Im}\chi(\mathbf{q},\omega) \sim \xi^2 \Phi(x,y), \tag{14}$$

$$\Phi(x,y) = \frac{x/\zeta^2(x)}{(1+c_q y^2)^2+[x/\zeta^2(x)]^2}, \tag{15}$$

where c_q is a constant.

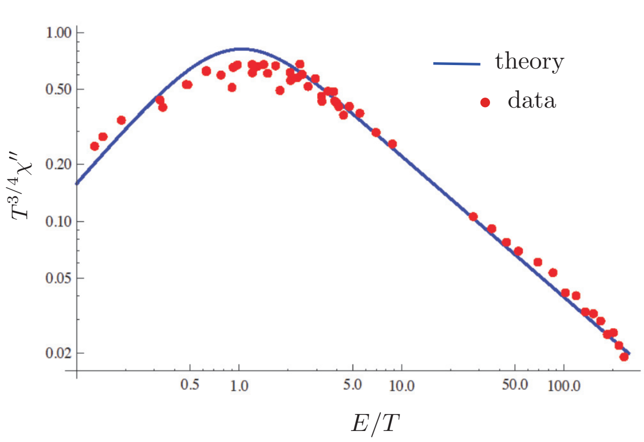

FIG. 2. (Color online) Inelastic neutron scattering: Comparison of theory Eq. (16) and experimental data [20] for $CeCu_{6-x}Au_x$ at the critical concentration $x = 0.1$.

At the ordering wave vector, $y = 0$ so the spin excitation spectrum obeys ω/T scaling inside the critical cone:

$$\mathrm{Im}\chi(\mathbf{Q},\omega) \sim T^{-2/z}\frac{\omega/T\zeta^2(\omega/T)}{1+[\omega/T\zeta^2(\omega/T)]^2}. \tag{16}$$

A comparison of this scaling form with neutron scattering data on CeCuAu is shown in Fig. 2, where we used $d = 2$, so that $z = 8/3$ and $\eta = 1/8$.

VI. FREE ENERGY

The critical part of the free energy density may be derived from the expression for the entropy density in terms of the self-energy [21]:

$$\frac{S}{V} = \frac{1}{2\pi}N(0)\int \frac{d\omega\omega}{T^2\cosh^2\frac{\omega}{2T}}[\omega - \mathrm{Re}\Sigma(\omega)]. \tag{17}$$

Substituting the critical self-energy found above and integrating over temperature, we find the scaling form of the free energy density in the case of d-dimensional spin fluctuations $(d = 2,3)$ in a 3D metal

$$f(H,T) = \xi^{-(2d+1)}\Phi_f(r_0\xi^{1/\nu},T\xi^z). \tag{18}$$

The correlation volume $V_c \sim \xi^{(2d+1)}$ is understood as follows: The underlying critical degrees of freedom in the very low temperature Anderson lattice picture are the heavy-fermionic quasiparticles described by the propagator $G(k,\omega)^{-1} = \omega - vk - \Sigma(\omega)$ with $\Sigma(\omega) \propto \omega^{1-\eta}$. Therefore, their dynamical exponent $z_f = 1/(1-\eta)$ and their dimensionality is $d_f = 1$ [22]. The entropy of the system is determined by hyperscaling for the fermions: $S \propto T^{d_f/z_f}$. Therefore, since $\xi \propto T^{-1/z}$, where $z = 4d/3$, the free energy density $f \propto T^{1+d_f/z_f} \sim \xi^{2d+1}$. Here, z and d are the bosonic exponents discussed above.

