$z = 3$ antiferromagnetic quantum critical point: U(1) slave-fermion theory of Anderson lattice model

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(Dated: June 9, 2009)

We find the dynamical exponent $z = 3$ antiferromagnetic (AF) quantum critical point (QCP) in the heavy fermion quantum transition beyond the standard framework of the Hertz-Moriya-Millis theory with $z = 2$. Based on the U(1) slave-fermion representation of the Anderson lattice model, we show the continuous transition from an antiferromagnetic metal to a heavy fermion Fermi liquid, where the heavy fermion phase consists of two fluids, differentiated from the slave-boson theory. Thermodynamics and transport of the $z = 3$ AF QCP are shown to be consistent with the well-known non-Fermi liquid physics such as the divergent Grüneis ratio with an exponent $2/3$ and temperature-linear resistivity. In particular, the uniform spin susceptibility turns out to diverge with an exponent $2/3$, the hallmark of the $z = 3$ AF QCP described by deconfined bosonic spinons.

PACS numbers: 71.10.Hf, 71.10.-w, 71.10.Fd, 71.30.+h

The continuous quantum transition from an antiferromagnetic (AF) metal to a heavy fermion (HF) Fermi liquid has been one of the central interests in strongly correlated electrons since its quantum critical point (QCP) is beyond the description of the Landau's Fermi liquid theory and Landau-Ginzburg-Wilson’s framework for phase transitions, two cornerstones in modern theory of metals [1]. Thermodynamics such as the divergent Grüneisen ratio with an exponent $2/3$ [2] and non-Fermi liquid transport of temperature-linear resistivity [3] are difficult to describe in the standard framework based on the weak coupling approach, that is, Hertz-Moriya-Millis (HMM) theory for the AF transition [4].

Recently, critical hybridization fluctuations described by the dynamical exponent $z = 3$ were proposed in the U(1) slave-boson description for the HF transition [5, 6], explaining both the thermodynamics [7] and transport [8] qualitatively well. However, quantum fluctuations of spin dynamics are overestimated in the slave-boson representation, giving rise to the so-called fractionalized Fermi liquid [8] instead of an AF metal. In addition, introduction of the hybridization order parameter allows an artificial finite temperature transition, not observed but identified with the crossover to the HF phase in experiments.

In this paper we revisit the AF to HF quantum transition, based on the U(1) slave-fermion representation incorporating AF correlations well. On the contrary to the common wisdom, we show that the slave-fermion description allows the HF liquid, resorting to the Luttinger theorem [10] and an explicit mean-field analysis. In particular, the artificial HF transition at finite temperatures does not appear in the slave-fermion representation, where the HF phase is not described by band hybridization, different from the slave-boson theory.

Our main result is that critical spin dynamics described by bosonic spinons is governed by the dynamical exponent $z = 3$ resulting from Landau damping of conduction electrons and fermionic holons, basically the same as critical hybridization fluctuations in the slave-boson theory [5, 6] but completely different from the HMM theory with $z = 2$. As a result, the slave-fermion theory reproduces the anomalous thermodynamics [7] and non-Fermi liquid transport [8] of the slave-boson description.

The hallmark of the $z = 3$ AF QCP is seen from the uniform spin susceptibility diverging with an exponent $2/3$, consistent with an experiment $0.72 \pm 0.05$ [11]. This result turns out to originate from the bosonic nature of fractionalized spinon excitations. Scaling of several quantities is shown for various scenarios in Table I.

| & $z \& \nu$ & $\Gamma(T)$ & $\chi(T)$ & $\rho(T)$ |
|---|---|---|---|---|
| SF QCP | $3 \& 1/2$ | $T^{-2/3}$ | $T^{-2/3}$ | $T \ln(2T/E^*)$ |
| KB QCP | $3 \& 1/2$ | $T^{-2/3}$ | const. | $T \ln(2T/E^*)$ |
| Local QCP | $-\infty \& ??$ | $T^{-w}$ | $T^{-w,\nu}$ | ?? |
| HMM QCP | $2 \& 1/2$ | $T^{-1}$ | const. | $T^{3/2}$ |

TABLE I: Scaling of Grüneisen ratio $\Gamma(T)$, uniform spin susceptibility $\chi(T)$, and resistivity $\rho(T)$ with dynamical $z$ and correlation-length $\nu$ exponents in $d = 3$ for the slave-fermion (SF), Kondo breakdown (KB), Local, and Hertz-Moriya-Millis (HMM) QCP scenarios, respectively.

