

Emergent soft-gap Anderson models at quantum criticality in a lattice Hamiltonian within dynamical mean field theory

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Local quantum criticality in itinerant fermion systems has been extensively investigated through the soft-gap Anderson impurity model, wherein a localized, correlated impurity hybridizes with a broad conduction band with a singular, $|\omega|^r$, density of states. However, lattice models hosting quantum critical points (QCPs) do not appear to have such a spectrum emerging at the QCP. In this work, we report the emergence of such a singular form of the density of states in a three-orbital lattice model, within dynamical mean field theory, precisely at a quantum critical point, separating a gapless, Fermi liquid (FL) metallic phase from a gapped, Mott insulating phase. A temperature-dependent exponent, α , defined using the corresponding Matsubara self-energy, is found to vary from $+1$ deep in the FL regime, to -1 in the Mott insulator regime. Interestingly, we find that α becomes temperature-independent, and hence isosbestic, precisely at the QCP. The isosbestic exponent is shown to lead to an emergent soft-gap spectrum, $|\omega|^r$, at the QCP, where $r = |\alpha_{\text{iso}}|$. We discuss the implications of our findings for non-Fermi-liquid behavior in the quantum critical region of the phase diagram.

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I. INTRODUCTION

Quantum phases and their critical nature continue to be a leading field of study in condensed-matter physics [1]. Particularly challenging and interesting is the class of quantum phase transitions (QPTs) that defy the traditional Landau-Ginzburg-Wilson framework [2–5]. These include topological phase transitions [6–9] and QPTs involving the presence of both locally critical modes and long-wavelength fluctuations [3,5], commonly observed in heavy fermion systems [10–12]. Other systems hosting local quantum critical points (QCPs) are correlated impurity systems with a pseudogapped host [3,13–15] and lattice Dirac systems in two dimensions [16–23]. For example, in the soft-gap Anderson model (SGAM), the local (boundary) QCP is governed by the intrinsic critical local moment fluctuations that are further sensitized in the presence of the vanishingly small host density of states [3,24–29]. From a field-theoretical perspective, local QCPs represent interacting fixed points when the exponent, r , of the vanishing density of states (DOS) is less than 1 [3,30]. Previous studies have shown that the phase transition in the single-impurity Kondo problem with a pseudogap host can be understood within a Ginzburg-Landau framework involving the locally critical modes describing local moment fluctuations [30]. In the lattice context, a Kondo lattice system can be self-consistently mapped onto the Bose-Fermi Kondo model (with a power-law bosonic bath), and the critical nature of the Kondo to local moment phase transition is associated with a magnetic ordering of the conduction electrons [31,32].

An intriguing scenario would arise if such gapless fermionic excitations naturally emerge precisely at the QCP instead of being existent from the outset. For example, the deconfined Mott transition is associated with the emergence of a gapless spin liquid state with a spinon Fermi surface representative of neutral spin-1/2 quasiparticles while the charge excitations are gapped [33]. Disorder-induced power-law gaps have also been observed across an insulator-metal Mott transition [34]. Identifying new models and the underlying universality classes will broaden our current understanding of QPTs beyond the Landau-Ginzburg-Wilson framework. Particularly enlightening would be the expansion of this class of local QPTs representing metal-insulator transitions, across naturally occurring lattice settings to aid experimental verification. In principle, the paramagnetic metal to paramagnetic insulator Mott transition could represent such fermionic criticality via the emergence of scale-invariant power law spectra [35–37]. However, as shown in a recent study, a strictly power law spectrum down to zero temperature has not been observed in the most basic version of the Hubbard model [36]. Concomitantly, the critical nature of the Mott transition is indeed observable, but only beyond a typical finite-temperature scale [38]. A recent experiment on a moire lattice also demonstrated a continuous Mott transition [39]. Theoretically, a strictly zero temperature, continuous Mott transition was indeed observed in a three-orbital lattice model consisting of a localized flat band of interacting (f) electrons hybridizing with two independent bands of itinerant electrons (c) [40]. This model has recently been studied in other contexts and can also be viewed as a modified periodic Anderson model in a layered configuration [41–43].

In this work, we revisit this model to analyze the signatures of quantum criticality at nonzero temperatures. We

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demonstrate the pristine nature of a continuous Mott transition in this model within dynamical mean field theory (DMFT) [44] using the numerically exact continuous time quantum Monte Carlo method [45–51]. The QPT occurs as the quasiparticle excitations continuously evolve into non-Fermi-liquid and critical gapless states manifested in the form of a power law spectrum down to the lowest energy scales. Specifically, the critical spectra represent emergent soft-gap Anderson models with a characteristic exponent for the soft-gap density of states. Interestingly, this exponent is independent of temperature over a given QCP, but it is nonuniversal and varies over the line of quantum critical points.

The paper is organized as follows: The model and method are presented in Sec. II, followed by results and discussions in Sec. III. Here we identify the quantum critical points and demonstrate the presence of an isosbestic exponent and quantum criticality through the analysis of the low-frequency form of the self-energy. We also relate these observations to an emergent soft-gap density of states and hybridization function at the QCP. In Sec. IV, we conclude and discuss some future directions.

II. MODEL AND FORMALISM

The three-orbital model system [40] comprises a localized, correlated f orbital hybridizing with a conduction band (c) of itinerant electrons via the hybridization energy, V ; the latter couples to a third, delocalized, noninteracting (M) orbital via hopping energy, $t_\perp$. The Hamiltonian, H , is thus given by $H = H_f + H_c + H_M + H_{fc} + H_{cM}$, and the individual terms are represented in standard second quantized notation as

$$H_f = \epsilon_f \sum_{i\sigma} f_{i\sigma}^\dagger f_{i\sigma} + U \sum_i n_{fi\uparrow} n_{fi\downarrow}, \quad (1)$$

$$H_c + H_M = \sum_{k\sigma} \epsilon_k (c_{k\sigma}^\dagger c_{k\sigma} + c_{Mk\sigma}^\dagger c_{Mk\sigma}), \quad (2)$$

$$H_{fc} = V \sum_{k\sigma} (f_{k\sigma}^\dagger c_{k\sigma} + \text{H.c.}), \quad (3)$$

$$H_{cM} = t_\perp \sum_{k\sigma} (c_{k\sigma}^\dagger c_{Mk\sigma} + \text{H.c.}). \quad (4)$$

In the absence of c - M mixing ($t_\perp = 0$), this is simply a standard periodic Anderson model, which has been employed extensively to investigate heavy fermion systems [44,52–56]. In a previous study [40], two of the authors employed the local moment approach [57] within DMFT at zero temperature, and they identified a surface of quantum critical points, in the U - $t_\perp$ - V space, separating a gapless Fermi liquid phase from a Mott insulator phase. For a fixed- V , the line of critical points was found to be roughly hyperbolic in the $t_\perp$ - U plane, with the asymptotes being $t_\perp = 1$ and $U = 0$. However, the finite-temperature signatures of the critical transition and underlying mechanism of the QCP were not addressed. Hence, in this work, we use continuous-time quantum Monte Carlo, as implemented in the TRIQS open source package [45–51], to investigate the nature of this quantum criticality and the manifestation of the zero-temperature QCPs in the finite-temperature phase diagram. We work in the particle-hole symmetric, paramagnetic regime, with $\epsilon_f = -U/2$, thus avoiding the fermion sign problem.

The local f -Green's function, in this model, is given by

$$G_f(i\omega_n) = \int d\epsilon \rho_0(\epsilon) \frac{1}{i\omega_n - \frac{V^2}{i\omega_n - \epsilon - \frac{t_\perp^2}{i\omega_n - \epsilon}} - \Sigma(i\omega_n)}, \quad (5)$$

where $\Sigma(i\omega_n)$ is the k -independent (within DMFT) self-energy [40]. We choose a generic, semielliptic conduction-band density of states, $\rho_0(\epsilon) = 2\sqrt{1 - \epsilon^2/D^2}/\pi D$, with D being the half-bandwidth. It is important to note the non-singular choice of the density of states, which is in contrast to the choice made in the soft-gap Anderson model ($|\epsilon|'$). The Weiss field, $\Delta(i\omega_n)$, is the self-consistent hybridization function representing the DMFT bath for the f -electrons, and it is related to the host Green's function, $\mathcal{G}(i\omega_n)$, by $\Delta(i\omega_n) = i\omega_n - \mathcal{G}^{-1}(i\omega_n)$, which in turn can be obtained from the self-energy, $\Sigma_f(i\omega_n)$, and the f -Green's function through Dyson's equation $\mathcal{G}^{-1}(i\omega_n) = G_f^{-1}(i\omega_n) + \Sigma_f(i\omega_n)$. Thus, for a given $\Delta(i\omega_n)$, we compute the self-energy and Green's function of the impurity using a hybridization-expansion CTQMC as implemented in TRIQS [45–51]. We use the Padé approximant method [58] to analytically continue the Matsubara f -Green's function to real frequencies, and hence we obtain the real-frequency f -spectrum. In this work, we use a fixed $V = 0.44D$ and two representative interaction strengths, namely $U = 1.75D$, $1.2D$, with the unit of energy being $D = 1$ to analyze the phase transition as a function of $t_\perp$. In fact, it should be noted that for each V , this model exhibits a line of quantum critical points in the $t_\perp$ - U plane [40]. The parameter sets used in this work to study the finite-temperature signatures of the QPT driven by tuning $t_\perp$ thus represent only two such points on a surface of QCPs existing in this model.