The specific heat coefficient follows as

$$C/T \propto \begin{cases} T^{(2d+1-2z)/z}, & \text{critical regime,} \\ r_0^{\nu(2d+1-2z)}, & \text{Fermi liquid regime.} \end{cases} \tag{19}$$

For the critical part of the magnetization we find

$$M - M(H_c,0) \propto \begin{cases} -T, & \text{critical regime,} \\ -r_0^{\nu(2d+1)-1}, & \text{Fermi liquid regime.} \end{cases} \tag{20}$$

The susceptibility has a critical part

$$\chi - \chi(H_c,0) \propto \begin{cases} -T^{1-1/\nu z}, & \text{critical regime,} \\ -r_0^{\nu(2d+1)-2}, & \text{Fermi liquid regime.} \end{cases} \tag{21}$$

Using $\partial M/\partial T = -$constant, we find the Grüneisen ratio in the critical regime:

$$\Gamma_G = -\frac{\partial M/\partial T}{C} \propto \frac{1}{C} \propto T^{(z-2d-1)/z}, \tag{22}$$

while in the Fermi liquid regime, we have the universal result

$$\Gamma_G = -\frac{G_r}{H-H_c}, \quad G_r = -\left(z - \frac{2d+3}{3}\right)\nu. \tag{23}$$

The critical scaling of transport properties is obtained by observing that the quasiparticle relaxation rate scales as

$\Gamma \propto \xi^{-z}\Phi_\Gamma(r_0\xi^{1/\nu},T\xi^z)$. Then the resistivity behaves as

$$\rho - \rho(H_c,0) \propto \frac{m^*}{m}\Gamma \propto \begin{cases} T^{(z+2)/2z}, & \text{critical regime,} \\ -|r_0|^{(2-3z)\nu/2}T^2, & \text{Fermi liquid regime.} \end{cases} \tag{24}$$

For the thermopower S we get, using $S \propto m^*T$, $S \propto C$ in both the critical regime and the Fermi liquid regime.

VII. SCALING PROPERTIES WITHIN THE SPIN-FERMION MODEL

The results of the phenomenological theory, presented in the previous sections, can alternatively be derived within an approach based on the spin-fermion model [11,12], assuming fermions ψ to couple to a spin-1 boson field $\boldsymbol{\phi}$ describing collective antiferromagnetic spin fluctuations according to

$$S_{\rm int} = g\int d^dx\,\psi^\dagger\boldsymbol{\sigma}\psi\cdot\boldsymbol{\phi}. \tag{25}$$

As mentioned in Sec. I, the role of critical fluctuations for the fermionic spectrum was traditionally studied at and near hot spots or lines of the Fermi surface, where $\varepsilon_{\mathbf{k}_F} = \varepsilon_{\mathbf{k}_F+\mathbf{Q}}$ with magnetic ordering vector $\mathbf{Q}$. For example, the self-energy in one-loop approximation at hot spots behaves [11] as $\Sigma_h(\omega) \propto g^2 i\omega|\omega|^{\frac{d-3}{2}}$ for a d-dimensional system. Note that in this section, ω is a Matsubara frequency. Thus for $d \leqslant 3$ one obtains deviations from Fermi liquid behavior [23], $\Sigma_{FL}(\omega) \propto i\omega$, for hot momenta. Up to order g^2, Fermi liquid behavior occurs for generic, cold quasiparticles. However, Hartnoll *et al.* [6] demonstrated that higher order processes, involving fermions which effectively couple via off-shell intermediate states to $\boldsymbol{\phi}^2$, affect the cold regions as well, albeit with less strong singularities in the single-particle excitation spectrum. Generalizing their findings to arbitrary dimension, one finds a self-energy contribution on the cold parts of the Fermi surface $\Sigma_c(\omega) \propto g^4 i\omega|\omega|^{d-\frac{3}{2}}$, as we previously obtained in Eq. (4). Even though this behavior is subleading with respect to Fermi liquid behavior for $d > \frac{3}{2}$, it constitutes a singular correction. It is at the heart of our theory to show how this singular correction may be boosted within a self-consistent approach.

