Magnetic-field-induced quantum phase transitions in the two-impurity Anderson model

Lijun Zhu and Jian-Xin Zhu

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Lijun Zhu and Jian-Xin Zhu
Theoretical Division and Center for Nonlinear Studies,
Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

In the two-impurity Anderson model, the inter-impurity spin exchange interaction favors a spin singlet state between two impurities leading to the breakdown of the Kondo effect. We show that a local uniform magnetic field can delocalize the quasiparticles to restore the Kondo resonance. This transition is found to be continuous, accompanied by not only the divergence of the staggered (antiferromagnetic) susceptibility, but also the divergence of the uniform spin susceptibility. This may imply that the magnetic field induced quantum phase transitions in Kondo systems are in favor of the local critical type.

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I. INTRODUCTION

The study on quantum phase transitions and critical phenomena has been an extraordinarily active area of research in condensed matter physics and quantum field theory. One example which has been extensively studied in experiments is the magnetic quantum phase transition (QPT) in heavy fermion metals.[1] Two theoretical scenarios are suggested for this QPT: the spin-density-wave picture based on itinerant quasiparticles,[2–4] and the Kondo breakdown picture mandating the localization of quasiparticles.[5–8] Although it is well accepted that, to address the nature of this QPT, the competition between the onsite Kondo coupling and the intersite spin exchange interaction, namely, the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, plays the determinant role, there are few theoretical methods which can handle them on an equal footing. Interestingly, the two-impurity Anderson (or Kondo) model presents a minimal model for such a competition effect in an exactly solvable way.[9–17] With the Kondo coupling, the impurity spin forms a Kondo singlet state with the spins of the conduction electrons and a quasiparticle resonance peak develops at the Fermi energy, which is described by the Kondo effect. When the inter-impurity spin exchange interaction is antiferromagnetic and strong enough, the two impurity spins tend to form a singlet by themselves, against the formation of Kondo singlets, leading to the localization of quasiparticles. As a result, the quasiparticle spectra have a "pseudogap" at low energies.[11,17] It is found that, the phase transition between the Kondo resonance state and the inter-impurity spin singlet state can be continuous.[10,11,17]

A magnetic field has been serving as one of the most important tuning parameters to investigate the magnetic properties of strongly correlated electron materials. Naturally, it is also relevant to the two-impurity Anderson model. However, a detailed analysis of the magnetic field effect in this model, especially close to the characteristic scales of the two-impurity quantum critical point (QCP), is still lacking, which is the purpose of this study. We note that there are some existing theoretical studies[18–20] targeting the double quantum dot, but they are limited to the cases with large magnetic fields, in which the physical properties follow the Zeeman splitting effect.[18–20] Although it is known that a local staggered magnetic field can induce a QPT as it directly couples to the critical staggered spin fluctuations,[12–14,16] the role of a local uniform magnetic field has not been explored. Such a uniform magnetic field is usually applied in experimental studies.[21]

In this Article, we report the first observation of a magnetic field induced quantum phase transition in the two-impurity Anderson model from a numerical study. We find that a local uniform magnetic field applied on the two impurity spins can drive a transition from the inter-impurity spin singlet state to the Kondo resonance state, leading to the delocalization of quasiparticles. We further show that this transition is *continuous*, accompanied by the abrupt change of the quasi-particle spectral weight at the Fermi energy and the divergence in staggered spin susceptibility, which are also features of the two-impurity QCP at zero field tuned by RKKY interaction. In sharp contrast, the uniform spin susceptibility is also found to diverge at this magnetic-field-induced QCP. The new observation is suggestive that the field-induced QCP in heavy fermion systems[21] does have the local nature, as advocated in recent QCP theories.[1,5]

The rest of the paper is outlined as follows: In Sec. II, we present a two-impurity Anderson model under a uniform magnetic field. Such dynamical quantities as spectral density and spin susceptibility are defined. The method to solve the model is also explained. In Sec. III, we analyze the scattering phase shift as a function of the magnetic field. The magnetic field dependence of the spectral density and dynamical susceptibility are also discussed. The characterization of these quantities enables us to identify a field-induced QCP. A summary is given in Sec. IV.