We point out that our present study generalizes the slave-fermion description for ferromagnetism in the Anderson lattice model [12] into the case of antiferromagnetism and the slave-fermion study for the two impurity problem [13] into the case of an impurity lattice, respectively. The $z = 3$ AF QCP is consistent with the previous slave-fermion study [14], where both the existence of the QCP and dynamics of holons are assumed, but not fully justified.

We start from the U(1) slave-fermion representation of
an effective Anderson lattice model

\[
Z = \int Dc_{i\sigma} Db_{i\sigma} Df_i D\Delta_{ij} D\chi_{ij}^0 D\lambda_e e^{-\frac{\beta}{\hbar} \int_0^\beta dt L},
\]

\[
L = L_c + L_f + L_h + L_V + L_0,
\]

\[
L_c = \sum_i c_{i\sigma}^\dagger (\partial_\tau - \mu) c_{i\sigma} - t \sum_{(ij)} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.),
\]

\[
L_f = \sum_i f_i^\dagger (\partial_\tau + i\lambda_i) f_i + \alpha t \sum_{(ij)} (f_i^\dagger \chi_{ij}^0 f_j + H.c.),
\]

\[
L_h = \sum_i b_{i\sigma}^\dagger (\partial_\tau + \epsilon_f + i\lambda_i) b_{i\sigma} - \alpha t \sum_{(ij)} (b_{i\sigma}^\dagger \chi_{ij}^0 b_{j\sigma} + H.c.),
\]

\[
L_V = V \sum_i (c_{i\sigma}^\dagger b_{i\sigma} f_i + H.c.),
\]

\[
L_0 = \alpha t \sum_{(ij)} (\chi_{ij}^0 f_i + H.c.) + N J \sum_{(ij)} |\Delta_{ij}|^2
\]

\[
- \frac{i}{\hbar} \sum_{ij} 2NS\lambda_i, \quad (1)
\]

where the hybridization term \( V \) competes with the AF correlation term \( J \) for localized electrons, modelled as the nearest neighbor spin-exchange interaction. \( L_c \) describes dynamics of conduction electrons \( c_{i\sigma} \), where \( \mu \) and \( t \) are their chemical potential and kinetic energy, respectively. \( L_f \) and \( L_h \) govern dynamics of localized electrons, decomposed with fermionic holons \( f_i \) and bosonic spinons \( b_{i\sigma} \), where local AF correlations \( \Delta_{ij} \) are introduced in the Sp(N) representation for the spin-exchange term \( J \) with an index \( n = 1, \ldots, N \) and an almost flat band with \( \alpha \ll 1 \) is allowed to describe hopping of holons \( \chi_{ij} \) and spinons \( \chi_{ij}^0 \), respectively. \( \epsilon_f \) is an energy level for the flat band, and \( \lambda_i \) is a Lagrange multiplier field to impose the spin-fermion constraint. \( L_V \) is the hybridization term, involving conduction electrons, holons, and spinons. \( L_0 \) represents condensation energy with \( N = 1 \) and \( S = 1/2 \) in the physical case.

In the limit of \( V \to 0 \) the slave-fermion Lagrangian is reduced to two decoupled sectors for conduction electrons and spinons, where ferromagnetic (FM) correlations \( \chi_{ij}^0 \) vanish in the spinon sector, recovering the Schwinger-boson theory for the half filled quantum antiferromagnet [10]. In this respect the present problem generalizes the Schwinger-boson theory, turning on hybridization fluctuations to cause "hole doping" in the localized band, represented by fermionic holons. Particularity, hybridization fluctuations give rise to FM correlations, weakening AF correlations \( \Delta_{ij} \) and destroying the AF order \( \langle b_{i\sigma} \rangle = 0 \).

The resulting paramagnetic phase turns out to be a HF metal, differentiated from that of the slave-boson theory described by band hybridization, where the localized band is decoupled with the conduction band due to gapping of spinons \( \langle b_{i\sigma} \rangle = 0 \). Instead, the effective chemical potential denoted by \( \lambda_v \) is changed by the hybridization coupling constant \( V \), filling holons to the almost flat band. In this respect the HF phase of the slave-fermion representation consists of two kinds of fluids, corresponding to light fermions of conduction electrons and heavy fermions of holons, respectively.

The presence of the HF phase in the slave-fermion description can be argued from the Luttinger theorem. Inserting the total electric charge \( \delta = c_i^\dagger c_i - f_i^\dagger f_i \) into the single occupancy constraint \( b_{i\sigma}^\dagger b_{i\sigma} + f_i^\dagger f_i + 2N\Delta_{ij}^0 \Delta_{ij} \) vanishes but antiferromagnetic correlations \( \Delta \) still exist.