To extract this important physics, we "patch" the Fermi surface into hot and cold regions (h,c) and start from a bare action that sums over the patches (whose details are described in what follows):

$$S = \sum_{j=h,c}\int\left[\psi_j^\dagger(i\omega - \varepsilon_{\mathbf{k}}^j)\psi_j + g\psi_j^\dagger\boldsymbol{\sigma}\psi_j\cdot\boldsymbol{\phi} + \lambda\psi_j^\dagger\psi_j\boldsymbol{\phi}\cdot\boldsymbol{\phi}\right] + \frac{1}{2}\int(r_0+q^2)\boldsymbol{\phi}\cdot\boldsymbol{\phi}. \tag{26}$$

Here, and in what follows, the boson field $\boldsymbol{\phi}$ has momentum $\vec{q}$, the fermion field ψ_j has momentum $\vec{k}$ within the patch j, and the integrations are over all these momenta. In Eq. (26), λ is the coupling of quasiparticles to a pair of bosons via intermediate off-shell fermionic states [6], as mentioned above. If we couple an external magnetic field to the electron spin, $\int\mathbf{h}\cdot\psi^\dagger\boldsymbol{\sigma}\psi$, we may shift $\boldsymbol{\phi}' = \boldsymbol{\phi} - \mathbf{h}/g$ and obtain the relation $\chi(\mathbf{q},\omega) = D(\mathbf{q},\omega) - r_0^{-1}$, which connects the spin susceptibility $\chi(\mathbf{q},\omega)$ and the propagator $D(\mathbf{q},\omega)$ of the bosons. Let $\Pi(\mathbf{q},\omega)$ be the full bosonic self-energy. Then

$$D(\mathbf{q},\omega) = \frac{1}{r_0 + q^2 - \Pi(\mathbf{q},\omega)}.$$

Close to the critical point at the ordering vector ($q=0$), $r_0 \simeq \Pi(\mathbf{Q},0)$. This model is valid up to the bandwidth, W.

We now set up a matching procedure by first integrating out all states down to an energy $\Lambda < W$. This introduces boson and (hot and cold) fermion self-energies into the bare action of Eq. (26) as well as renormalized couplings Γ among the fields. The effective low-energy action is

$$S_{\rm low} = \sum_{j=h,c}\int\psi_j^\dagger[i\omega - vk - \Sigma_j^>(k,\omega) + \Gamma_{j,g}^>\sigma\cdot\phi]\psi_j + \frac{1}{2}\int[r_0 + q^2 - \Pi^>(q,\omega)]\boldsymbol{\phi}^2 + \int\Gamma_\lambda^>\psi_c^\dagger\psi_c\boldsymbol{\phi}^2. \tag{27}$$

We have taken the bare Fermi velocities of both hot and cold electrons to be equal, for simplicity. The relevant bare couplings are g and $\lambda \simeq g^2/E_F$. Here $\Sigma_j^>(k,\omega)$, etc., refer to scattering processes that involve energies above Λ. The behavior in the high-energy region is governed by the bare action [Eq. (26)], while the behavior for energies below Λ is governed by $S_{\rm low}$. In what follows, we shall match the low- and high-energy sectors at Λ.

We parametrize the self-energy and vertex functions as

$$\begin{aligned}\Sigma_j^>(k,\omega) &= (1 - Y_{j,\omega})i\omega + v(Y_{j,k}-1)k,\\ \Gamma_{j,g}^>(k,q,\omega,\Omega) &= gY_{j,g},\\ \Gamma_\lambda^>(k,q,\omega,\Omega) &= \lambda Y_{c,g}^2Y_\lambda.\end{aligned} \tag{28}$$

The Y_j are all functions of Λ.