II. MODEL AND METHOD

The Hamiltonian for the two-impurity Anderson model can be written as

$$\begin{aligned} H &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma,(i=1,2)} \left(\frac{V_{\mathbf{k}}}{\sqrt{N_c}} e^{i\mathbf{k}\cdot\mathbf{r}_i} c^\dagger_{\mathbf{k}\sigma} f_{i\sigma} + h.c. \right) \\ &+ \sum_{(i=1,2),\sigma} \epsilon_f f^\dagger_{i\sigma} f_{i\sigma} + \sum_{(i=1,2)} U n_{fi\uparrow} n_{fi\downarrow} \\ &+ I\mathbf{S}_{f1}\cdot\mathbf{S}_{f2} + h(S_{f1z}+S_{f2z}) \; . \end{aligned} \tag{1}$$

This model describes two interacting local orbitals $f_{i\sigma}$ (Anderson impurities) in hybridization with a non-interacting conduction electron band $c_{\mathbf{k}\sigma}$ with the strength $V_{\mathbf{k}}$ at each impurity site $\mathbf{r}_i$. The variables ϵ_f and U are the energy level and onsite Coulomb interaction for the local orbitals, respectively, and I is a direct spin exchange interaction between two impurities. We here consider a uniform magnetic field B which acts on the impurity spins only.[22] Therefore, $h \equiv g\mu_B B$ has the dimension of energy, where g, μ_B are Landé factor and Bohr magneton, respectively. This model has been shown[10,11,17] to be equivalent to a two-impurity two-channel model, with degrees of freedom cast into the even (e) and odd (o) parity channels. The local orbitals become

$$f_{e,o} = (f_1 \pm f_2)/\sqrt{2} \; , \tag{2}$$

and the hybridization functions for these two channels are given by

$$\Gamma_{e,o}(\omega) = (1/2N_c)\sum_{\mathbf{k}} V^2_{\mathbf{k}} |e^{i\mathbf{k}\cdot\mathbf{r}} \pm e^{-i\mathbf{k}\cdot\mathbf{r}}|^2 \delta(\omega - \epsilon_{\mathbf{k}}) \; , \tag{3}$$

where $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)/2$. The inter-site spin exchange interaction can be generated by considering specific forms of $V_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}$ (RKKY interaction), or provided by the direct spin exchange term I. We adopt the numerical renormalization group (NRG)[23] method with the complete-Fock-space NRG (CFS-NRG) method[24,25] for calculations of dynamical quantities at zero temperature, including the spectral function

$$A_{f,p\sigma} = -\mathrm{Im} G_{f,p\sigma}(\omega) \; , \tag{4}$$

the uniform and staggered spin susceptibilities

$$\chi_{u,a} = \langle\langle S_{1z} \pm S_{2z}; S_{1z} \pm S_{2z} \rangle\rangle \; . \tag{5}$$

We follow the same numerical procedure as in Ref. 17. As in standard NRG,[23] we discretize $\Gamma_{e,o}(\omega)$ into two separate semi-infinite chains in decreasing energy scale $\Lambda^{-(i-1)/2}$, where i is the chain site and $\Lambda > 1$ the discretization parameter. While the impurities only couple to the head sites of each chain, we can solve the Hamiltonian by an iterative diagonalization procedure incorporating gradually low energy sites. As the size of the eigen space increases exponentially, in general, only certain number of low energy states are kept in each iteration for further iterations. In our calculations, we choose $\Lambda = 2$ and keep 4000 states for each iteration. In practice, we find that choosing a smaller Λ or keeping more states (therefore more accurate) improves the low energy spectrum weight (therefore the Friedel's sum rule), but does not affect the determination of the low energy scales. We typically take 100 iterations (the length of the chain), reaching an energy scale $\sim 10^{-15}$ in unit of the electron bandwidth. Because this energy scale is related to an effective temperature, our calculations are therefore in the zero-temperature limit. In the vicinity of critical points where the characteristic energy scale approaches zero, we increase the number of iterations to ensure that the effective temperature is smaller than the characteristic energy scale, i.e., the fixed point being reached.

In traditional NRG, the dynamical quantities are calculated from the kept states from each iterations. The CFS-NRG method[24,25] instead calculates the dynamical quantities in terms of the discarded states (including all states from the last iteration), which form a complete Fock space conserving the total spectral weight. We adopt this method in our calculations and find that it is indeed advantageous to the traditional method for the two-impurity problem with the enlarged basis. An explicit comparison is shown in Ref. 17. In addition, it has also been argued that the CFS-NRG method is particularly suitable for the problem with a finite magnetic field.[20,26] In practice, we follow the $T = 0$ calculation procedure as in the single-impurity Anderson model,[25] to adopt a backward iterative process determining the reduced density matrix between the discarded states and calculating the imaginary parts of the dynamical quantities from the Lehmann representation. We then use Kramers-Kronig relation to determine their real parts. Due to the exponentially decreasing energy scales in NRG, the delta function in the Lehmann representation is commonly broadened in the log-Gaussian form,[23]

$$\delta(\omega-\omega_n)\rightarrow\frac{e^{-b^2/4}}{b\omega_n\sqrt{\pi}}e^{-\ln^2(\omega/\omega_n)/b^2}, \tag{6}$$

where b is a broadening parameter. For $\Lambda=2$, we take $b=0.6$, as commonly adopted.[23]

