Quantum phase transition in a two-dimensional Kondo-Heisenberg model: a Schwinger-boson large-\(N\) approach

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Strange metal behavior arises in heavy fermion metals close to antiferromagnetic transitions. An increasing amount of experiments indicates a link of such behavior to a Kondo breakdown quantum critical point. To shed light on this intriguing problem, we study the 2D Kondo-Heisenberg model using a dynamical large-\(N\) multichannel Schwinger boson approach. We identify and characterize the quantum phase transition from an antiferromagnetically ordered ground state to a Kondo-dominated paramagnetic state, and attribute a jump in certain phase shift to Kondo breakdown. In addition, we calculate transport and thermodynamic quantities and discuss them in the context of the experimental observations in quantum critical heavy fermion systems.

“Strange metal (SM)” behavior, which is characterized by a linear-in-temperature resistivity and logarithmic-in-temperature specific heat coefficient, has been reported in many strongly correlated electron systems close to metallic quantum phase transitions due to competing orders, such as in cuprate superconductors [1] and heavy fermion systems [2]. The microscopic origin of this common phenomenology remains an outstanding issue.

A particularly interesting class of materials with SM features are heavy fermion materials, such as YbRh\(_2\)Si\(_2\) [3–5], CeCu\(_{6-x}\)Au\(_x\) [6–9], and CeMIn\(_5\) with \(M = \) Co, Rh [10–12], where the systems can be tuned from an antiferromagnetically (AF) ordered phase to a paramagnetic Kondo-screened heavy Fermi liquid (FL) state through a quantum critical point (QCP) [13]. Low-temperature measurements such as the spin susceptibility of the majority of these materials indicate that the effective degrees of freedom are two-dimensional despite the overall 3D crystal structure [10, 13–15]. Moreover, many experimental findings strongly suggest Kondo breakdown (KB) [16, 17] to occur at the AF QCP, most notably the enlargement of the Fermi volume observed via Hall effect measurements [18, 19], the \(\omega/T\) scaling in the dynamical susceptibility [8] and the optical conductivity [20], and STM measurements [21]. These findings go beyond the standard Hertz-Millis type of spin-density-wave theory [22], critical quasiparticle approaches [23], and phenomenological approaches [24].

To account for the nature of the QCP, Doniach’s framework for heavy fermion systems where the Kondo effect competes with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in the form of a Kondo-Heisenberg (KH) model is an appropriate starting point. Kondo breakdown in the KH model has been extensively studied by the EDMFT method [16, 25, 26], which covers the antiferromagnetically ordered and Kondo-screened heavy Fermi liquid phases as well as the dynamical \(\omega/T\) scaling in the quantum critical regime that reflects the dynamical competition between the RKKY and Kondo interactions. Several other techniques have also been used to study this problem [27–30], which capture aspects of the Kondo breakdown physics. In this work, we take a dynamical large-\(N\) Schwinger boson approach to the 2D KH model, generalized from the two-impurity Kondo model [31]. A simplified version of this approach on a 1D Kondo lattice model was recently studied [32, 33]. This method is able to

FIG. 1. (a) Phase diagram mapped out using the specific heat coefficient. The AF and heavy FL ground states are separated by a QCP at \(\xi \approx 0.635\). Note that the AF-LRO phase only exists at \(T = 0\) for the 2D KH model (bold solid line). (b) Temperature dependence of the magnetic short range order, \(|\Delta|^2\), at different \(\xi = T_K/J_H\) marked by \(A\) to \(D\) in (a). (c) \(|\Delta|^2\) and the holon phase shift \(\delta_K/\pi\) as functions of \(\xi\).
describe both the antiferromagnetic phase through the condensation of bosons as well as the heavy FL phase. We identify the antiferromagnetic-Kondo breakdown (AF-KB) QCP (see Fig. 1(a)) via the holon phase shift linked to the Kondo hybridization and condensation of bosonic spinons. Near this transition, we find a SM region at finite temperatures in between the quantum critical fan and the heavy FL state. We further link the SM behavior to the 2D nature of the critical Kondo and resonating valence bond (R VB) correlations.