III. RESULTS AND DISCUSSION

A. Identification of quantum critical points

We utilize the temperature-dependent, Matsubara quasiparticle fraction, $Z_0(T) = [1 - \text{Im} \Sigma(i\omega_0)/\omega_0]^{-1}$, with $\omega_0 = \pi T$ being the lowest Matsubara frequency, for locating the QCP [59,60]. In the zero-temperature limit, $\lim_{T \rightarrow 0} Z_0(T) = Z$ is simply the zero-temperature quasiparticle renormalization factor, defined for a conventional, real-frequency, Fermi-liquid self-energy, as $\Sigma_{\text{FL}} = \Sigma(0) + \omega(1 - 1/Z) + O(\omega^2)$. Naturally, at finite temperatures, and over the Mott insulator regime, the $Z_0(T)$ does not have a direct physical interpretation. Nevertheless, it has proven to be a quick diagnostic for identifying a QCP [59–62]. Considering U and V to be 1.75 and 0.44 (in units of D), respectively, and for various values of $t_\perp$, the computed $Z_0(T)$ are shown in Fig. 1. We have performed calculations for many more $t_\perp$ values, but we have not displayed the results to avoid cluttering. The low T Matsubara quasiparticle fraction $Z_0(T)$ clearly changes its character as $t_\perp$ increases through $t_\perp/D = 1.033$, in a way that parallels the finding in a two-dimensional Hubbard model close to optimal doping [59] that had employed the dynamical cluster approximation framework [63]. The data for $t_\perp < t_{\perp c}$ have a convex curvature as $T \rightarrow 0$ and have a finite positive intercept at $t_{\perp c}$, while $Z_0(T)$ for $t_\perp > t_{\perp c}$ bends downwards displaying a concave curvature approaching a value close to zero at finite temperature. We identify the QCP as the value of

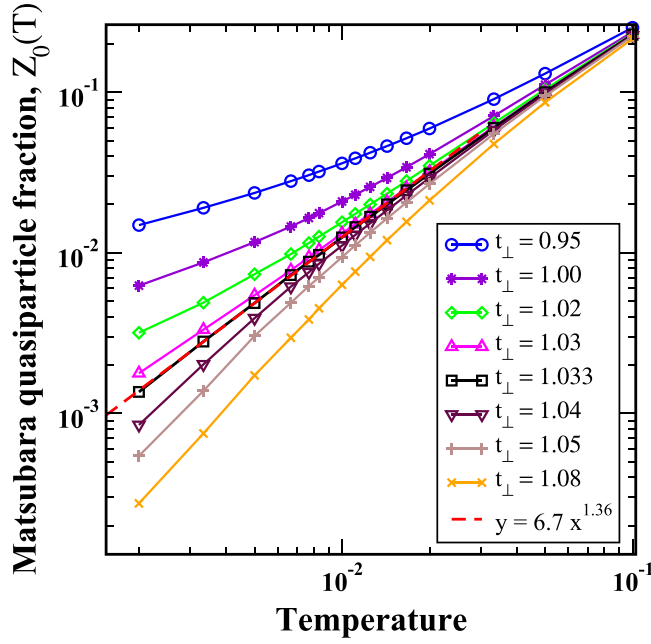


FIG. 1. The Matsubara quasiparticle fraction $Z_0(T)$ defined as $Z_0(T) = [1 - \text{Im}\Sigma(i\omega_0)/\omega_0]^{-1}$, calculated using CTQMC, is plotted as a function of temperature T for a selection of $t_\perp$ values. The dashed red line is a power law fit to the $t_\perp = 1.033$ data. The fit is seen to be valid over almost two decades.

$t_\perp$ at which such a vivid change in the dependence of Z_0 on T occurs; specifically at the parameter $t_{\perp,c}/D = 1.033 \pm 0.001$, the $Z_0(T) \sim T^{1.36 \pm 0.005}$ has a power law form. The behavior indicates a crossover from a Fermi liquid phase for $t_\perp < t_{\perp,c}$ to a Mott insulator phase for $t_\perp > t_{\perp,c}$ [40]. A parallel analysis for $U = 1.2D$ yields $t_{\perp,c}/D = 1.077 \pm 0.001$ and $Z_0(T) \sim T^{1.38 \pm 0.004}$ [64].

To consolidate the finding of a quantum critical point, we must show that the characteristic scales on the two sides of the QCP vanish simultaneously, implying the absence of a coexistence region. The scale on the Fermi liquid side can be taken to be the zero-temperature quasiparticle weight $Z_0(T = 0)$. We extract this quantity as a y-axis intercept of a simple fit of the $Z_0(T)$ data [using a form $Z_0(0) + CT^\gamma$] for a range of $t_\perp < 1.033D$. On the Mott insulator side, a natural choice of the characteristic scale is the spectral gap, the determination of which requires analytical continuation, a mathematically ill-defined problem. As an alternative to analytic continuation from imaginary to real frequencies for determining the Mott spectral gap, we use a protocol that employs the reverse route, which is well-defined, albeit approximate. This protocol is described briefly here, and details have been provided in Appendix A.

A real-frequency gapped density of states is *designed* with certain unknown parameters. Using three constraints, namely the spectral sum rule, getting the density of states value at $\omega = 0$ directly from CTQMC as $A(\omega = 0) = -G_f(\tau = \beta/2)/(\pi T)$, and a geometric constraint between the parameters, we reduce the number of unknown parameters to just two, from which we can obtain the zero-temperature gap, Δ_{g0} , and an effective bandwidth, W . We also obtain a finite temperature spectral gap, which we call Δ_{gT} , such that at

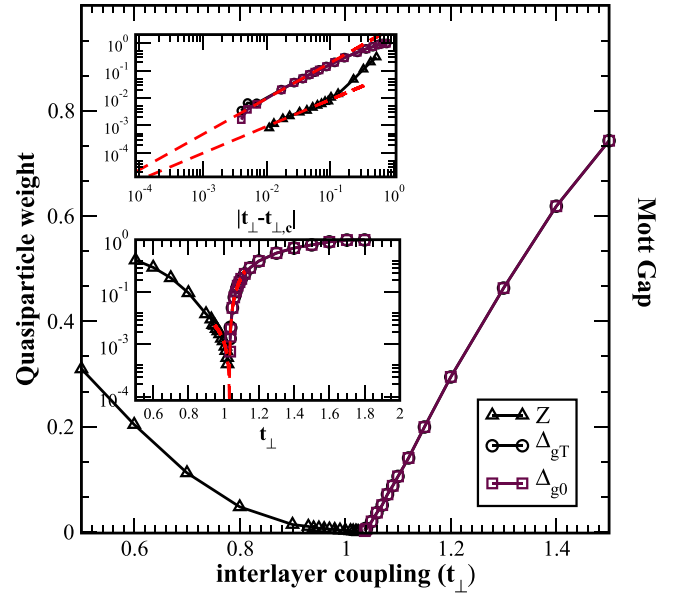


FIG. 2. Vanishing of the zero-temperature quasiparticle weight (Z) and zero- (finite-) temperature Mott gap, denoted as Δ_{g0} (Δ_{gT}) as we approach the QCP ($t_{\perp,c} \approx 1.033$) plotted on a linear scale (main panel) and evaluated at $U/D = 1.75$ and $T/D = 0.002$. Inset, bottom panel: The same data in the main panel are shown on a linear-log scale for the region close to the QCP to highlight that the scales vanish as a power law, with $Z \sim |t - t_{\perp,c}|^{a_1}$ and $\Delta_{g0} \sim |t - t_{\perp,c}|^{a_2}$ (with $a_1 = 0.97 \pm 0.02$, $a_2 = 1.30 \pm 0.02$). The power law fit to the CTQMC data is shown as red dashed lines. The Fermi liquid scale Z and the zero-temperature Mott gap Δ_{g0} vanish simultaneously, at $t_{\perp,c} \approx 1.033D$, which thus represents a QCP. Inset, upper panel: The x-axis is rescaled to $|t_\perp - t_{\perp,c}|$, and the scales are plotted on a log-log scale.