As a result, the Luttinger theorem holds, given by \( \frac{\delta}{2\pi} = 1 + \delta - 2\Delta^2 \) and implying the large Fermi surface, where \( V_{FS} \) is the volume of the electron Fermi surface and \( \delta \) is the density of conduction electrons in the decoupling limit. It is interesting to observe that the area of the Fermi surface is not \( 1 + \delta \) but smaller owing to the presence of AF correlations.

Performing the mean-field approximation of uniform hopping \( \chi_{ij} \to \chi_{ij}^0 \), pairing \( \Delta_{ij} \to \Delta \), and chemical potential \( \lambda_v \to \lambda \), we find the slave-fermion mean-field phase diagram for the Anderson lattice model (Fig. 1). Actually, we see that the spinon condensation amplitude vanishes at the critical hybridization strength \( V_c \). In the AF phase \( (V < V_c) \) band hybridization is allowed, but the area of the Fermi surface will be small, proportional to \( \delta \) because the effective chemical potential of holons is almost on the top of the holon band and the density of holons is vanishingly small. Enhancing the hybridization coupling constant, the holon chemical potential shifts to the lower part, filling holons into the flat band and causing heavy fermions. In this description the HF transition at finite temperatures turns into crossover, where the crossover temperature \( T_{FL} \) is given by gap of spinon excitations \( T_{FL} \sim \xi_s^{-1} \) with the correlation length \( \xi_s = \left[(\lambda - 2\delta \epsilon_f)^2 - (2\Delta)^2\right]^{-1/2} \) since scattering of conduction electrons and holons with spinon fluctuations is suppressed below this temperature allowing Fermi liquid physics.

Thermodynamics around the slave-fermion AF QCP can be understood from the scaling expression of the free energy

\[
f_s(r, T) = b^{-(d+z)} f_s(rb^{1/\nu}, T b^z), \quad (2)
\]
where \( r \propto |V - V_c| \) is an external parameter associated with mass for critical fluctuations and \( b \) is a scaling parameter with dimension of length. The dynamical exponent \( z \) tells the nature of critical fluctuations, i.e., their dispersion relation \( \Omega \propto q^z \), and the correlation-length exponent \( \nu \) gives how the correlation length \( \xi \) changes with respect to the external parameter \( r \), i.e., \( \xi \propto |r|^{-\nu} \). Our main problem is to derive this scaling free energy from the slave-fermion theory. Actually, this was performed in the slave-boson context, constructing the Luttinger-Ward (LW) functional in the Eliashberg approximation \([17]\), where momentum dependence in fermion self-energies and vertex corrections are neglected, allowing us to introduce one loop-level quantum corrections fully self-consistently. It was explicitly demonstrated that the Eliashberg framework is “exact” in the large \( N \) limit \([18]\).

Our main discovery is that dynamics of spinon fluctuations is described by \( z = 3 \) critical theory due to Landau damping of electron-phonon polarization above an intrinsic energy scale \( E^* \), while by \( z = 1 \) O(4) nonlinear \( \sigma \) model \([19]\) below \( E^* \). The energy scale \( E^* \sim \alpha D(q^*/k_F)^3 \) originates from the mismatch \( q^* = |k_F - k_F^c| \) of the Fermi surfaces of the conduction electrons \( k_F^c \) and holons \( k_F \), shown to vary from \( \mathcal{O}(10^4) \) \( mK \) to \( \mathcal{O}(10^2) \) \( mK \) \([3, 8]\). Actually, inserting the Landau damping self-energy \( \Pi_b(q, i\Omega) = \gamma_b(q/\Omega^2) \) with the damping coefficient \( \gamma_b = \frac{\pi k_F^2}{v_F^2} \) into the spinon’s full propagator, where \( \rho_c \) is the density of states for conduction electrons and \( v_F \) is the holon velocity, we find their \( z = 3 \) dynamics

\[
\Im D_b(q, \Omega) \approx -\frac{\gamma}{2\gamma_b q^6 + \gamma^2 \Omega^2} \tag{3}
\]

with \( \gamma \equiv (2\gamma_b)(2d \Delta / v_s^2) \), where \( v_s = \sqrt{2[\alpha t \chi_f(\lambda - 2d \alpha t \chi_f) + (2d \Delta)]} \) is the velocity of spinons. Then, the correlation-length exponent is given by the usual mean-field value \( \nu = 1/2 \) since the critical theory is above its upper critical dimension in \( d = 3 \).