Model- We start with the KH model \( H = H_0 + H_K + H_J \) in which the Kondo coupling \( J_K = J_K \sum_i S_i \cdot \sigma_i \) and the AF RKKY interaction \( J_H (H_J = J_H \sum_{i,j} S_i \cdot S_j) \) are treated to be independent of each other for generality. Here, \( H_0 = \sum_{p} \varepsilon_p \psi^\dagger_{pa} \psi_{pa} \) describes the non-interacting conduction electron bath with \( \psi^\dagger_{pa} \psi_{pa} \) being the creation operator of a conduction electron with quasi-momentum \( p \) with channel index \( \alpha \in \{1,K \} \) and spin index \( \alpha \in \{-N\frac{\pi}{2},-N\frac{\pi}{2} + 1, \ldots, N\frac{\pi}{2} - 1, N\frac{\pi}{2} \} \). The large-N [Sp(N)] generalization of \( H \) via Schwinger bosons reads [31]:

\[
H \rightarrow H_0 + \sum_{i,p} \left[ \frac{1}{\sqrt{N}} (b^\dagger_{i\alpha} \psi_{1\alpha}) \chi_{ia} + h.c. + \frac{[\chi_{i\alpha}]^2}{J_K} \right] + \sum_{\langle i,j \rangle} \left[ sgn(\alpha) b_{i\alpha} b_{j,-\alpha} \Delta_{ij} + h.c. + \frac{N[\Delta_{ij}]^2}{J_H} \right] + \sum_{i} \lambda_i (b^\dagger_{i\alpha} b_{i\alpha} - 2S) .
\]

In Eq. (1), \( \psi^\dagger_{1\alpha} \) is the Fourier component of \( \psi^\dagger_{pa} \) with \( i \) being the site index. The Schwinger boson operator \( b^\dagger_{i\alpha} \) creates a spinon of spin \( \alpha \). Note that the large-N generalization to the local spin operator \( S_i \) at site \( i \) can be expressed in terms of either the \( N \)-flavored bilinear fermions [34] or bosons [31–33, 35]. The Kondo hybridization, \( \chi_{i\alpha} \propto \sum_{p} \psi^\dagger_{1\alpha} \psi_{pa} \), is a charged, spinless fermionic holon field obtained as a Hubbard-Stratonovich field through decoupling of the original Kondo term. Unlike its bosonic counterpart in the pseudo-fermion representation of spins, the \( \chi_{i\alpha} \) field cannot Bose-condense, i.e. \( \langle \chi_{i\alpha} \rangle = 0 \), its fluctuating nature develops an energy gap in both the spinon and holon spectrum which protects the Kondo singlets from being destroyed by thermally excited spinons [36]. As a result, various physical quantities will exhibit Fermi-liquid behavior over a finite temperature window.

The AF Heisenberg \( H_J \) is expressed in terms of the Sp(\( N \))-invariant RVB term, \( sgn(\alpha) b_{i\alpha} b_{j,-\alpha} \Delta_{ij} \) where \( \Delta_{ij} = -\frac{N}{J_H} \sum_{p} (sgn(\alpha) b^\dagger_{j\alpha} b^\dagger_{i\alpha}) \) is the AF short-range order (SRO) parameter. The SRO bosonic spin liquid is a suitable description of systems with strong magnetic frustration and/or disorder. The AF long-range order (LRO) phase is represented in terms of the boson condensate, \( \langle b_{i\alpha} \rangle \) [37]. The capability of describing both LRO and SRO is a major advantage of our approach over the fermionic representation. The last term in \( H \) reads \( n_b(i) = \sum_{\alpha} (b^\dagger_{i\alpha} b_{i\alpha}) = 2S \), with \( 2S = K \) corresponding to full Kondo screening [31]. The Lagrange multiplier, \( \lambda_i \), also serves as the temperature-dependent chemical potential of the spinons. Numerically, we treat \( \lambda_i = \lambda, \Delta_{i,i+\hat{x}} = \Delta_{i,i+\hat{y}} = \Delta \) as homogeneous variational \( c \)-numbers. The ratio \( K/N \) is kept constant (0.2 in this work [38]) as we take the large-N limit.