Introducing quasiparticle operators $\psi_{j,r} = \psi_j Y_{j,\omega}^{1/2}$, we arrive at the low-energy quasiparticle action

$$S_r = \sum_{j=h,c}\int\left[\psi_{j,r}^\dagger(i\omega - v_j^*k)\psi_{j,r} + g_j^*\int\psi_{j,r}^\dagger\boldsymbol{\sigma}\psi_{j,r}\cdot\boldsymbol{\phi}\right] + \frac{1}{2}\int[r_0 - \Pi^>(q,0) + q^2]\boldsymbol{\phi}^2 + \lambda^*\int\psi_{c,r}^\dagger\psi_{c,r}\boldsymbol{\phi}^2 \tag{29}$$

that is governed by renormalized velocities and coupling constants: $v_j^* = vY_{j,k}/Y_{j,\omega}$, $g_j^* = gY_{j,g}/Y_{j,\omega}$, and $\lambda^* = \lambda Y_{c,g}^2Y_\lambda/Y_{c,\omega}$. In the following, we shall label the self-energies of the ψ_r field by a subscript "qp".

There are no singular corrections to the boson self-energy; its nonsingular frequency and momentum behavior can be absorbed into the existing frequency and momentum dependence and it is unnecessary to introduce a renormalized $\boldsymbol{\phi}$ operator. Finally, the boson self-energy $\Pi_{qp}(q,\omega)$ is determined perturbatively; see below.

The renormalization of the coupling constant λ is a consequence of the composite nature of its coupling and reflects the fact that the coupling to energy-density fluctuations is affected by renormalizations Y_g of the coupling constant g.

The key idea is to develop a perturbation theory in the low-energy sector in terms of the renormalized coupling constants. To this end, we take advantage of the fact that the momentum dependence of the self-energy is weak, so that $Y_{j,k} \approx 1$. In addition we use the small-q Ward identity $Y_\lambda = Y_{c,\omega}$, which reflects energy conservation.

Making contact with the earlier sections, we introduce $Z_j^{-1} = Y_{j,\omega}$ for the quasiparticle weights. Z_c is to be identified with the Z of Secs. I–IV. We obtain $v_c^* = vZ_c$, $v_h^* = vZ_h$, $g_c^* = Z_c Y_{c,g}$, $g_h^* = gZ_h Y_{h,g}$, and $\lambda^* = \lambda Y_{c,g}^2$. This leaves us with three unknown renormalization factors. At a quantum critical point one expects power-law solutions of the kind $Y_{h,g} \propto Y_{c,g} \propto |\omega|^{-\phi}$ (we have assumed that the two Y_j are governed by the same exponent ϕ, which we leave undetermined until the end of this section), $Z_h \propto |\omega|^{\eta_h}$, and $Z_c \propto |\omega|^{\eta_c}$. These three exponents lead to corresponding dynamic scaling exponents of the critical degrees of freedom: spin fluctuations, hot quasiparticles, and cold quasiparticles. In the case of the fermionic degrees of freedom, we obtain dynamic scaling exponents $z_{f,c} = \frac{1}{1-\eta_c}$ for cold and $z_{f,h} = \frac{1}{1-\eta_h}$ for hot portions of the Fermi surface. For the bosonic self-energy due to a quasiparticle loop, it follows from low-energy perturbation theory that

$$\Pi_{qp}(q,\omega) \approx \Pi_{qp}(Q,0) - \gamma|\omega|$$

with the coefficient of the Landau damping $\gamma = (g_h^*/v_h^*)^2/Q = (gY_{h,g}/v)^2/Q$.

Inserting this result into the bosonic propagator, we find at the critical point the dynamic bosonic scaling exponent

$$z = \frac{2}{1-2\phi}. \tag{30}$$

As pointed out earlier, an anomalous dynamic critical exponent, as seen in the experiments by Schröder *et al.* [20], requires a nontrivial exponent ϕ in the vertex renormalization. A straightforward perturbation theory (at $T = 0$) with respect to λ^* yields the self-energy of renormalized quasiparticles on the cold parts of the Fermi surface:

$$\Sigma_{qp,c}(i\omega) \propto \frac{\lambda^{*2}}{v_c^*}\gamma^{d-5/2}\mathrm{sign}(\omega)|\omega|^{\frac{2d-1}{2}}, \tag{31}$$

while perturbation theory with respect to g_h^* yields for hot carriers

$$\Sigma_{qp,h}(i\omega) \propto \frac{g_h^{*2}}{v_h^*}\gamma^{d/2-3/2}\mathrm{sign}(\omega)|\omega|^{\frac{d-1}{2}}. \tag{32}$$