III. RESULTS

In our previous study on this model,[17] we have explicitly calculated a system with a well-defined two-impurity QCP (we refer the two-impurity QCP to this zero-field QCP in the following). Our results can be summarized as follows. We choose $\Gamma_{e,o}(\omega)=\Gamma_0$, for which no RKKY interaction is generated and the single-impurity Kondo temperature T_K can be determined. We then add the direct spin exchange interaction I (to simulate RKKY interaction) to tune the competition between the Kondo effect and the inter-impurity spin exchange interaction. Below a critical value I_c, the low energy properties are still due to the Kondo effect, $A_f(0)\approx 1/(\pi\Gamma_0)$ and $\chi'_u(0)\sim 1/T_K$, but $\chi'_a(0)\sim 1/T_F^*$ with T_F^* the reduced (local) Fermi liquid temperature. Above I_c, it is the inter-impurity spin singlet state with vanishing $A_f(0)$. It differs from the Mott gap in the fact that there are still finite spectral weights at low energies: $A_f(\omega)\sim\omega^2$ for $\omega<T_F^*$ and a non-Fermi liquid form for $T_F^*<\omega<T_{sf}$, where T_F^* and T_{sf} (spin fluctuation scale) correspond respectively to the two energy scales T_L and T_H identified in our previous work.[17] For $\Gamma_0=0.045\pi D$, and $\epsilon_f=-U/2=-D$, it is found that the single-impurity Kondo temperature $T_K=1.0\times10^{-3}D$ and the critical value $I_c\approx 0.0023464D\approx 2.3T_K$. Here D is the half bandwidth of the conduction electrons. At I_c, there is a sudden change of the spectral weight at the Fermi energy, but the transition is still *continuous*. This is evidenced by the uniformly vanishing $T_F^*\sim(I-I_c)^2$ with the divergence of the staggered spin susceptibility $\chi'_a(0)$. However, the uniform spin susceptibility $\chi'_u(0)$ remains finite through the transition. These results are consistent with earlier studies.[11,12]

We add a local uniform magnetic field h to the above system to examine its effects. In Fig. 1, we show the results of the scattering phase shift $\delta_{p\sigma}(0)$ at the Fermi energy, determined from the expression:

$$A_{f,p\sigma}(0)=(1/\pi\Gamma_0)\sin^2\delta_{p\sigma}(0)\ , \tag{7}$$

as functions of h for various values of I. For $I=0$, this is equivalent to a single-impurity Kondo problem and indeed our results are in agreements with those obtained for the single-impurity Kondo model.[29] The scattering phase shift by the exact Bethe-Ansantz method is $\delta_h(0)\sim\pi/2-h$ for $h\ll T_K$ while $\delta_h(0)\sim 1/\log(h/T_K)$ for $h\gg T_K$.[30] The latter relation is in agreement for all finite Is but with $1/\log(h/T_{sf})$, where $T_{sf}\approx I$ when $I\gg T_K$.[17] For $I<I_c$, i.e., in the Kondo regime, $\delta_h(0)$ is always finite. For the same h, $\delta_h(0)$ is enhanced with a small I. For $I>I_c$, $\delta_h(0)$ vanishes when $h=0$, characterizing the inter-impurity spin singlet state. A finite but small h induces a small $\delta_h(0)$ or a small quasiparticle weight at the Fermi energy: it is found that $\delta_h(0)\sim h$ as verified by a log-log plot (not shown). When h is increased to a critical value h_c, we observe a sudden jump of the phase shift from a tiny value to a large value of the order unity, which indicates a transition rather than a crossover between the inter-impurity spin singlet state and the Kondo resonance state. The relation between h_c and $I-I_c$ is shown in the inset of Fig. 1. We find that $h_c\sim(I-I_c)^{1/2}$ for $(I-I_c)/I_c\ll 1$ and a noticeable deviation for $(I-I_c)/I_c>0.1$. Such a deviation is also identified in $T_F^*\sim(I-I_c)^\alpha$ when $h=0$.[17]

The effect of the magnetic field is to align spins along its direction to gain the Zeeman energy. While it can directly reduce the the inter-impurity singlet to triplet excitation gap (determined by I), it does not destroy the Kondo effect, only to shift the Kondo resonance peak position to the Zeeman energy to suppress the spectral weight at the Fermi energy.[29–31] As a result, the magnetic field can destroy the inter-impurity spin singlet state ($I>I_c$) to recover a Kondo resonance state. To illustrate this and further show that it is a continuous phase transition, we present a detailed analysis for the $I=3.0T_K$ case. In Fig. 2, we show the results of the spectral functions $A_{f,p\sigma}(\omega)$, and the uniform and staggered spin susceptibilities $\chi_{u,a}(\omega)$. For a small magnetic field, for instance $h=1.2T_K$, the spectral weight at the Fermi energy is only slightly enhanced. When h increases, $A_f(0)$ increases as well. But such change is not uniform, having a sudden jump at a critical value $h_c\approx 1.2814T_K$, as also indicated in Fig. 1. At $h=1.4T_K$, $A_f(0)$ is comparable with the full Kondo resonance weight $1/(\pi\Gamma_0)$, indicating the Kondo resonance regime. When the magnetic field is further increased, for instance $h=6T_K>\max(I,T_K)$, $A_f(0)$ decreases. This is similar to the single-impurity Kondo model in the presence of a large magnetic field. Spin-up and spin-down resonance peaks are located at positive and negative energies, respectively, and the energy difference (or the gap) is $2h$, which is the hallmark of the Kondo resonance.[31] However, $A_{f,p\sigma}(0)$ is still finite. The sudden jump of $A_f(0)$ at h_c is similar to that in the two-impurity QCP at zero-field. The staggered spin susceptibility has the same behavior as well: it becomes divergent when $h\rightarrow h_c$. Correspondingly, the associated energy scale T_h (as the effective Kondo scale or the Fermi