Method- To solve Eq. (1), we exploit the self-consistent Dyson-Schwinger equations in terms of the fully dressed Green’s functions and self energies of various fields. To make further progress, we assume that all the self energies are momentum independent, i.e. \( \Sigma (i\omega, p) \rightarrow \Sigma (i\omega) \), similar to what is used in the DMFT. The resulting local Green’s functions read

\[
G_{c\alpha} (i\omega) = \sum_{p} \frac{1}{i\omega - \varepsilon_p} ,
\]

\[
G_{x} (i\omega) = [-1/J_K - \Sigma_{x} (i\omega)]^{-1} ,
\]

\[
G_{b} (i\nu) = \frac{1}{\gamma_{b} (i\nu)} \frac{2}{\pi} \frac{E_K (16|\Delta|^2)}{\gamma_{b} (i\nu) \gamma_{b} (-i\nu)} ,
\]

\[
\Sigma_{x} (i\nu) = \sum_{\gamma} \frac{G_{c\alpha} (i\nu - i\omega) G_{b} (i\nu)}{
u} ,
\]

\[
\Sigma_{b} (i\nu) = -\kappa \sum_{\omega} G_{c\alpha} (i\nu + i\omega) G_{x} (i\omega) .
\]

In the above equations, \( \omega \equiv \pi (2n + 1)/\beta \) and \( \nu \equiv 2\pi n/\beta \) denote the fermionic and bosonic Matsubara frequencies, and \( \varepsilon_p \) the conduction electron dispersion. In Eq. (2), \( \gamma_{b} (z) \equiv z - \lambda - \Sigma_{b} (z) \), and the complete elliptic integral of the first kind, \( E_K (z) \equiv \int_0^1 \frac{1}{\sqrt{1-z \sin^2 \theta}} d\theta \), comes from the 2D momentum integral [39]. We keep the leading terms in \( \Sigma_{b} \) and \( \Sigma_{x} \) of order of unity (Fig. 2), but ignore the vertex corrections and the conduction electron self energy \( \Sigma_{c} \), which are of higher order in \( 1/N \).

Two constraints for the Green’s functions are obtained by minimizing the free energy of the system with respect to \( \lambda \)
and $\Delta$:

$$\kappa = -\int \frac{dz}{\pi} n_B(z) \text{Im} G_b(z),$$

$$\frac{1}{J_H} = \int \frac{dz n_B(z)}{2\pi^2 |\Delta|^2} \text{Im} E_K \left[ \frac{16|\Delta|^2}{\gamma_b(z) \gamma_b(-z)} \right].$$  (4)

Here, $n_B(z)$ is the Bose function. The unknowns, $G_X$, $G_b$, $\Sigma_X(\omega)$, $\Sigma_b(\nu)$, $\lambda$, and $\Delta$ are obtained self-consistently through Eqs. (2) to (4).

Global phase diagram- Our main results are summarized in Fig. 1(a): a phase diagram in terms of the tuning parameter $\xi \equiv T_K/J_H$ ($T_K = D e^{-D/J_K}$ is the bare Kondo temperature with $D$ being the half bandwidth of the conduction electrons) and the temperature $T/J_H$ is mapped out via the specific heat coefficient $C_V/T$. At $T = 0$, a QCP at $\xi = \xi_c$, separating the AF-LRO phase at small $\xi$ and the paramagnetic FL ground state at large $\xi$ is clearly identified via the low-temperature evolution of various quantities. The AF-LRO phase can be inferred from the spinon spectral function showing a non-zero weight of massless mode (or condensation of bosons $|b\rangle \neq 0$), while the heavy FL phase is identified through the linear-in-$T$ entropy and the holon phase shift, defined as

$$\frac{\delta \Sigma}{\pi} = -\text{Im} \ln \left[ 1 + J_K \Sigma_X \left( 0^+ \right) \right].$$  (5)

Within this phase, the magnetic SRO vanishes, and both the spinons and holons develop gaps in their spectral functions. The abrupt jump of holon phase shift $\delta \Sigma/\pi$ (Fig. 1(c)) and the vanishing of $|\Delta|^2$ as $T \to 0$ for $\xi > \xi_c$ (Fig. 1(b)) indicate a reconstruction of the Fermi surface at the QCP, which is consistent with the Kondo breakdown observed in various heavy fermion compounds including YbRh$_2$Si$_2$ [18, 19] and CeCu$_{6-x}$Au$_x$ [8, 9]. In addition, the AF-SRO is completely suppressed in the heavy FL phase, different from the previous studies for the two-impurity and the 1D Kondo lattice model [31–33]. We find an AF-LRO phase to persist at finite temperatures [Fig. 3(a)]. However, this finite temperature LRO phase is ruled out by the Mermin-Wagner theorem [40] and thus is an artifact of our approach [41]. Above the LRO phase, an RVB-dominated region, where $|\Delta|$ is significantly enhanced, is found. Near the QCP, the SM behavior, characterized by a logarithmic-in-$T$ specific heat coefficient and linear-in-$T$ resistivity, is clearly seen within a narrow region on the Kondo side (marked as “SM” in Fig. 1(a)). As further explained in the Discussion section, we believe that the SM region being rather narrow and tilted towards the Kondo-screened side is an artifact of our approach.