Thus far, high- and low-energy processes have been treated rather differently. Yet, they meet at the scale Λ. The matching is realized as follows: For each sector (hot, cold), the Green's function G generated by the action S_{low} is matched to G_{qp}, the one generated by the low-energy "quasiparticle" action S_r of Eq. (29). We find

$$G(\omega = \Lambda) = Z_s(\omega = \Lambda)G_{qp}(\omega = \Lambda), \tag{33}$$

where $1/Z_s(\omega) = 1 - \partial\Sigma^>(\omega)/\partial\omega$.

In a genuine strong-coupling regime, we expect that the quantum critical behavior is not confined to low energies but extends to high energies. Then the scale Λ is not a physically motivated crossover scale, but rather an arbitrary intermediate scale. Therefore, we can generalize Eq. (33) and request that for arbitrary ω,

$$\Sigma_{qp}(\omega) = Z_s(\omega)\Sigma^>(\omega), \tag{34}$$

where the left-hand side is given by the perturbative results of Eqs. (31) and (32). In addition, the matching yields that Z_s is identical to $Z = 1/Y_\omega$ of earlier paragraphs. Knowing the power-law behavior of Σ_{qp}, we may look for power-law solutions $Z_j \propto \omega^{\eta_j}$, with the result that

$$\eta_c = d - \frac{3}{2} + \phi(1-2d), \tag{35}$$

$$\eta_h = \frac{3-d}{2} + \phi(d-1). \tag{36}$$

Low-order perturbation theory within the spin-fermion model yields $\phi = 0$ for $d > 2$; i.e., there are no singular renormalizations of the fermion-boson coupling g and correspondingly no changes in the dynamic scaling exponent z, Eq. (30), from its mean-field value $z = 2$. In this limit, we obtain for hot carriers that $\eta_h(\phi = 0) = \frac{3-d}{2}$. Most interestingly, we do obtain a nontrivial result for the anomalous exponent of the cold carriers $\eta(\phi = 0) = d - 3/2$. Thus, even at the lowest level the self-consistent perturbation theory presented here yields genuine non-Fermi-liquid behavior on the entire Fermi surface.

Our phenomenological framework developed here allows furthermore to go beyond the spin-fermion model to include effects of higher order perturbation theory or due to additional interaction channels. For example, as shown recently [24], the actual derivation of the $q = 0$ Ward identity requires the resummation of an infinite class of diagrams, including, in particular, diagram structures of the Azlamazov-Larkin type [25]. Recently, new Ward identities for the spin vertex that are valid at any wave vector $\mathbf{q}$ have been discovered [18], which relate the spin vertex to the effective mass enhancement. As discussed above, we can explore the implications of this result, that the Ward identity for the spin-vertex at $\mathbf{q} = 0$ carries over to the vertex at momentum transfer $\mathbf{q} = \mathbf{Q}$, which means $Y_{h,g} = Z_c^{-1}$. This relation immediately implies $\phi = \eta_c$, which turns Eq. (35) into a self-consistent equation for η_c and yields

$$\eta_h = \frac{3+d}{4d}, \quad \eta_c = \frac{2d-3}{4d}, \tag{37}$$

as was obtained in the phenomenological theory presented above, in Eq. (7), including the dynamic scaling exponent z obtained earlier in Eq. (10). In fact, (Z_c, η_c) should be identified with (Z,η) of previous Secs. I–IV.