$T = 0$, $\Delta_{gT} = \Delta_{g0}$. The spectral representation may then be used to transform the above two-parameter real-frequency density of states to a Matsubara frequency Green's function, G_f^{model} , having two fitting parameters, which can be found simply by comparing against the numerically obtained Green's function. In Fig. 9 of Appendix A, we demonstrate a sample of the fitting of the CTQMC data with the two-parameter model Green's function. Utilizing the protocol described in Appendix A, and data for the lowest temperature reached in our simulations, i.e., $T/D = 0.002$, we have computed the spectral gap scales (Δ_{gT} and Δ_{g0}).

In Fig. 2 we show the quasiparticle weight, $Z \equiv Z_0(T = 0)$, and the MI gap scale Δ_{g0} (as well as Δ_{gT}) for $U/D = 1.75$, as a function of $t_\perp$ on a linear scale in the main panel and on a linear-log scale in the inset. The zero- and finite-temperature Mott gaps (Δ_{g0} and Δ_{gT} , respectively) are almost identical for all $t_\perp$ except in the proximity of the QCP, where they do differ. We have confirmed that the two scales, namely Z and Δ_{g0} , vanish simultaneously as a power law with $Z \sim |t_\perp - t_{\perp,c}|^{a_1}$ and $\Delta_{g0} \sim |t_\perp - t_{\perp,c}|^{a_2}$ ($a_1 = 0.97 \pm 0.02$, $a_2 = 1.30 \pm 0.02$) [64] at $t_{\perp,c} \approx 1.033D$ thus representing a QCP at $t_{\perp,c}$. Again, for the other parameter set, namely $U = 1.2D$, $t_{\perp,c} = 1.077D$, we find a similar vanishing of scales with $a_1, a_2 = 0.89 \pm 0.02, 1.01 \pm 0.01$ [64], confirming that this parameter set is also a QCP.

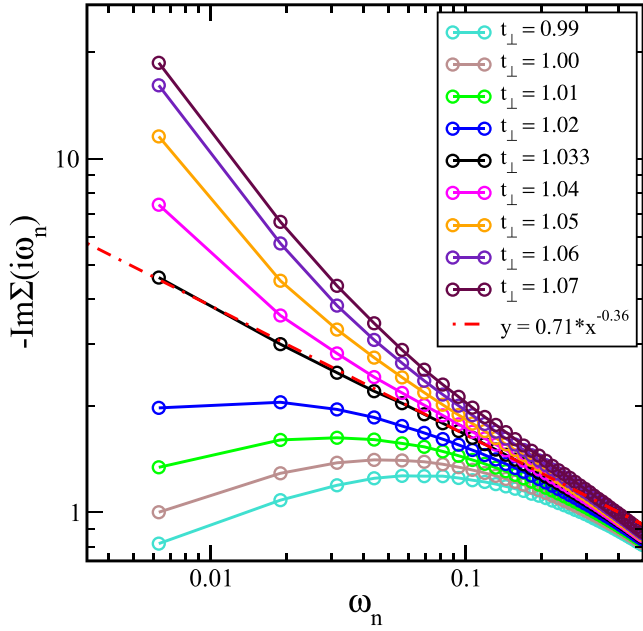


FIG. 3. The imaginary part of the Matsubara frequency self-energy, $\Sigma(i\omega_n)$, as a function of Matsubara frequency, ω_n , for various $t_{\perp}$ values (in units of D) evaluated at $T/D = 0.002$, $U/D = 1.75$, and $V/D = 0.44$. The power law ($\sim |\omega_n|^{-|\alpha|}$) form is observed at the QCP ($t_{\perp,c} \approx 1.033D$) with an exponent $\alpha = -0.36 \pm 0.005$ [64].

B. Isosbestic points and quantum criticality

For an ideal Fermi liquid and a Mott insulator, the imaginary part of the Matsubara self-energy may be represented as $-\text{Im}\Sigma(i\omega_n) \sim (\omega_n)^{\alpha}$ for $\omega_n \rightarrow 0^+$, with $\alpha = +1$ and -1 , respectively [65]. However, if the respective metal-insulator transition is a quantum-critical phase transition, then quantum-critical fluctuations at finite temperatures generally accompany classic non-Fermi-liquid signatures in the form of low-frequency power law behavior of the self-energy. As we move farther away from the QCP, these non-Fermi-liquid features cross over to the conventional features representing the stable metallic or insulating ground states on either side of the QCP. To understand whether our system projects similar characteristics, we plot $-\text{Im}\Sigma(i\omega_n)$ as a function of ω_n on a log-log scale for various values of $t_{\perp}$, evaluated at $U/D = 1.75$ and $T/D = 0.002$. As shown in Fig. 3, and as expected, a power-law behavior extending over a wide range of frequencies is observed at $t_{\perp,c} \approx 1.033D$.

As we move away from this parameter, the $-\text{Im}\Sigma(i\omega_n)$ deviates from its power law characteristic, especially at low frequencies. The magnitude of this deviation signifies the parametric distance from the QCP. We define a self-energy exponent, α , using a two-parameter fit of $y_n = -\text{Im}\Sigma(i\omega_n, t_{\perp}, T)$ at a fixed $t_{\perp}$ and T fitting only the first two Matsubara frequencies to $A|\omega_n|^{\alpha}$. The exponent may be obtained in closed form as $\alpha = \ln(y_1/y_0)/\ln(3)$. The Matsubara quasiparticle fraction $Z_0(T)$ acquires a physical meaning as the quasiparticle weight only at $T = 0$. Similarly, the exponent α acquires a physical meaning as the exponent of the emergent soft-gap DOS only at the QCP (as will be shown later). Nevertheless, as the change of curvature in the

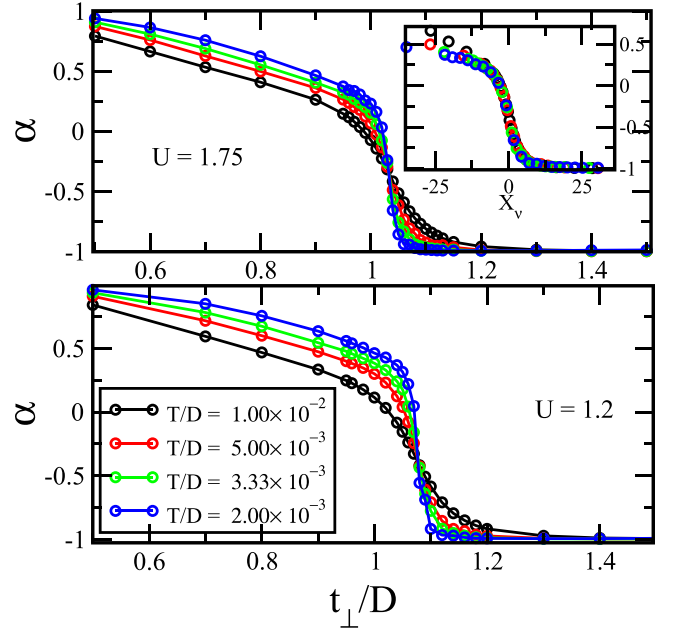


FIG. 4. The self-energy exponent α (defined in the text through the imaginary part of the self-energy) is plotted as a function of $t_{\perp}/D$ for (a) $U/D = 1.75$ (left panel) and (b) $U/D = 1.2$ (right panel) for different T/D . The exponent features an isosbestic point, at $t_{\perp,c}/D$. However, a closer look reveals a small spread along the vertical and horizontal axes. The isosbestic exponent, α_{iso} , reported here is located at the midpoint of this spread. We find $t_{\perp,c} \approx 1.033 \pm 0.0005$, $\alpha_{\text{iso}} = -0.35 \pm 0.01$ for $U/D = 1.75$ and $t_{\perp,c}/D \approx 1.077 \pm 0.001$, $\alpha_{\text{iso}} = -0.39 \pm 0.01$ for $U/D = 1.2$. Left (inset): A data collapse is achieved by a rescaling of the self-energy exponents shown in the main panel using the scaling ansatz, Eq. (6), reminiscent of scaling collapse in critical systems with a correlation length exponent $\nu = 1.11 \pm 0.001$ for $U/D = 1.75$ (see also Appendix B).

temperature dependence of $Z_0(T)$ leads to an identification of a QCP, the exponent α , as shown in the following, turns out to be an excellent diagnostic for identifying the QCP.

We find, as expected, that the exponent is nonintegral in a wide region around the QCP. In Fig. 4 we plot this exponent α as a function of $t_{\perp}$ for different temperatures. As illustrated in Fig. 4, the self-energy exponent (α) changes smoothly across the QCP from a positive value to a negative value close to -1 with increasing $t_{\perp}$. Furthermore, if the power-law form of the self-energy at $t_{\perp,c}$ is a genuine quantum effect, then α should be independent of T at this point; in other words, the exponent at $t_{\perp,c}$ should represent an isosbestic point in the α versus $t_{\perp}$ plot, as shown in Fig. 4. We label the isosbestic exponent as α_{iso} , where the exponent is independent of temperature. Indeed, as demonstrated in Fig. 4, an isosbestic point, $\alpha_{\text{iso}} = -0.35 \pm 0.01$, is found at $t_{\perp} \approx (1.033 \pm 0.0005)D$ for $U = 1.75D$ (left panel) and $\alpha_{\text{iso}} = -0.39 \pm 0.01$ at $t_{\perp} \approx (1.077 \pm 0.001)D$ for $U = 1.2D$ (right panel). The error bar in $t_{\perp,c}$ (α_{iso}) indicates the spread along the horizontal (vertical) axis.