Entropy and specific heat coefficient- Figure 4 shows the temperature dependence of the entropy, $S$ [42], and the specific heat coefficient, $\gamma \equiv C_V/T = \partial S/\partial T$ at different values of $\xi$. For $\xi > \xi_c$, the plateau at low temperatures in the specific heat coefficient associated with the linear-in-$T$ entropy reveals the formation of the FL phase. As $\xi$ approaches $\xi_c$ from the Kondo side, the temperature range of the plateau shrinks monotonically and vanishes at the QCP. Above the FL region, the specific heat coefficient increases till it reaches a “Schottky” peak [43]. Above the Schottky peak, the specific heat coefficient decreases logarithmically with increasing temperatures, with a scaling form $b(\xi)C_V/T \sim -\alpha(\xi) \ln(T/T^*)$ with $b$ and $\alpha \sim |\xi - \xi_c|^{-0.49}$ being two non-universal factors [39]. Similar strange metal behavior in $C_V/T$ has been observed in YbRh$_2$Si$_2$ [4] and CeCu$_{6-x}$Au$_x$ [7]. This logarithmic singularity in the specific heat coefficient is a characteristic of 2D bosonic critical fluctuations, reminiscent of similar features recently obtained via a fermionic large-$N$ approach to Ge-substituted YbRh$_2$Si$_2$ and CeMn$_2$ [44]. Note that, the peak temperatures (open circles in Fig. 1(a)) display a weakly first-order jump at the QCP, similar to that in Ref. [45] (see Discussion section for this point).

Magnetic susceptibility- The static local (momentum integrated) magnetic susceptibility $\chi_{loc}(T)$ as a function of temperature defined as

$$\frac{\chi_{loc}(T)}{N} = 2 \int \frac{dz}{\pi} n_B(z) G_b'(z) G_b''(z)$$  (6)

FIG. 3. (a) Temperature dependence of the local magnetic susceptibility, $\chi_{loc}(T)/N$ at different values of $\xi$. The dashed straight line corresponds to $\xi = \xi_c$. Inset: the spatial dependence of the spin susceptibility along the $x$-direction, $\chi_{sf}(N)$ (red dots), fitted to $g(r/a) \equiv (a^2/5r^2) \cos(3.21r/a)$ with $r_i - r_j \equiv (r, 0)$ and being the lattice constant (solid curve). (b) Electrical resistivity $\rho(T)$ versus $\xi$. Inset: Feynman diagram of the self energy of a conduction electron, $\Sigma_c$. The resistivity behaves as $\rho(T) \sim \exp(-J_H/T)$ ($\rho(T) \sim T$) in the lower (higher) temperature regime. The dashed lines in (a) and (b) schematically show the extrapolations of $\chi_{loc}$ and $\rho(T)$ at the QCP.
is plotted in Fig. 3(a) at different values of $\xi$ near the QCP. It shows two distinct properties corresponding to the two regimes $\xi > \xi_c$ and $\xi < \xi_c$ as $T/J_H \to 0$. In the Kondo limit, the susceptibility acquires a crossover from a saturated Pauli susceptibility at low temperatures, where all the local spins are fully screened, to a typical spin liquid behavior at high temperatures [46]. Meanwhile, both the local and the uniform susceptibility exhibit a Curie’s law at temperatures above the spin liquid region [39]. The quantum critical fan is identified through the power-law scaling of the local susceptibility [39]. Further experiments on inelastic neutron scattering or Knight shift measurements are needed to confirm this critical behavior.