VIII. COMPARISON WITH EXPERIMENTS ON $CeCu_{6-x}Au_x$

The above results, in the case of 3D fluctuations, are identical to the ones obtained by two of us previously, [7,8], where impurity scattering was invoked to give rise to a critical, weakly momentum-dependent self-energy. In particular, the Z exponent $\eta = 1/4$ found there, and the ensuing critical indices $z = 4, \nu = 1/3$, are the same as the ones found in the present work for the clean system. The excellent agreement of the theory [7,8] with the experimental data on $YbRh_2Si_2$ (YRS)

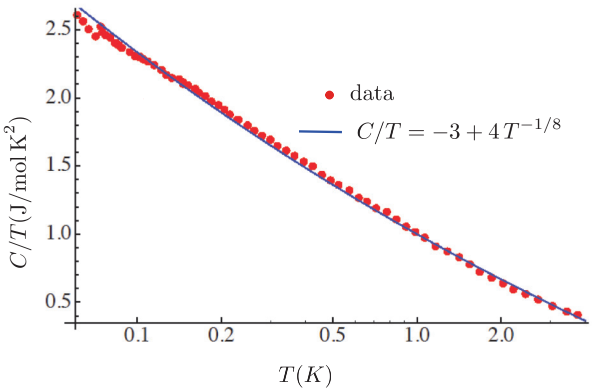

FIG. 3. (Color online) Specific heat: Comparison of theory Eq. (19) and experimental data [26] for $CeCu_{6-x}Au_x$ at the critical concentration $x = 0.1$.

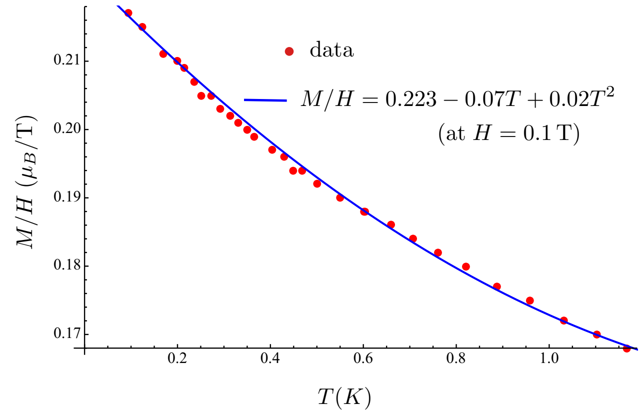

FIG. 5. (Color online) Uniform magnetization: Comparison of theory Eq. (20) and experimental data [26] for $CeCu_{6-x}Au_x$ at the critical concentration $x = 0.1$.

in the regime close to the QCP therefore applies to the present theory as well. In contrast to that earlier work, the present results do not depend on the impurity concentration. Indeed, in experiment, the critical parts of, e.g., the specific heat do not show a dependence on the impurity content of the sample.

We turn to a different case, $CeCu_{6-x}Au_x$ (CCA), for which a QCP has been found at the concentration $x = 0.1$ at ambient pressure in the absence of a magnetic field and at slightly different concentrations at a critical pressure and/or an applied critical field. As suggested by the neutron scattering data, the magnetic fluctuations there appear to be quasi-two-dimensional. We therefore compare our results for $d = 2$ with the available data. In doing this we keep in mind that generically in the case of quasi-two-dimensional spin fluctuations in a three-dimensional metal, the hot regions on the Fermi surface (the regions where both partners of a particle-hole excitation at $q = Q$ are near the Fermi surface ($\epsilon_{\mathbf{k}} \approx \epsilon_{\mathbf{k+Q}} \approx 0$) occupy a finite fraction of the Fermi surface (the scenario of quasi-two-dimensional fluctuations in the 3D metal CCA was first proposed by Rosch *et al.* [27] in the framework of Hertz-Millis theory). We assume this fraction to be sufficiently small, such that over a wide intermediate temperature range, quasiparticles on the cold parts of the Fermi surface dominate. However, below some crossover