Inserting Eq. (3) into the LW expression of the free energy, we find Eq. (2) with \( z = 3 \) and \( \nu = 1/2 \) for the singular part above \( E^* \) \([17]\). As a result, we obtain both the logarithmic divergent specific heat coefficient and power-law diverging thermal expansion coefficient, giving rise to the divergent Gruneisen ratio \( T^{-1/\nu} \) \( = 2 \) with an exponent \( 2/3 \) up to the logarithmic correction \([5]\).

An important result of the \( z = 3 \) slave-fermion QCP is that the dynamic uniform spin susceptibility diverges with an anomalous exponent \( 2/3 \). The transverse spin susceptibility is given by sum of both spinon and electron susceptibilities

\[
\chi^{++}_{k}(q, \Omega) = \frac{N}{J(q) - 1} \frac{1}{\chi_{0b}(q, \Omega)} + \chi^{--}_{k}(q, \Omega), \tag{4}
\]

where the spinon response is the standard RPA expression with the momentum dependent exchange coupling

\[
\Im \chi_{0b}^{-\pm}(q, \Omega) \approx \frac{C_s N^{5/3}}{8\pi^4 \gamma_b^2} \Omega^{2/3}, \tag{5}
\]

where \( C_s = \int_{-1}^{0} dy \int_{0}^{\infty} dx \frac{x^2}{x^2 + y^2} \frac{y^{(s+1)}(x+1)}{x^{(s+1)}} \approx 0.52 \). One can check that this expression coincides with the scaling theory, meaning that replacement of \( r \) with the uniform magnetic field \( h \) in Eq. (2) gives rise to \( \chi_b^c(h, T) = T^{(d+z)/z - 2/z\nu} \frac{\partial^2 f^c(|x|, 1)}{\partial x^2} \bigg|_{x=hT^{-1/\nu}} \propto T^{2/3} \) in \( d = 3 \).

On the other hand, the electron spin susceptibility is \( \chi_{0c}^{-\pm}(q, \Omega) = \chi_b^c + \gamma_c(q/\Omega) \) in \( |\Omega| \ll q \), where \( \chi_b^c \) is the Pauli susceptibility and the damping coefficient is \( \gamma_c = \frac{N \rho_c}{\nu_b} \).

As a result, critical spinon excitations contribute to the spin susceptibility dominantly, given by (Top in Fig. 2)

\[
\Im \chi^{+\pm}_{k}(q, \Omega) \approx \frac{2N^2}{(dJ_c)^2} [\Im \chi^{+\pm}_{0b}(q, \Omega)]^{-1} \propto \Omega^{-2/3},
\]

where \( J_c \) is the critical value for the slave-fermion QCP.

The diverging uniform spin susceptibility with the exponent \( 2/3 \) is identified with the hallmark of the \( z = 3 \) AF QCP described by ”deconfined" bosonic spinons. If the QCP falls into the universality class of the HMM theory, the exponent for divergence is half of the present value \([21]\). Strength of divergence is enhanced by fractionalization, giving rise to multiple correlations of deconfined degrees of freedom \([22]\). If spinon excitations were fermionic in nature, the uniform susceptibility would be governed by the Pauli susceptibility. In addition, the singular behavior of the uniform susceptibility is a special feature of

FIG. 2: (Color online) Top: Uniform dynamic spin susceptibility described by deconfined bosonic spinons scales with \( \Omega^{-2/3} \) in the \( z = 3 \) regime. Bottom: Temperature linear electrical resistivity. Right-inset: Resistivity from conduction electrons (Blue) and that from holons (Black).

\( J(q) \) and \( \chi^{-\pm\pm}_{0b}(q, i\Omega) \equiv -\left\langle S_b^{+}(q, i\Omega)S_b^{-}(q, -i\Omega)\right\rangle_c \) are bare spin susceptibilities for spinons and electrons, respectively, with the subscript \( c \) meaning ”connected”.

We find the spinon susceptibility

\[
\Im \chi_{0b}^{-\pm}(\Omega) \approx \frac{C_s N^{5/3}}{8\pi^4 \gamma_b^2} \Omega^{2/3}, \tag{5}
\]
the slave-fermion description because it is difficult to find in the HMM framework, although it allows the Curie-Weiss behavior at the AF wave vector in itinerant electrons \(^2\).