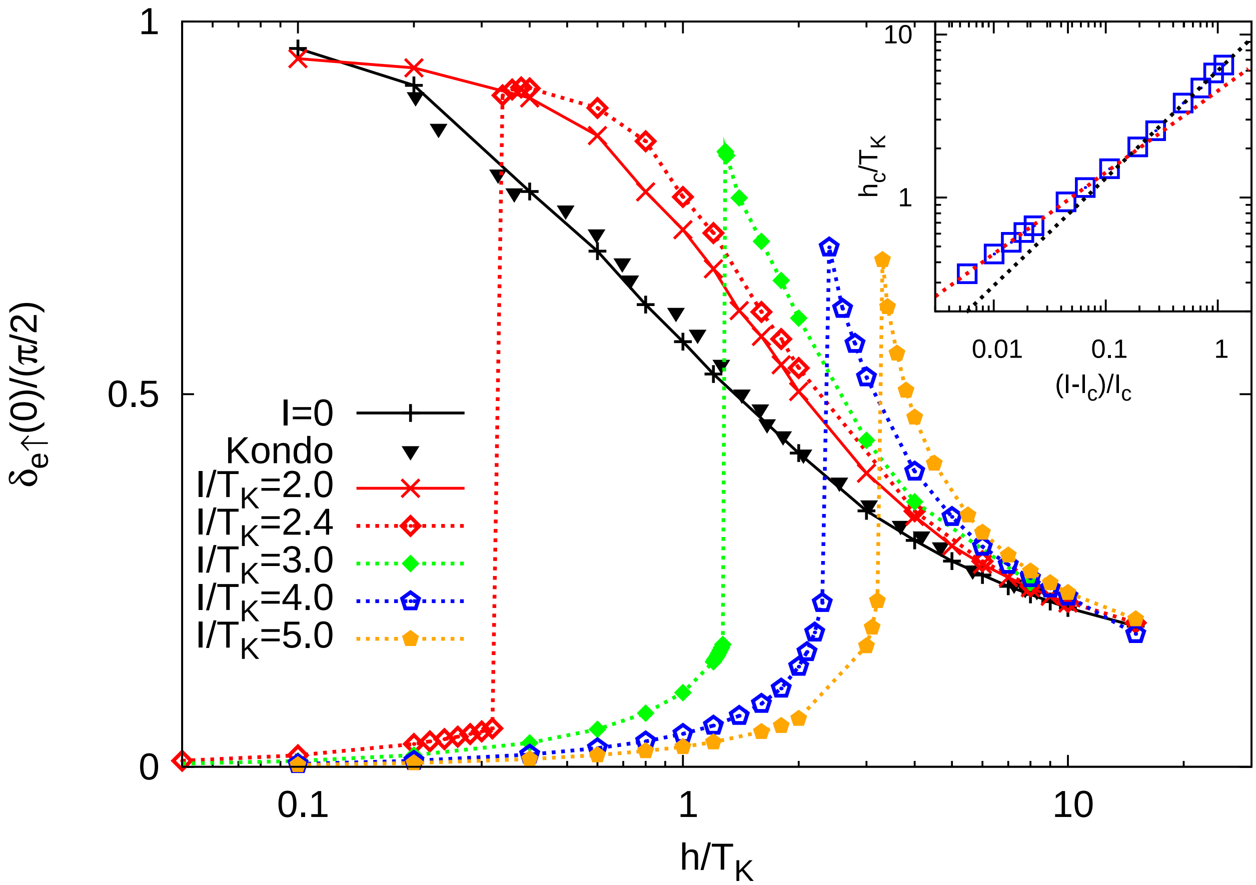

FIG. 1: (color online) The scattering phase shift $\delta_{e\uparrow}(0)$ as a function of h for different values of I. The phase shifts at the Fermi energy for different channels and spins are the same due to the symmetries $A_{e\sigma}(\omega) = A_{o\sigma}(\omega)$ and $A_{e\uparrow}(\omega) = A_{e\downarrow}(-\omega)$[27]. The data labelled with "Kondo" are subtracted from Costi's paper on the single-impurity Kondo model[29]. The inset shows the critical value h_c as a function of $I - I_c$ for $I > I_c$. Two dotted lines are $h_c = 4.5T_K(I/I_c - 1)^{1/2}$ (red) and $h_c = 6.0T_K(I/I_c - 1)^{2/3}$ (black).