From the Matsubara quasiparticle fraction analysis (as shown in Fig. 1) and the vanishing of the scales (Fig. 2), we know that the two parameter sets, namely $(U/D, t_{\perp}/D) = (1.75, 1.033)$ and $(1.2, 1.077)$, represent quantum critical

points. Combining this inference with the self-energy analysis shown in Fig. 4 yields the observation that the $t_{\perp}$ values corresponding to the quantum critical points are also isosbestic points. Indeed, it is well known that strongly correlated systems display *isosbestic* crossing points as a typical conspicuous feature in several observable quantities like the specific heat or the optical conductivity [66]. In quantum critical systems, the Binder cumulant obtained from local magnetization was shown to display such an intersection point that coincides with the QCP [67]. The identification of the QCP through an isosbestic point in the exponent that determines the Matsubara frequency dependence of the local, one-particle self-energy is one of the highlights of this work.

As is well-known for isosbestic points, a rescaling of the axes should yield a data collapse [68], and indeed, as seen in the inset of the left panel of Fig. 4, the exponents for $U = 1.75D$ collapse onto a universal curve for all temperatures, with the following scaling ansatz:

$$\alpha(t_{\perp}, T) = f_U \left(\frac{t_{\perp} - t_{\perp c}}{t_{\perp c} T^{1/\nu}} \right), \quad (6)$$

where f_U is the scaling function. A similar data collapse is observed for the exponents shown in the bottom right panel of Fig. 11 for $U = 1.2D$ in Appendix B. Furthermore, the scaling exponent ν that is typically associated with the correlation length exponent across a phase transition is found to be $\nu = 1.11 \pm 0.001$ (using a procedure discussed in Appendix B) for the parameter set $U/D = 1.75$, $t_{\perp c} \simeq 1.033D$, and $\nu = 1.03 \pm 0.01$ for the second parameter set $U = 1.2D$, $t_{\perp c} \simeq 1.077$. Perturbative renormalization-group studies on the pseudogap Anderson and Kondo model predict $\nu = 1$ for the pseudogap exponent, $r \geq 1$, when the solution is a level crossing transition and is therefore first-order. We will briefly prove that $r = -\alpha_{\text{iso}}$ for the model under investigation. In our case, we find $\nu > 1$ and $0 < r < 1/2$ for which the transition is known to be second order [3,30].

The CTQMC method is constrained to work at finite temperatures, and it becomes prohibitively expensive at lower temperatures. However, since the exponent α_{iso} at the quantum critical point is found to be an isosbestic, i.e., independent of temperature in the investigated range, we conjecture that the exponent remains the same down to $T = 0$, and such an extrapolation naturally leads to the inference that the self-energy has a power law form at the QCP, with a fractional exponent. In fact as Fig. 4 shows, as we traverse the $t_{\perp}$ axis, the α versus $t_{\perp}$ becomes steeper with decreasing temperature, and extrapolating such behavior down to $T = 0$, the exponent should be $+1$ in the FL phase, changing abruptly to the isosbestic fractional exponent at the QCP, and then changing again immediately thereafter to -1 in the Mott insulating phase. This suggests that the low-frequency self-energy changes from having an analytic form ($\sim -i\omega_n$) in the FL phase to a branch point [$\sim -i \text{sgn}(\omega_n) |\omega_n|^{\alpha_{\text{iso}}}$] at the QCP to a simple pole form ($1/i\omega_n$) in the Mott insulating phase. It is worth mentioning that further evidence of the interacting nature of the QCP could be provided via ω/T scaling of the one- and two-particle correlation functions evaluated on the real frequency axis. However, such analyses including the identification of the different critical exponents and their

relation to the critical self-energy exponent α_{iso} will be taken up in later work.

Until now, we have confined ourselves to the imaginary frequency axis. In the next two subsections, we will use simple analytical arguments to deduce the manifestation of the power law form of the Matsubara frequency self-energy at the QCP, and the density of states in the corresponding real-frequency quantities.

C. Self-energy as a function of real frequency: Behavior at low frequencies

The isosbestic exponent in the frequency dependence of the Matsubara frequency self-energy must manifest in the real-frequency dependence of the retarded self-energy. We show in this section that this is indeed the case. Using the arguments presented in the previous section, we may express the finite-temperature self-energy at the QCP as $\Sigma(i\omega_n \rightarrow i0^+) = -iA\omega_n^{-r}$, where $r = -\alpha_{\text{iso}}$ and $\omega_n > 0$. The corresponding real-frequency self-energy may be obtained using analytic continuation, but here we employ the reverse route. Using an ansatz of the self-energy on the real-frequency axis, and employing the spectral representation, we derive the Matsubara frequency quantity, which matches the corresponding, numerically obtained quantity, thus validating the real-frequency ansatz.

We consider a power law form as an ansatz for ρ_{Σ} , namely

$$\rho_{\Sigma}(\omega) = -\frac{1}{\pi} \text{Im} \Sigma(\omega) = B|\omega|^{-\gamma}, \quad B > 0, \quad (7)$$

and we ask if such a form, when substituted in the spectral representation, can yield the form $\Sigma(i\omega_n \rightarrow i0^+) = -iA\omega_n^{-r}$ ($A > 0$), thus avoiding analytic continuation. Indeed this is possible, as we show below. Consequently, we would also know the relation between γ and r .

We begin with the spectral representation of the Matsubara frequency self-energy, specifically for the particle-hole symmetric case under consideration here as

$$\Sigma(i\omega_n) = -2i\omega_n \int_0^{\infty} \frac{d\omega' \rho_{\Sigma}(\omega')}{\omega'^2 + \omega_n^2}, \quad (8)$$

where $\rho_{\Sigma}(\omega) = (-1/\pi) \text{Im} \Sigma(\omega)$, and $\Sigma(\omega)$ is the real frequency retarded self-energy. We can substitute Eq. (7) in Eq. (8) to get (for $\omega_n > 0$)

$$\begin{aligned} \Sigma(i\omega_n) &= -2iB\omega_n \int_0^{\Lambda} \frac{\omega'^{-\gamma} d\omega'}{\omega'^2 + \omega_n^2} \\ &= -2iB\omega_n^{-\gamma} \int_0^{\Lambda/\omega_n} \frac{dx}{x^{\gamma}(1+x^2)}, \end{aligned}$$

where Λ is a UV-cutoff scale. For $T \rightarrow 0$, $\Lambda/\omega_n \rightarrow \infty$ and since the integrand vanishes as $x^{2+\gamma}$ ($\gamma > 0$) for large x , the upper limit of the integral can be considered to be ∞ . Thus,

$$\Sigma(i\omega_n) = -2iB \text{sgn}(\omega_n) |\omega_n|^{-\gamma} \int_0^{\infty} \frac{dx}{x^{\gamma}(1+x^2)}. \quad (9)$$

From the numerically evaluated self-energy, we know that, at the isosbestic point,

$$\Sigma(i\omega_n \rightarrow 0) = -i \text{sgn}(\omega_n) A |\omega_n|^{-r}. \quad (10)$$

Comparing Eq. (9) with Eq. (10), we get $\gamma = r$ and $\rho_\Sigma(\omega) = B|\omega|^{-r}$. Now, given that the imaginary part of the self-energy has the form $\rho_\Sigma(\omega) = B|\omega|^{-r}$, we can derive the real part, $\text{Re}\Sigma(\omega)$, through the Kramers-Kronig transform $\text{Re}\Sigma(\omega) = -\mathcal{P} \int d\omega' \rho_\Sigma(\omega')(\omega - \omega')^{-1}$, and we get $\text{Re}\Sigma(\omega) \simeq -B' \text{sgn}(\omega)|\omega|^{-r}$. Combining the real and imaginary parts, we get the limiting low-frequency self-energy as

$$\Sigma(\omega) = -[B' \text{sgn}(\omega) + i\pi B]|\omega|^{-r} = -\bar{B}|\omega|^{-r}, \quad (11)$$

with $B, B' > 0$. In the following subsection, we will show that the above form of the self-energy translates to a soft-gap form of the density of states.