The \(z = 3\) AF QCP results in the temperature linear resistivity. Electrical conductivity is given by the Ioffe-Larkin composition rule due to the single occupancy constraint \(^2\).

\[
\sigma_{cl} = \sigma_c + \frac{\sigma_f(\sigma_b + \sigma_\Delta)}{\sigma_f + \sigma_b + \sigma_\Delta} \approx \sigma_c + \sigma_f, \quad (6)
\]

where the subscript represents each field and the last expression resorts to \(\sigma_\Delta \to \infty\). This result is reasonable because only conduction electrons and holons carry electric charges.

Using the Kubo formula expressed by the current-current correlation function, we obtain

\[
\sigma_c(T) \approx \frac{2CN}{\pi} \frac{\rho_0 v_F^2}{3\Sigma_{c}(k_F, T)}, \quad \sigma_f(T) \approx \frac{C}{\pi} \frac{\rho_F v_F^2}{\Sigma_{f}(k_F, T)} \quad (7)
\]

in the one loop approximation with \(C = \int_{-\infty}^{\infty} dy \gamma_{\pi}^{(y^2 + 1)^{1/2}} = \frac{\pi}{2}\), where \(3\Sigma_{c,f}(k_F, T)\) are imaginary parts of the self-energies \(^2\). Scattering of fermions with \(z = 3\) critical fluctuations results in

\[
3\Sigma_{c}(T > E^*) = \frac{\gamma}{2\gamma_b} \frac{V^2}{12\pi^2 v_F^2} \ln \left(\frac{2T}{E^*}\right),
3\Sigma_{c}(T < E^*) = \frac{\gamma}{2\gamma_b} \frac{V^2}{12\pi^2 v_F^2} \frac{T^2}{E^*} \ln 2 \quad (8)
\]

for conduction electrons and

\[
3\Sigma_{f}(T > E^*) = 2N \frac{\gamma}{2\gamma_b} \frac{V^2}{12\pi^2 v_F^2} \ln \left(\frac{2T}{E^*}\right),
3\Sigma_{f}(T < E^*) = 2N \frac{\gamma}{2\gamma_b} \frac{V^2}{12\pi^2 v_F^2} \frac{T^2}{E^*} \ln 2 \quad (9)
\]

for holons, basically the same as those of the slave-boson theory \(^3\).

Bottom in Fig. 2 shows the quasi-linear behavior in temperature for electrical resistivity above \(E^*\), resulting from the dominant \(z = 3\) scattering with spinon fluctuations. The \(T\) linear relaxation time in transport is typical of the scaling of the free energy with \(z = 3\) and \(\nu = 1/2\), provided a mechanism for decaying the current is present in the theory \(^3\).

In the present study gauge fluctuations associated with spin collective modes are not taken into account, particularly, in the heavy fermion phase. Actually, this consideration is protected in the low temperature regime, where gauge fluctuations are gapped. The U(1) gauge symmetry is reduced to \(Z_2\) owing to the presence of both AF (\(\Delta\)) and FM (\(\chi_f\)) correlations. Introducing two energy scales of \(T_\Delta \propto J\Delta^2\) for AF correlations and \(T_\chi \propto \alpha T_\chi \chi_f\) for FM fluctuations, \(T_\Delta \gg T_\chi\) is expected because it is indeed true in the decoupling limit and \(\alpha \ll 1\) preserves this expectation. In the regime of \(T \leq T_\chi\), \(Z_2\) gauge fluctuations are gapped, justifying our treatment, where our rough estimate tells \(T_\chi \sim O(10^3)K\) larger than \(E^*\). Even in \(T \geq T_\chi\), dynamics of gauge fluctuations will be described by \(z = 3\) due to Landau damping of holon excitations, which cannot change our present results qualitatively, but modifying those quantitatively \(^2\), \(^2\).

In this paper we find \(z = 3\) AF QCP in the slave-fermion description for the HF quantum transition, where the HF phase is composed of both light conduction electrons and heavy holons. The \(z = 3\) quantum criticality turns out to result from fractionalization of spin excitations, giving rise to the well known anomalous thermodynamics \(^2\) and non-Fermi liquid transport \(^3\). In particular, the bosonic nature of deconfined spinons was shown to cause the divergent uniform spin susceptibility with an anomalous scaling exponent \(2/3\), the hallmark of the present theory, qualitatively consistent with an experiment \(^1\).

K.-S. Kim thanks C. Pépin for introducing this problem and helpful discussions on the initial stage. Fruitful discussions with T. Takimoto are appreciated.

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