liquid temperature[17]) uniformly vanishes. The significant difference lies in the uniform spin susceptibility: it is also divergent at h_c in this field-induced QCP compared with finite $\chi_u(0) \sim 1/T_{sf}$ in the two-impurity QCP. While we can subtract the energy scales from $1/[4\chi_{u,a}(0)]$ (shown in inset of Fig. 2(b)) as determining T_K, a more reliable method to determine the low energy scale is from a scaling analysis, which is shown in Fig. 3, for $\chi''_a(\omega)$. Once the energy is scaled with a certain scale T_h for different h, the low energy part of $\chi''_a(\omega)$ falls into a universal curve. T_h serves as the onset scale for Fermi liquid behaviors (T^*_F). Similar behavior can be observed in $\chi''_u(\omega)$, but its high energy part does not appear to scale (or not universal). We further plot the obtained T_h as a function of $|h - h_c|$: T_h can be fitted as $T_h \sim |h - h_c|^2$ for both $h < h_c$ and $h > h_c$. The uniformly vanishing scale T_h, the divergence in both the staggered and uniform spin susceptibilities, as well as the scaling property, are clear evidences that this magnetic field induced QPT is continuous.

When $I \to I_c$, h_c vanishes and the field-induced QCP merges with the two-impurity QCP at zero-field. We then need to understand why the divergence in χ_u vanishes in the latter case. The results for the spectral functions and the spin susceptibilities for $I = 2.3T_K$ are shown in Fig. 4. Indeed, any small h induces the full Kondo resonance at the Fermi energy with the finite Fermi temperature T_h, which is fitted as $T_h \sim h^4$. We also observe an enhancement of uniform spin fluctuations, which is manifested as a flat part above T_h, $\chi''_u(\omega) \sim C_h$. C_h increases as h increases. When T_h vanishes as $h \to 0$, C_h also vanishes. As a result, χ_u is not divergent. However, for any $I > I_c$ and tuning h to a critical value h_c, as C_h remains finite at low energies, χ_u indeed diverges. The variation of C_h also explains that $\chi''_u(\omega)$ does not scale for $\omega > T_h$ [cf. Fig.3].

The continuous QPT induced by a local uniform magnetic field in the two-impurity Anderson model was not