Electrical resistivity- Figure 3(b) show the electrical resistivity obtained through the Boltzmann formula [47],

$$\rho^{-1}(T) = \frac{ne^2}{m} \int \tau(\omega) \frac{\partial n_F(\omega)}{\partial \omega} d\omega,$$

where $n_F(x) = [\exp(x/T) + 1]^{-1}$ denotes the Fermi function and $\tau^{-1}(\omega) = -2\Sigma''(\omega)$ is the scattering rate of the conduction electrons [of order of $O(1/N)$, see inset of Fig. 3(b)]. In the Kondo limit, we observe a typical NFL linear-in-$T$ dependence of the electrical resistivity $\rho(T) = a + bT$ with $a$ and $b$ being constants [inset of Fig. 3(b)]. The $T$-linear resistivity is more clearly featured as the system approaches the QCP, suggesting its link to the critical Kondo fluctuations [44], similar to what is seen in pure YbRh$_2$Si$_2$ [3, 4], Ge-substituted YbRh$_2$Si$_2$ [5], and CeMn$_5$ [10, 11]. On the AF side, insulating behavior is observed at low temperatures. Note that, to the leading order in $N$, the expected $T^2$ Fermi liquid behavior is replaced by an exponential decay [inset of Fig. 3(b)], due to the finite holon and spinon gaps [36].

$\omega/T$ scaling- The $\omega/T$ scaling has initially been observed in the dynamical spin response [8], and connected to the critical Kondo Breakdown [30]. More recently, dynamical scaling has also been demonstrated in the charge response [48] and observed in optical conductivity measurements on YbRh$_2$Si$_2$ [20], which is thus believed to be induced by the emergent critical charge fluctuations at the KB QCP. This observation is supported by the $\omega/T$ scaling of the critical valence fluctuations in $G'$ at the KB QCP, i.e. $G'_\chi(\omega, T) = -T^{0.56}f(\omega/T)$ with $f(\omega/T)$ being an universal function [39], consistent with the linear-in-$T$ behavior of $\Sigma''(\omega = 0, T)$, i.e. $\Sigma''(\omega = 0, T) \sim T$.

Discussions- Before concluding, we would like to make some remarks. Firstly, at non-zero temperatures, the region in the parameter space with non-zero RVB strength ($|\Delta| \neq 0$) extends to the quantum critical region. As a result, the SM behavior can only be observed within a narrow region on the Kondo side of the QCP. We attribute this feature to the bosonic representation of impurity spins where the holon field $\chi$ cannot get Bose-condensed, giving rise to an overestimated RVB mean field $\Delta$. We expect that introducing a combined boson-fermion supersymmetric representation of spins [49], where $\chi$ and $\Delta$ are treated on equal footing, may remedy this artifact. Secondly, weakly first-order transitions usually exist in the Schwinger boson mean-field theories due to the attractive quartic term of order $O(\Delta^4)$. This term can be cancelled via including a small repulsive biquadratic term $J''_H(S_i \cdot S_j)^2$ with $J''_H \ll J_H$ in the Hamiltonian and thus the second-order phase transitions can be restored [32]. Thirdly, the finite-temperature AF-LRO phase we find here is likely due to an overestimated Kondo-induced long-range RKKY interaction [41], as manifested by the long-range correlated position-dependent magnetic susceptibility [inset of Fig. 3(a)]. Nonetheless, this long-range order will be stabilized in the form of 3D long-range order in real materials due to weak inter-layer coupling and the calculated 2D long-range order will emerge as quasi-long-range order in the corresponding renormalized classical regime [50].

Conclusions- We have explored the quantum phase transition and the quantum criticality of heavy fermion compounds based on the antiferromagnetic Kondo-Heisenberg model on a two-dimensional square lattice via the large-$N$ ($\text{Sp}(N)$) multichannel Schwinger boson approach. The global phase diagram and the behavior of various physical observables therein show a close resemblance to YbRh$_2$Si$_2$ [3–5, 18–20] and CeCu$_6$–$x$Au$_x$ [6–9]: At $T = 0$, an antiferromagnetic-Kondo breakdown quantum critical point, which separates the antiferromagnetic long-range order phase from the Kondo-screened heavy Fermi-liquid phase, is identified via the low temperature evolution of several physical observables. The strange metal state with $T$-linear electrical resistivity and a logarithmic divergence in the specific heat coefficient is also observed. The universal critical scaling of the local susceptibility further underpins the existence of a quantum critical region. Further studies to generalize our work to the supersymmetric dynamical large-$N$ approach are needed.

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Our approach does obey the Mermin-Wagner theorem in the 2D...