Equation (10) is also seen to be consistent with the results shown in Fig. 1. To see this, we note that, for $n = 0$, $\Sigma(i\omega_0) = -i|\omega_0|^{-r}$, but since $\omega_0 = \pi T$ and $Z_0(T) = [1 - \Sigma(i\omega_0)/i\omega_0]^{-1}$, we get $Z_0(T) = (1 + |\omega_0|^{-(r+1)})$, which, in the low-temperature limit, reduces to $Z_0(T) \simeq T^{-(1+r)}$. As Fig. 1 shows, the exponent deduced from the power law is 1.36, which is equal to $1 - \alpha_{\text{iso}}$ deduced from the results of the left panel of Fig. 4. A similar analysis has been carried out for $U = 1.2D$, and we find $Z_0(T) \approx T^{-(1+r)}$, with $r = 0.38 \pm 0.004$, which is consistent with the $r = -\alpha_{\text{iso}} = 0.39 \pm 0.01$ obtained for $U = 1.2D$ from the right panel of Fig. 4.

D. Emergent soft-gap density of states at the QCP

We can now use the real-frequency power law form of the self-energy [Eq. (11)] to derive the low-frequency form of the f -electron Green's function on the real axis. Starting from the Green's function expression,

$$G_f(\omega) = \int d\epsilon \frac{\rho_0(\epsilon)}{z - \frac{V^2}{\omega^+ - \epsilon - \frac{t_\perp^2}{\omega^+ - \epsilon}}}, \quad (12)$$

and using $\Sigma(\omega) = -\bar{B}|\omega|^{-r}$, with $z = \omega^+ - \Sigma(\omega) \rightarrow \bar{B}|\omega|^{-r}$ as $\omega \rightarrow 0$, we get, to leading order,

$$G_f(\omega) \approx \int d\epsilon \frac{\rho_0(\epsilon)}{\bar{B}|\omega|^{-r}} = \frac{|\omega|^r}{\bar{B}},$$

by considering the most divergent term in the denominator. Thus, the spectral function of the f -density of states is given by

$$\rho_f(\omega) = -\frac{1}{\pi} \text{Im} G_f(\omega) = \frac{\text{Im} \bar{B} / \pi}{(\text{Re} \bar{B})^2 + (\text{Im} \bar{B})^2} |\omega|^r.$$

The above expression shows that $\rho_f(\omega)$ has a soft-gap form with the exponent r . The arguments presented in Secs. III C and III D establish the link between the isosbestic exponent and the soft-gap exponent. Namely, if $\Sigma_{\text{QCP}}(i\omega_n \rightarrow 0) \approx -i \text{sgn}(\omega_n)|\omega_n|^{-r}$, then $\rho_f(\omega) \approx |\omega|^r$. The isosbestic exponent and the soft-gap exponent of the spectrum have the same magnitude but the opposite sign. This emergent soft-gap density of states at the QCP represents our most important result. Additionally, the emergent soft-gap model is non-symmetry-breaking in nature unlike the QCPs in the soft-gap Anderson models studied earlier [30–32,69].

The inference of a soft-gap density of states can be further consolidated by analytically continuing the CTQMC Green's

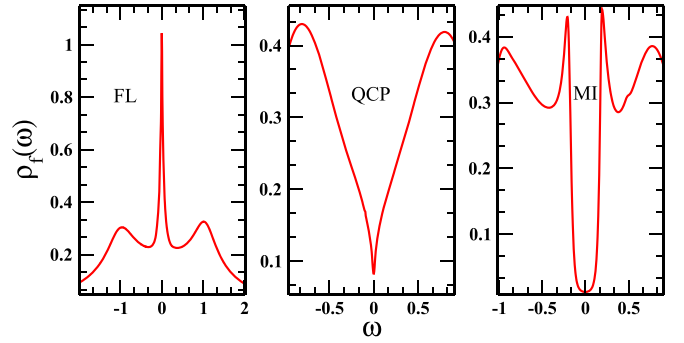


FIG. 5. The single-particle density of states $\rho_f(\omega)$ obtained via analytic continuation of the Matsubara frequency Green's function $G_f(i\omega)$ using the Padé approximation is shown for the Fermi liquid region (left panel) with $t_\perp/D = 0.8$, the quantum critical point (middle panel) with $t_\perp/D = 1.033$, and the Mott insulator (right panel) with $t_\perp/D = 1.08$. The parameters used to obtain $G_f(i\omega)$ are $U/D = 1.75$, $V/D = 0.44$.

function. Here we have used the Padé approximation as implemented in Ref. [58] to get the real frequency spectra, $\rho_f(\omega)$. The analytically continued f -spectra are shown in Fig. 5 for the parameters $t_\perp = 0.8$ in the left panel, $t_\perp = 1.033 = t_{\perp c}$ in the middle panel, and $t_\perp = 1.08$ in the right panel. In the left panel, $\rho_f(\omega)$ is peaked around $\omega = 0$, which is the Kondo resonance, characteristic of the FL phase. The MI phase (right panel) exhibits a gapped $\rho_f(\omega)$, representing a Mott insulator. Particularly at $t_\perp = 1.033 = t_{\perp c}$, the single-particle density of states (DOS) $\rho_f(\omega; T = 0.002) \sim |\omega|^r + a_0$ exhibits a power law, soft-gap DOS in agreement with the previous discussion. Thus, we have shown that, while the density of states has a Kondo resonance in the FL phase, and a gap in the MI phase, it has an emergent soft-gap at the QCP.

Finally, it is straightforward to show that a soft-gap density of states of the form $\rho_f(\omega) = |\omega|^r \theta(\Lambda - |\omega|)$, with Λ as a ultraviolet cutoff, results in a power law form in the Matsubara time dependence of the Green's function, namely $G_f(\tau) \propto -\tau^{-(1+r)}$ for $\tau, \beta \gg 1$ (see Appendix C for the derivation). Such a power law is indeed observed in the numerically obtained CTQMC results, as shown in Fig. 6, which shows $-G_f(\tau)$ as a function of τ as obtained for $U = 1.75D$ and temperatures of 0.01 (purple), 0.005 (blue), 0.003 (red), and 0.002 (green). The $\tau \gg 1$ behavior is clearly seen to be a power law, and the fit (dashed line) is seen to be valid over more than a decade for all the temperatures. The extracted exponent r from each of the fits is $\sim 0.35 \pm 0.01$, which is temperature-independent and is seen to be the negative of the isosbestic exponent found from the self-energy analysis (Fig. 4). Furthermore, as expected, the power law form does not fit the results obtained away from the QCP as shown in Fig. 14 of Appendix C.

E. The self-consistent hybridization function

Within DMFT, the lattice model is mapped onto a self-consistent impurity Anderson model, and our findings at the QCP indicate that a soft-gap Anderson model is emergent at the QCP. We confirm this by showing that the imaginary part of the self-consistent hybridization is indeed a power law at

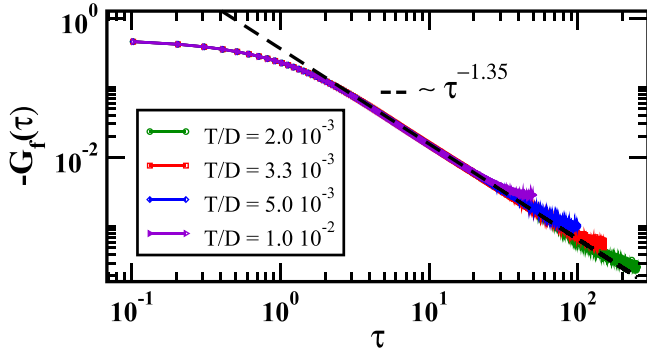


FIG. 6. The imaginary-time Green's function $-G_f(\tau)$ as a function of the Matsubara time τ for $t_{\perp} = t_{\perp,c} = 1.033$, $U = 1.75D$ and three different temperatures: (a) $T/D = 0.01$ (purple), (b) $T/D = 0.005$ (blue), (c) $T/D = 0.003$ (red), and (d) $T/D = 0.002$ (green) at the QCP. The $\tau \gg 1$ behavior is seen to fit very well to a power law ($\sim \tau^{-(1+r)}$) (black dashed line) over more than a decade, and the extracted exponent, r , as obtained via this comparison is $r \approx 0.35 \pm 0.01 \approx -\alpha_{\text{iso}}$ [64], which is also independent of the temperature.

the QCP. To show this analytically, we need to revisit the arguments of Sec. III D, and compute subleading corrections to the Green's function for $T \rightarrow 0$ and $\omega_n \rightarrow 0^+$, and connect that to the DMFT hybridization function.