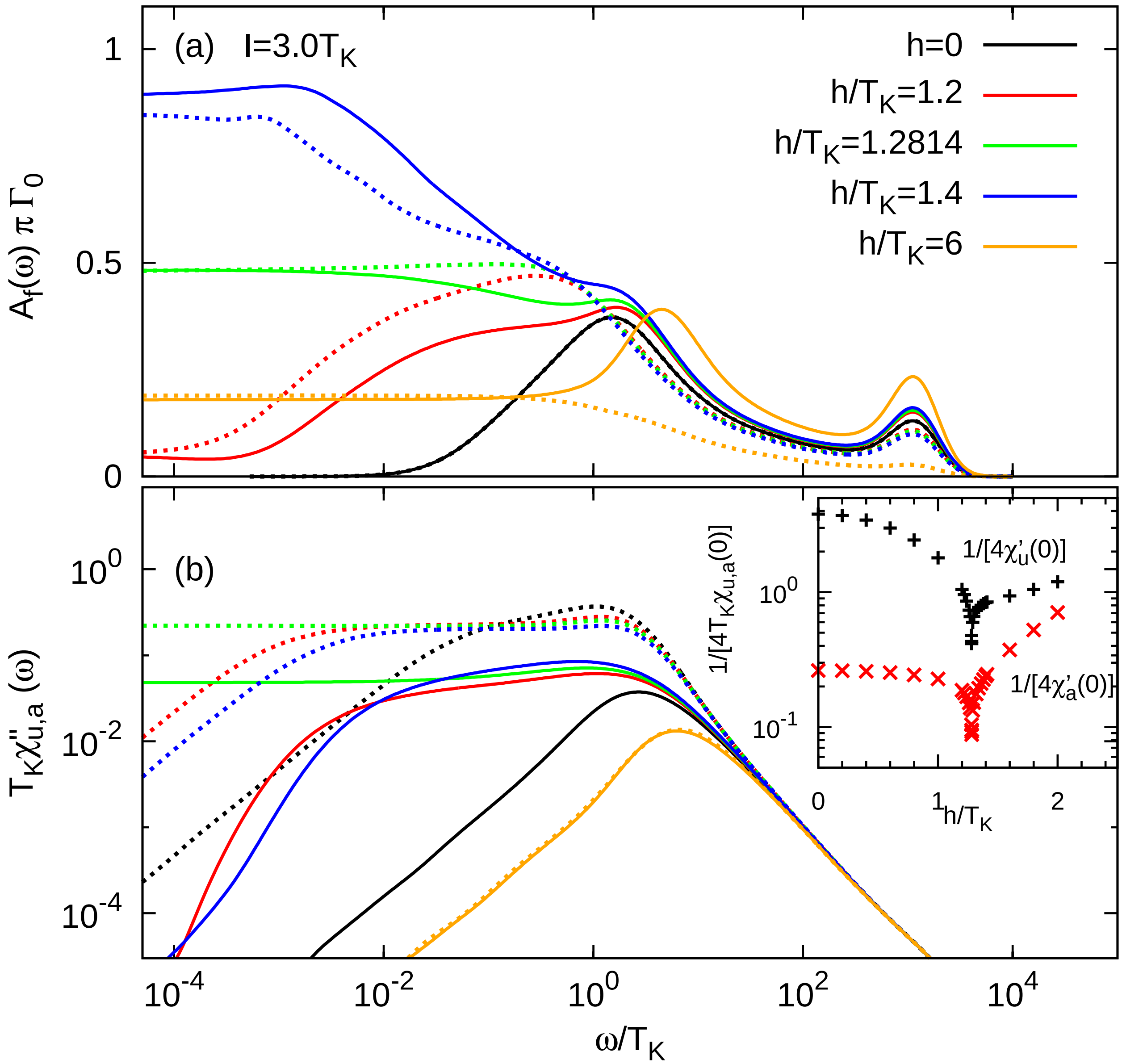

FIG. 2: (color online) Spectral functions $A_f(\omega)$ (a) and the imaginary parts of the uniform and staggered spin susceptibilities (b) as functions of energy for different values of h in the inter-impurity singlet regime, $I = 3.0T_K$. In (a), the solid and dotted lines represent $A_{f,p\uparrow}(\omega)$ and $A_{f,p\downarrow}(\omega)$, respectively [$A_{f,e\sigma}(\omega) = A_{f,o\sigma}(\omega)$ as the parity symmetry is not broken with a uniform magnetic field h]. In (b), they respectively represent $\chi''_u(\omega)$ and $\chi''_a(\omega)$. The inset shows $1/[4\chi'_{u,a}(\omega = 0)]$ (static) as functions of h.

predicted by either the conformal field theory[13] or the bosonization construction.[14,16] Compared with the two-channel QCP where $T_h \sim h^{228}$, the analogy of the magnetic field in the two-channel Kondo impurity model is the staggered magnetic field in the two-impurity model, i.e., $h_s(S_{1z} - S_{2z})$, which directly couples to the critical staggered spin fluctuations. It is commonly anticipated that a staggered magnetic field h_s is a relevant perturbation as it couples to $S_{1z} - S_{2z}$, the critical degrees of freedom. Our results suggest that the uniform magnetic field h also couples effectively to $S_{1z} - S_{2z}$, as evidenced from the divergence of χ_a. While an analytical analysis regarding this coupling is highly desirable, we can make the following reasoning on this coupling term based on our results. 1) The control parameter is modified as $I - I_c - ah^2$, to be consistent with the exponents deduced from our numerical data in different regimes. In other words, the field-induced QCP is the same in nature as the two-impurity QCP at zero field, having the same critical exponents. From another perspective, for a given finite h, tuning I can also lead to a QPT but the critical value of I_c is shifted up. 2) It involves the uniform spin fluctuations as h is directly coupled to. This also accounts for the divergence of the uniform spin susceptibility, which is induced rather than the driving mechanism. 3) It vanishes