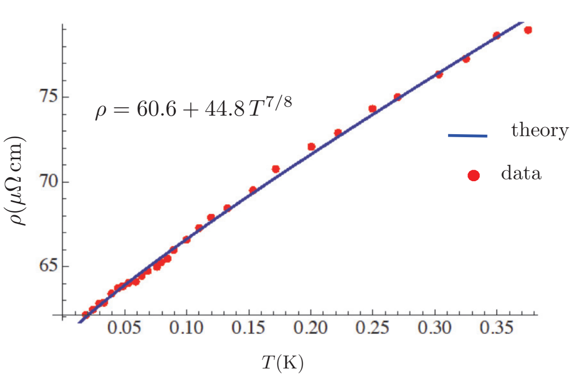

FIG. 4. (Color online) Resistivity: Comparison of theory Eq. (24) and experimental data [28] for $CeCu_{6-x}Au_x$ at the critical concentration $x = 0.1$.

temperature the critical behavior in that case will be governed by the hot quasiparticles. In Fig. 2, we have already compared theory and experiment for the dynamical spin susceptibility. In Fig. 3, we show the specific-heat data [26] in comparison with $C/T \propto T^{-1/8}$ as obtained above in Eq. (19). The resistivity result $\rho(T) - \rho(0) \propto T^{7/8}$ of Eq. (24) is fitted to the data in Fig. 4.

Our prediction for the uniform magnetization is $M(T) = M(0) - aT + bT^2$, from Eq. (20) augmented by a Fermi liquid correction $\propto T^2$. It fits the data [26] well, as shown in Fig. 5.

IX. CONCLUSION

We presented a semi-phenomenological theory of quantum criticality near a critical point that separates antiferromagnetic and paramagnetic phases of a metal. Starting from the assumption that the Landau quasiparticle effective mass diverges on approaching the critical point, giving rise to critical quasiparticles, we identified the corresponding renormalization of the dynamical spin susceptibility near the antiferromagnetic wave vector. Critical contributions to the electron self-energy induced by antiferromagnetic fluctuations in a clean system are known to be strongly anisotropic (confined to the "hot spots"). However, impurity scattering may be shown [7,8] to distribute the effects of critical scattering all over the Fermi surface. Here we have shown that even in a clean system, the critical antiferromagnetic fluctuations give rise to a critical self-energy uniformly over the Fermi surface. This is because the magnetic fluctuations generate energy fluctuations, which diverge in the long-wavelength limit. The scattering of quasiparticles off these energy fluctuations leads to a contribution to the effective mass which is nominally proportional to a positive power of energy, but is strongly enhanced by factors of the effective mass itself. This leads to a self-consistency relation for the effective mass (or the quasiparticle Z factor), which may have a strong-coupling solution provided the initial value of Z at the appropriate high-energy scale is sufficiently small (as may be caused by precursor fluctuations leading to a weakly diverging effective mass). While the critical quasiparticles living on the "cold" parts of the Fermi surface dominate most of the observable quantities, the "hot" quasiparticles may be shown to be even more singular; e.g., in $d = 3$, we find the equivalent of the Z-factor exponent η to be $= 1/2$. In this context, it is interesting to observe that the observed critical behavior of CCA depends on whether the QCP is tuned by varying the Au concentration, the pressure, or the magnetic field. It is conceivable that in the case of magnetic field tuning the precursor fluctuations necessary to access the strong-coupling regime are too weak so that the system remains in the weak-coupling regime, as is apparently observed. A further condition for the applicability of the self-consistent solution is that the effective dimension of the bosonic fluctuations, $z + d$, is sufficiently above the upper critical dimension of the appropriate field theory (e.g., ϕ^4 theory), such that boson-boson-interaction effects may be neglected.