A detailed derivation is provided below. The main aim is to derive a relation between the isosbestic exponent (α_{iso}) and the hybridization exponent at the QCP. Given the Green's function,

$$G_f(i\omega_n) = \int \frac{d\epsilon \rho_0(\epsilon)}{\Omega_n - f_n(\epsilon)}, \quad (13)$$

where $\Omega_n = i\omega_n - \Sigma(i\omega_n)$ and $f_n(\epsilon) = V^2[i\omega_n - \epsilon - t_{\perp}^2/(i\omega_n - \epsilon)]^{-1}$, we can substitute the low-frequency form of $\Sigma(i\omega_n)$ to get $\Omega_n \simeq i(\omega_n + A|\omega_n|^{-r})$ (with $r > 0$ and $r = -\alpha_{\text{iso}}$), which is divergent for $T \rightarrow 0$ or $\omega_n \rightarrow 0$. Hence, we can use Taylor's expansion to rewrite $G_f(i\omega_n)$ as

$$G_f^{-1}(i\omega_n) = \Omega_n - M_1 + \frac{(M_1^2 - M_2)}{\Omega_n} + \mathcal{O}\left(\frac{1}{\Omega_n^2}\right), \quad (14)$$

where the k th moment is given by $M_k = \int d\epsilon \rho_0(\epsilon) f_n^k(\epsilon)$. The self-consistent hybridization function is given by

$$\Delta(i\omega_n) = i\omega_n - \Sigma(i\omega_n) - G_f^{-1}(i\omega_n), \quad (15)$$

and thus, to lowest order in $1/\Omega_n$, the hybridization is given by $\Delta(i\omega_n) = M_1 - (M_1^2 - M_2)/\Omega_n$.

For $\omega_n \rightarrow 0^+$, M_1 and M_2 are real constants, and it is easy to show that $M_1 = 0$, and M_2 is finite and positive-definite (see Appendix D). Hence,

$$\Delta(\omega_n \rightarrow 0^+) = -\frac{iM_2|\omega_n|^r}{A}, \quad (16)$$

thus yielding a low-frequency power law form for the self-consistent hybridization function. We emphasize that a divergent and dominant form of the self-energy and a vanishing $M_1 = \int d\epsilon \rho_0(\epsilon) f_n(\epsilon)$ are important to ensure the validity of the moment expansion of the Green's function. Furthermore, the functional form of $f_n(\epsilon)$ in our model ensures that we will always have a vanishing M_1 , and the low-frequency

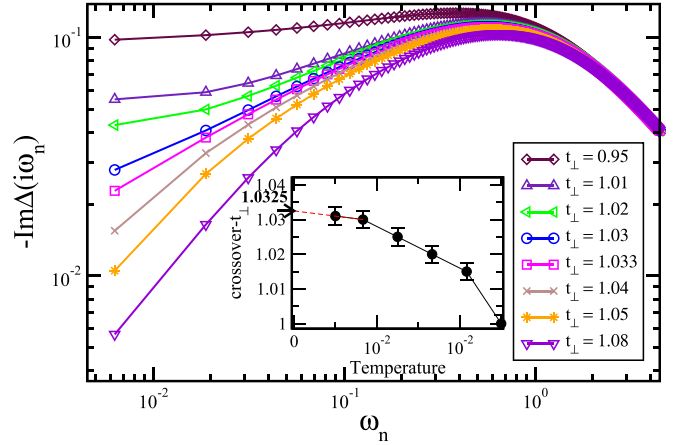


FIG. 7. Main: The imaginary part of the self-consistent hybridization, $\Delta(i\omega_n)$, as a function of Matsubara frequency, for various $t_{\perp}$ values (in units of D) and $\beta = 500$. Inset: The $t_{\perp}$ at which the imaginary part of the hybridization $[-\text{Im}\Delta(i\omega_n)]$, at a given temperature, obeys a power-law at the maximum number of points is identified as the crossover point. The inset shows the crossover $t_{\perp}$ as a function of temperature. The red dashed line shows a linear extrapolation to zero temperature, where the limiting value is seen to be the quantum critical value ($t_{\perp,c}$) within numerical resolution. The error bar represents the x -axis resolution to which the calculation is performed.

power-law form of the self-energy [Eq. (11)] will always be the most singular function in the Hilbert transform. This is not true for other models like the standard periodic Anderson model [32,70,71], where the self-energy vanishes as $\omega_n \rightarrow 0$.

We emphasize that the above analysis is correct only in the zero-temperature limit. In other words, a genuine power law vanishing (soft-gap) hybridization function is obtained at sufficiently low temperatures when $\omega_n \rightarrow 0$ makes true sense. At any nonzero temperature, the moments appearing in Eq. (14) are dependent on ω_n (see Fig. 15 and the discussion in Appendix D) and contribute to the low-energy frequency behavior of the hybridization function inducing deviations from a pristine power-law expected at the QCP, i.e., $t_{\perp} = t_{\perp,c}$. Nonetheless, this frequency dependence becomes negligibly small as $T \rightarrow 0$, where $M_1 \rightarrow 0$ and M_2 becomes purely real and positive-definite, producing a soft-gap hybridization function, $\Delta(i\omega_n \rightarrow 0) = -iA^{-1}M_2|\omega_n|^r$, as $T \rightarrow 0$ and $\omega_n \rightarrow 0$ (see Fig. 16 in Appendix D for more details).

In Fig. 7, we plot the numerically obtained $-\text{Im}\Delta(i\omega_n)$ as a function of ω_n for different $t_{\perp}$'s and a fixed $U/D = 1.75$ and $T/D = 0.002$. The data in the main panel clearly demonstrate a change of curvature as the $t_{\perp}$ is tuned, similar to the Matsubara quasiparticle fraction (Fig. 1) and the imaginary part of the self-energy (Fig. 3), indicating a finite-temperature crossover from a gapped to a metallic bath seen by the electrons as $t_{\perp}$ is decreased. Taking a closer look at the data suggests that this crossover occurs at a value of $t_{\perp}$ that is not equal to the $t_{\perp,c}$ at $\beta = 500$. In fact, this crossover value is temperature-dependent, and only in the limit of $T \rightarrow 0$ does it approach the quantum critical value, $t_{\perp,c}$, as the $T \rightarrow 0$ limiting value, represented by the red dashed line in the inset of Fig. 7 shows.

The error bars for the crossover $t_{\perp}$ are estimated by the resolution at which the numerical calculations were performed.

The finding of a power law form in the hybridization function at a $t_{\perp} \neq t_{\perp,c}$ is thus seen to be a finite-temperature effect, and as argued above, the impurity spectral function, the self-energy, and the hybridization function acquire the same exponent only at $T \rightarrow 0$. We do not have a complete physical understanding of this finite-temperature mismatch between hybridization and self-energy. We emphasize that this observation should not be interpreted as nonconverged DMFT self-consistency since we have checked very carefully for convergence of the self-energy and the hybridization (please see the discussion in Appendix D and Fig. 17). Instead, it should be regarded as evidence that temperatures as low as $T/D = 10^{-4}$ need to be accessed to find the same exponent in the hybridization at $t_{\perp,c}$ within numerical resolution. However, we do not have the resources required to access such low temperatures at present.

We note that the hybridization as well as the density of states have a vanishing form as $T \rightarrow 0$, namely $\sim |\omega|^r$ ($r > 0$) in the three-orbital model considered in this work, a behavior that is quite distinct from the SGAM. In the latter, the hybridization has a vanishing form by choice for any temperature, and, while the generalized FL phase has a divergent DOS, the local moment phase has a vanishing DOS, precisely as found here and in the critical Mott insulator in the single-band Hubbard model close to U_{c1}^+ [36]. We have also investigated a few other points on the line of QCPs, and the soft-gap exponent appears to vary monotonically over the line of QCPs, in the $t_{\perp}$ - U plane, thus giving rise to a family of soft-gap Anderson models. A detailed investigation of the emergent family of the soft-gap Anderson models is underway and will be reported later.

IV. OUTLOOK

Extensive investigations of quantum criticality in the soft-gap Anderson model (SGAM) over the past two decades have shown the QCP to be an interacting, non-Fermi-liquid fixed point with a wide quantum critical scaling (ω/T) region [30,72–75], with a nonvanishing local magnetic response. In contrast, the critical properties of the emergent SGAM derived through DMFT treatment of the three-orbital model investigated here are non-symmetry-breaking. Thus, an important future direction would be to extensively investigate the quantum critical scaling (ω/T) region for the current model.

The emergent nature of the continuous transition is reminiscent of a deconfined QCP [33], where low-energy fractional particles that are absent on either side of the QCP naturally emerge at the QCP. The low-frequency form of the self-energy having a branch point at the QCP was also found in a dilaton gravity model using gauge-gravity correspondence [76], thus yielding a natural explanation of non-Fermi-liquid behavior emanating from the QCP. It would be interesting to explore how the emergent low-energy critical modes interplay with long-range magnetic fluctuations [41,77], which would be predominantly relevant in lower dimensions. The particle-hole asymmetric SGAM with $r > 1/2$ hosts a QCP between a Kondo screened and a local moment phase otherwise absent in the symmetric case.