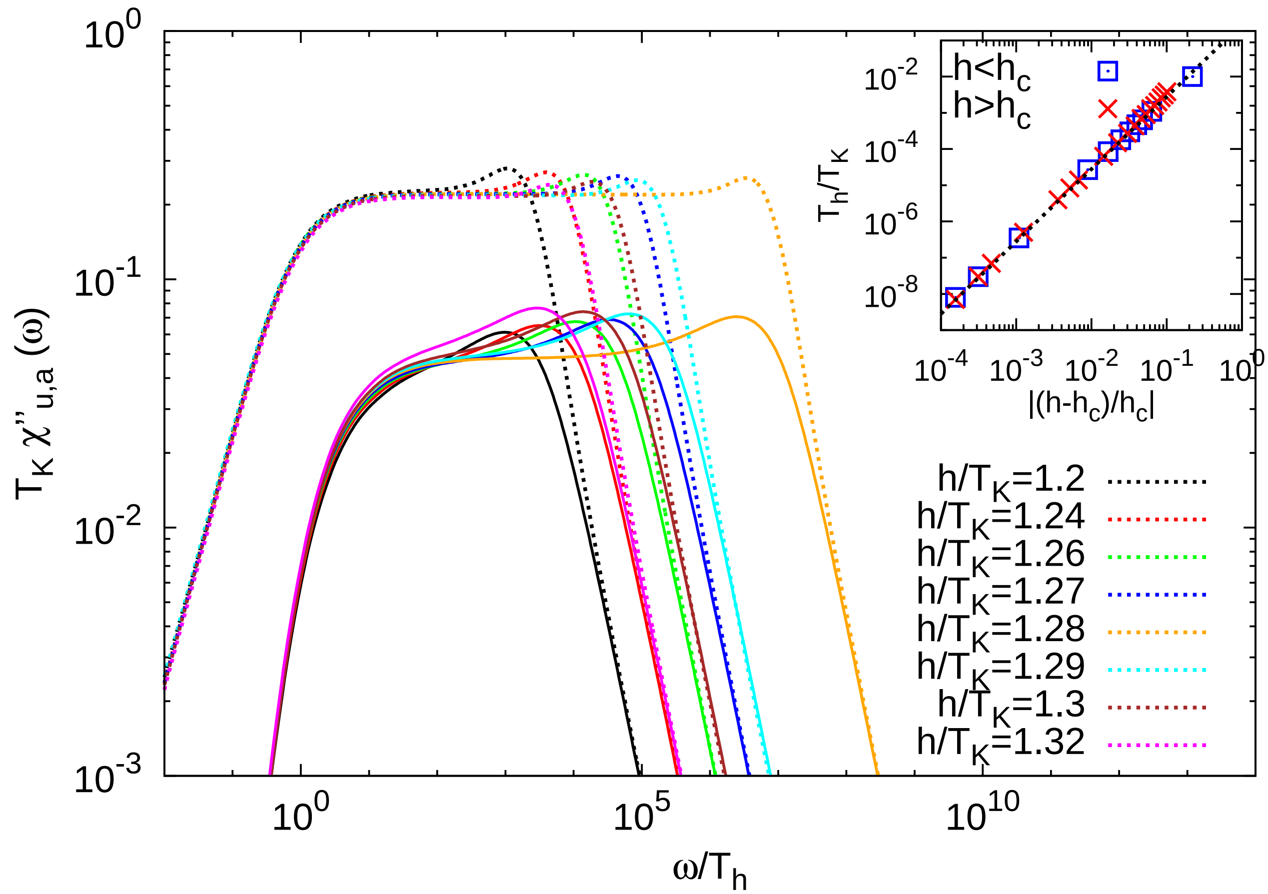

FIG. 3: (color online) Scaling behavior of the staggered spin susceptibility (dotted lines) for various values of h near h_c. The rescaled uniform spin susceptibility (solid lines) is also shown. From the scaling, T_h can be obtained and is plotted in the inset as a function of $|h - h_c|/h_c$. The line is a fitting $T_h/T_K = 0.28|h/h_c - 1|^2$.

or becomes irrelevant as h vanishes, as necessary to explain the loss of divergence in χ_u at the two-impurity QCP.

IV. SUMMARY

This magnetic-field-induced QPT, especially the divergence in $\chi_u(0)$, sheds new insights on understanding the two-impurity Kondo physics and quantum criticality in general. However, we notice that such a continuous transition depends on the symmetry between the even and odd channels, i.e., two identical impurities and the absence of parity-splitting charge-transfer term, i.e., $V_-(\tilde{f}^\dagger_{1\sigma}\tilde{f}_{2\sigma} + h.c.)$ for quasiparticles. Otherwise, one might not observe a sharp transition with an applied magnetic field, which has been discussed in Refs. 18–20. This is primarily due to the fact that V_- always contributes to a finite FL scale, $T^*_F = a(I - I_c)^2 + bV_-^2$,[11,32] even when $I = I_c$, and finite spectral weight at the Fermi energy even in the RKKY dominated regime. An applied magnetic field, to restore the Kondo resonance state, therefore can never tune a continuous transition. However, when temperature (or energy) is larger than bV_-^2, one still observes the scaling behavior associated with the two-impurity quantum critical point.[32] This issue is also relevant to the antiferromagnetic quantum critical points in heavy fermion materials. In a cluster DMFT solution based on two sites, it is suggested that the self-consistency condition transforms the crossover into a true phase transition, which shares the same property as the two-impurity quantum critical point.[33] In this approach, the uniform and staggered spin susceptibilities for the cluster correspond to the lattice spin susceptibility at momentum points, for example, $Q_0 = (0, 0, 0)$ and $Q_\pi = (\pi, \pi, \pi)$ for a three-dimensional (3D) lattice. The antiferromagnetic QCP in a lattice is signified by the divergence of magnetic susceptibility at Q_π, which may or may not involve the divergence of the local spin susceptibility, a sum of contributions from all momentum points. In a two-dimensional