Application of our theory to the cases of 3D and 2D fluctuations in a three-dimensional metal leads to a critically diverging effective mass $m^* \propto T^{-\eta}$ with $\eta = 1/4$ (3D) and $\eta = 1/8$ (2D), in good agreement with experimental data on the two heavy-fermion compounds YRS and CCA, where neutron scattering showed the presence of 3D and 2D AFM fluctuations. Our theory obeys hyperscaling, taking into account the scaling of the critical fermions. Further comparisons of our theory with experimental data on YRS and CCA show good agreement. In particular the universal behavior of the Grüneisen ratio in the quantum-disordered regime measured in YRS is in excellent agreement with our result [8].

Finally, we emphasize that we assumed the heavy quasiparticles to be robust, though modified by scattering from critical spin fluctuations. There is no breakdown of the Kondo effect nor an associated collapse of part of the Fermi surface in our scenario. Experimental features, such as the crossover behavior observed in transport properties (and, to a lesser extent, in the thermodynamic quantities) across the "T^* line" in the T-H phase diagram of YRS, may be accounted for by a change in quasiparticle scattering strength associated with thermal activation of the (ESR) spin resonance as well as by single-quasiparticle spin-flip scattering [29,30].

While the good agreement of our theory with experiment across the board is encouraging, there is a need to put the phenomenological assumptions it involves on a firm microscopic basis. Work in this direction is in progress.

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APPENDIX: CORRELATION LENGTH

The control parameter r in Eq. (1) that describes the distance to the critical point has a nonanalytic contribution from the irreducible spin polarization $\Pi(q,\omega)$, which generates the full susceptibility:

$$\chi(q,\omega) = \frac{\Pi(q,\omega)}{1 + \Gamma^{\omega}(q)\Pi(q,\omega)}, \tag{A1}$$

where $\Gamma^{\omega}(q)$ is an irreducible quasiparticle-quasihole scattering vertex that has a minimum at $\mathbf{q} = \mathbf{Q}$. Schematically,

$$\Pi(Q,\omega_m) = \sum_{k,n} \lambda_Q^2 G(k,\varepsilon_n)G(k + Q,\varepsilon_n + \omega_m), \tag{A2}$$

where λ_Q is the spin vertex part discussed in the text, Eq. (1).

The imaginary part of Π arises from Landau damping and is renormalized by the λ_Q vertices:

$$\mathrm{Im}\,\Pi(Q,\omega) \propto N_0\lambda_Q^2(\omega/v_F Q). \tag{A3}$$

In contrast, the real part of Π is governed by high-energy contributions and its leading contribution is unrenormalized $\mathrm{Re}\,\Pi(Q,\omega) \propto N_0(1 + \ldots)$. There is, however, a nonanalytic subleading contribution to $\mathrm{Re}\,\Pi$, which may be seen from the Kramers-Kronig transform on $\mathrm{Im}\,\Pi$ to be of the form

$$\mathrm{Re}\,\Pi(Q,0) \propto N_0\lambda_Q^2 T.$$

This contribution is responsible for the T dependence of the correlation length in the critical region: $1/\xi(T) \propto \lambda_Q(T)T^{1/2}$.

We turn now to the dependence of ξ on the tuning field, say H. The scattering vertex Γ^{ω} is analytic in H, but we expect $\Pi(Q,\omega = 0)$ to be nonanalytic at the critical field H_c. This may be seen by examining the behavior of $\partial\Pi/\partial H$. From Eq. (A2), one sees that this involves a factor $\partial G/\partial H$ that contains a ($\mathbf{q} = \mathbf{0},\omega \to \mathbf{0}$) spin vertex, which is $\propto 1/Z$, from a Ward identity related to particle number and spin conservation. Outside the critical cone, $Z(H) \propto (H - H_c)^{\eta z\nu}$, so that integrating $\partial\Pi/\partial H \propto 1/Z(H)$, we find $\mathrm{Re}\,\Pi(H) \propto (H - H_c)^{1-\eta z\nu}$. By equating $\mathrm{Re}\,\Pi$ and $\xi^{-2} \propto (H - H_c)^{z\nu}$, we determine the correlation length exponent as

$$\nu = \frac{2}{2 + z\eta}. \tag{A4}$$

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