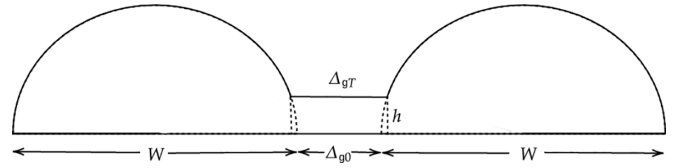


FIG. 8. Model DOS chosen to extract the Mott gap Δ_{g0} .

So a question remains as to the fate of the Mott QCP in the presence of particle-hole asymmetry. We anticipate that a renormalization-group approach [78,79] may uncover the Hamiltonian flows of this three-orbital model, and hence lead to the underlying reasons for the emergence of the soft-gap Anderson models at quantum criticality.

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APPENDIX A: DETERMINATION OF MOTT GAP

To extract the zero-temperature Mott gap from the Matsubara Green's function obtained through CTQMC, we design a model density of states on the real frequency axis having certain unknown parameters, one of them being the $T = 0$ Mott gap. The model DOS is then “Wick-rotated” onto the imaginary frequency axis, compared with the CTQMC Green's functions, and the Mott gap as well as the other parameters are obtained through a best fit. The procedure is detailed below.

A model, gapped density of states (DOS) is shown in Fig. 8, which has semielliptic bands flanking the gap. Such a model DOS is relevant for this work since our simulations consider a semielliptic DOS and therefore the Hubbard bands of the Mott insulator spectral function are semielliptic in form. Nonetheless, the strategy outlined should be applicable to any form of the Hubbard bands. This model DOS is used as an ansatz for the putative real-frequency spectral function of the Mott insulator at a certain $t_{\perp}$, U and temperature, T , with the $T = 0$ Mott gap being denoted by Δ_{g0} . At $T \neq 0$, we expect thermal filling of the Mott insulating gap. Let us denote the finite-temperature “Mott gap” as Δ_{gT} . Thus, at $T = 0$, $\Delta_{gT} = \Delta_{g0}$. To mimic this finite-temperature effect, we include a nonzero spectral weight at and around the Fermi level. Therefore, we modify the model spectral function by considering a parameter h that mimics the Fermi level spectral weight. A mathematical representation for the model DOS is

the following:

$$\rho_f^{\text{model}}(\epsilon) = \begin{cases} h, & \forall |\epsilon| \leq \Delta_{gT}/2, \\ \frac{4N}{\pi W} \left[1 - \left(\frac{|\epsilon| - (W + \Delta_{g0})/2}{W/2} \right)^2 \right]^{1/2}, & \forall \Delta_{gT}/2 \leq |\epsilon| \leq W + \Delta_{g0}/2. \end{cases} \quad (\text{A1})$$

We note that the model DOS written above has five unknown parameters: h , N , W , Δ_{gT} , Δ_{g0} . However, there are three constraints we can use to reduce the number of unknowns to just two:

(i) The finite-temperature spectral density h may be obtained directly from CTQMC as $h = -G_f(\tau = \beta/2)/(\pi T)$.

(ii) The constant N may be determined in terms of the other parameters through the observation [from Eq. (A1) and Fig. 8] that at $|\epsilon| = \frac{\Delta_{gT}}{2}$, $\rho_f^{\text{model}}(\epsilon) = h$ representing continuity of the model DOS:

$$N = \frac{h\pi W}{4 \cos \theta}, \quad (\text{A2})$$

where $\sin \theta = 1 - (\Delta_{gT} - \Delta_{g0})/W$.

(iii) The spectral sum rule, i.e., $\int d\epsilon \rho_f^{\text{model}}(\epsilon) = 1$, represents the third condition, and yields

$$\frac{2N}{\pi} \left[\frac{\pi}{2} + \theta + \frac{\sin(2\theta)}{2} \right] + h\Delta_{gT} = 1. \quad (\text{A3})$$

Using Eq. (A2) in (A3), we get $W = 4 \cos \theta \frac{(1/h) - \Delta_{gT}}{\pi + 2\theta + \sin(2\theta)}$. Thus, we are left with only two fitting parameters, namely θ and Δ_{gT} .

The strategy for obtaining the unknowns, i.e., Δ_{gT} and θ , is as follows:

(i) Using the spectral representation, $G_f^{\text{model}}(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{\rho_f^{\text{model}}(\epsilon)}{i\omega_n - \epsilon}$, the corresponding Matsubara Green's function may be calculated.

(ii) The model Green's function obtained in the first step above is then compared to the numerically obtained $G_f(i\omega_n)$ through CTQMC to get the two unknown fitting parameters through a best-fit procedure.

As mentioned in step (i) above, using the spectral representation, the model Matsubara Green's function may be obtained as

$$G_f^{\text{model}}(i\omega_n; \Delta_{gT}, W) = -2i\hbar\omega_n \left[\frac{W}{2 \cos \theta} \int_{-\theta}^{\pi/2} \frac{\cos^2 \bar{\theta} d\bar{\theta}}{\omega_n^2 + \frac{W^2}{4} (\sin \theta + \sin \bar{\theta} + \frac{\Delta_{gT}}{W})^2} + \frac{1}{\omega_n} \tan^{-1} \left(\frac{\Delta_{gT}}{2\omega_n} \right) \right]. \quad (\text{A4})$$

Equation (A4) represents a two-parameter model Green's function, which may be used for fitting the imaginary part of the numerically obtained CTQMC Green's function, $G_f(i\omega_n)$, to get Δ_{gT} and θ . For each combination of Δ_{gT} and θ , the effective bandwidth is found through $W = 4 \cos \theta (1/h - \Delta_{gT})/[\pi + 2\theta + \sin(2\theta)]$. The best fit then yields the zero-temperature Mott gap Δ_{g0} through $\sin \theta = 1 - (\Delta_{gT} - \Delta_{g0})/W$. Figure 9 demonstrates the imaginary part of the f -electron Matsubara Green's function calculated within DMFT-CTQMC fitted against the analytical form given in Eq. (A4) for $t_{\perp} = 1.037$ (top panel), $t_{\perp} = 1.04$ (middle panel), and $t_{\perp} = 1.05$ (bottom panel). The agreement is seen to be excellent.

Ideally, the Δ_{g0} obtained from the above fitting should be independent of temperature, i.e., $\Delta_{g0}(T)/\Delta_{g0}(0.002D) \sim 1$ as we vary T . In Fig. 10, therefore, we plot $\Delta_{g0}(T)/\Delta_{g0}(0.002D)$ as a function of temperature for $t_{\perp} = 1.037$ (top panel) and $t_{\perp} = 1.08$ (bottom panel). As observed from these plots, for $t_{\perp} \rightarrow t_{\perp c}$, $\Delta_{g0}(T)/\Delta_{g0}(0.002D)$ very quickly deviates from 1 as we vary T , unlike a $t_{\perp}$ that is far away from the QCP. More investigations are required to understand this rapid deviation, close to the QCP.

APPENDIX B: DETERMINATION OF THE CORRELATION-LENGTH EXPONENT, ν , THROUGH A SCALING COLLAPSE OF THE ISOBESTIC (α VERSUS $t_{\perp}$)

The α versus $t_{\perp}$ curves shown in Fig. 4 display an isobestic point at a certain $t_{\perp c}$. If this point is to be identified as a quantum critical point, then all the curves passing through the isobestic point must collapse onto a single curve when

the $t_{\perp}$ is rescaled as

$$X_{\nu}(\beta) = \beta^{1/\nu} (t_{\perp}/t_{\perp c} - 1). \quad (\text{B1})$$

However, the determination of ν , the correlation length exponent, that determines the best scaling collapse, is not straightforward. The first step in this direction is to determine α as a function of X_{ν} , given the known function $\alpha(t_{\perp})$. The mapping of $t_{\perp}$ to X_{ν} is linear, for a fixed β and ν , but the slope is temperature- and ν -dependent, and care must be taken when trying to interpolate/extrapolate $\alpha(t_{\perp})$ to $\alpha(X_{\nu})$.

For any given ν , when we rescale the $t_{\perp}$ axis, the window of the rescaled axis [$X_{\nu}(t_{\perp}, \nu)$ axis] increases with an increase in β for $\nu > 0$. Since the smallest window is obtained for high temperatures, in order to use only interpolation and avoid extrapolation of the data at lower temperatures, we consider $\beta_r = 100$ as the reference inverse temperature. For a given ν , and $(t_{\perp}/t_{\perp c} - 1) \in [-\delta, \delta]$ window, we construct an $X_{\nu} \in \beta_r^{1/\nu} [-\delta, \delta]$ mesh with N_x points for the reference β_r . Given the one-to-one correspondence between $t_{\perp}$ and X_{ν} for a given ν and β , it is straightforward to obtain α on the X_{ν} mesh. In practice, we calculate the corresponding self-energy exponent $\alpha(\beta, X_{\nu, i})$ using the Akima spline interpolation of the α versus $t_{\perp}$ data. Note that a direct interpolation of α versus X_{ν} is prone to error, hence it should be avoided. We repeat this procedure for different β values.