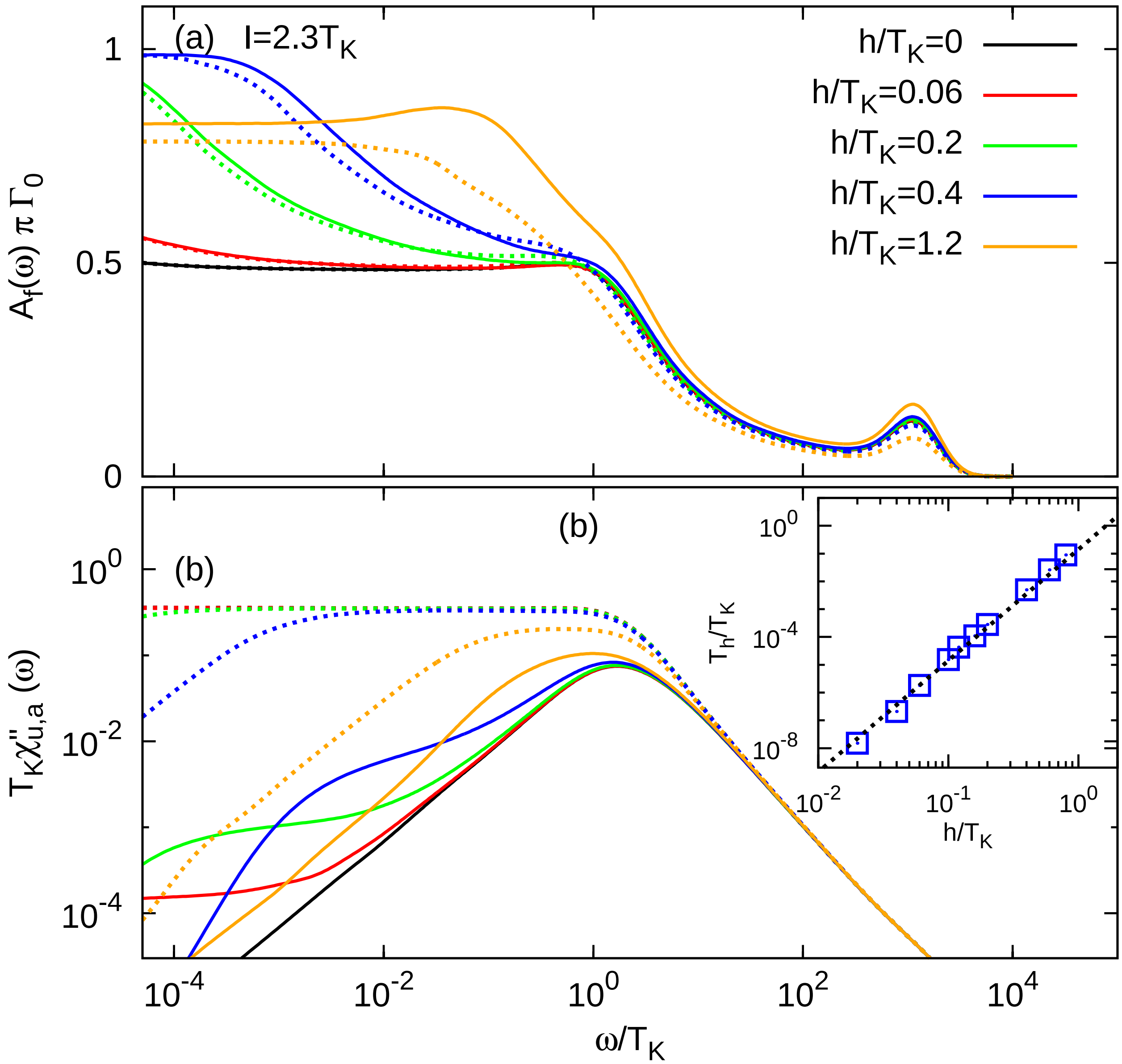

FIG. 4: (color online) Spectral functions $A_f(\omega)$ (a) and the imaginary parts of the uniform and staggered spin susceptibilities (b) as functions of energy for different values of h in the two-impurity quantum critical regime, $I = 2.3T_K$. The line representations in (a) and (b) are the same as in Fig. 2. The inset shows T_h as a function of h, which is obtained the same way as in Fig. 3. The line is a fitting $T_h/T_K = 0.18(h/T_K)^4$.

lattice, such divergences are related to each other due to finite spin density of states near Q_π. In a magnetic-field driven QPT, the local spin susceptibility can diverge even for 3D, arising from the divergence near Q_0. This favors the local critical type of transitions with the delocalization of quasiparticles, a feature shared with the two-impurity QCP. The divergence of the uniform spin susceptibility induced by the magnetic field might be related to the pronounced ferromagnetic fluctuations observed in field-drive transition in $YbRh_2Si_2$.[34]

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