We do a visual inspection of α versus X_{ν} for a range of ν values, and we observe that, within a chosen window around the QCP, as the ν is increased, the α versus X_{ν} for $\beta = 100$ and 500 cross each other with the QCP being the pivot (see the top two panels of Fig. 11). This observation suggests that in order to determine the scaling exponent that yields the best “scaling collapse,” we should look for a zero crossing of a

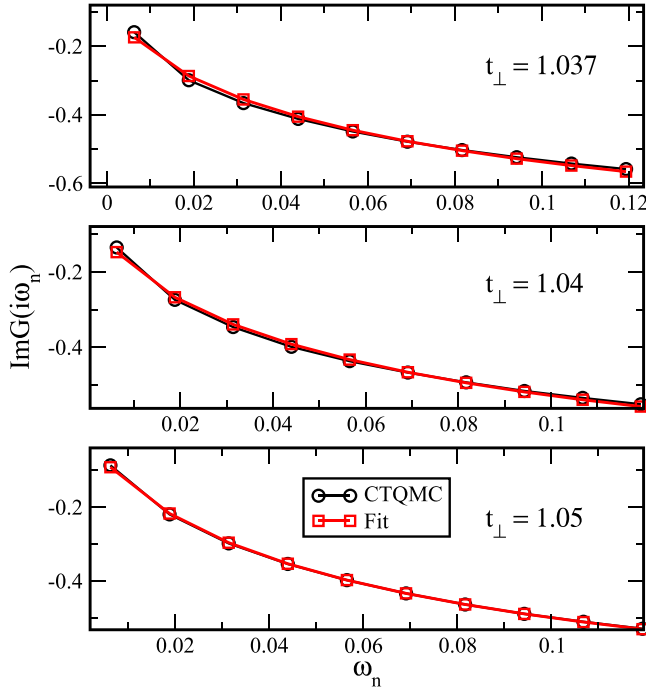


FIG. 9. Matsubara Green's function is calculated using CTQMC for $T/D = 0.002$, and $t_{\perp}/D = 1.037$ (top panel), 1.04 (middle panel), 1.05 (bottom panel), $U/D = 1.75$, and $V/D = 0.44$ and is fitted with the analytically calculated Matsubara Green's function in Eq. (A4), and hence the Mott gap (Δ_{gT}) and effective bandwidth W are obtained.

spread function defined as

$$L(\nu) = \sum_{i=1}^{N_x} [2\theta(X_{v,i}) - 1][\alpha(100, X_{v,i}) - \alpha(500, X_{v,i})], \quad (\text{B2})$$

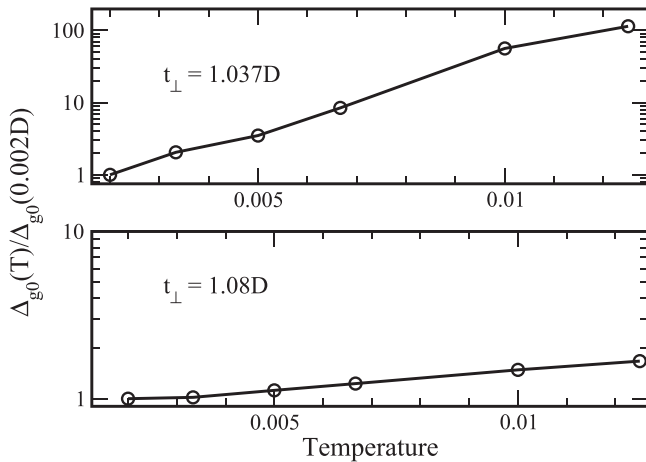


FIG. 10. $\Delta_{g0}(T)/\Delta_{g0}(0.002D)$ is plotted as a function of temperature for $t_{\perp} = 1.037D$, $1.08D$. Δ_{g0} is obtained by fitting the Matsubara Green's function obtained from CTQMC to the analytically calculated Matsubara Green's function in Eq. (A4).

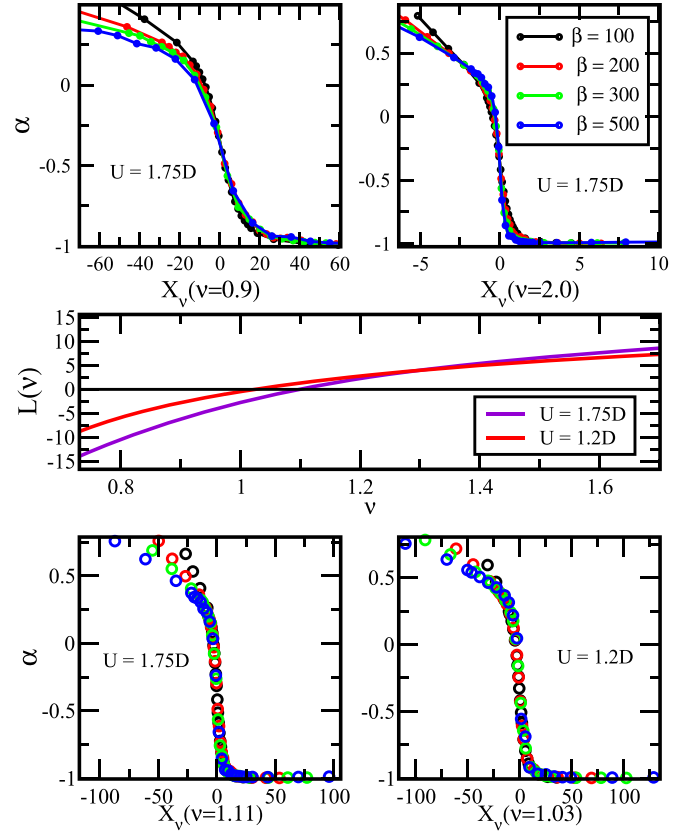


FIG. 11. The top two panels show α versus X_v for $\nu = 0.9$ (left) and $\nu = 2.0$ (right) corresponding to $U = 1.75D$. The middle panel shows the spread function $L(\nu)$ as a function of ν for both $U = 1.75D$ and $1.25D$. The ν that yields the zero crossing of the spread is identified as the correlation length exponent. The bottom two panels show the scaling collapse (of Fig. 4) for $U = 1.75D$ (left) and $U = 1.2D$ (right) with the corresponding correlation length exponent $\nu(U = 1.75) = 1.11 \pm 0.001$ and $\nu(U = 1.2) = 1.03 \pm 0.01$. The error in ν is found out from the corresponding error in determining the $t_{\perp,c}$ from the isosbestic plot in Fig. 4.

where $\theta(x)$ is a step-function. The finally obtained ν value corresponds to the root of $L(\nu)$, which also gives us the best scaling collapse around the QCP, as shown in Fig. 11.

The choice of the window $[-\delta, \delta]$ around the QCP for computing the spread function is also made through the visual inspection of the crossings, as shown in the top two panels of Fig. 11. For $U = 1.75D$ and $1.2D$, we chose $\delta = 0.133$ and 0.377 , respectively. The error associated in the determination of ν arises from the error in the estimation of $t_{\perp,c}$. In other words, we repeat the analysis for the maximum and minimum probable value of $t_{\perp,c}$ and associate the respective spread in the ν obtained as the error. We have verified that the exponent ν is quite robust with respect to a variation of δ .

APPENDIX C: MANIFESTATION OF A SOFT-GAP DENSITY OF STATES WITH EXPONENT τ IN THE MATSUBARA TIME DEPENDENCE OF THE GREEN'S FUNCTION $G_f(\tau)$

In this Appendix, we show that a real-frequency, soft-gap DOS implies a power law dependence of the Matsubara

Green's function, $G_f(\tau)$, on the imaginary-time (τ) axis. And the observation of power laws in the CTQMC derived $G_f(\tau)$ may then be traced back to the existence of a real-frequency soft-gap DOS through this proof, as done in Fig. 6 and the discussion associated with it.

Our starting point is a soft-gap density of states of the form

$$\rho_f(\omega) = A|\omega|^r \Theta(D - |\omega|), \quad (\text{C1})$$

where $|\omega| < D$, and A may be found through normalization of the DOS as $A = (r+1)/2D^{r+1}$. The Matsubara Green's function can be found by taking the Hilbert transform of the DOS [Eq. (C1)] as

$$G_f(i\omega_n) = \int_{-\infty}^{\infty} A \frac{|\omega|^r}{i\omega_n - \omega} \Theta(D - |\omega|) d\omega. \quad (\text{C2})$$

Fourier transforming the above, the Matsubara time Green's function, $G_f(\tau)$, can be represented in terms of $G_f(i\omega_n)$ as

$$G_f(\tau) = \frac{1}{\beta} \sum_n G_f(i\omega_n) e^{-i\omega_n \tau}. \quad (\text{C3})$$

Using Eqs. (C1), (C2), and (C3), we get

$$\begin{aligned} G_f(\tau) &= - \int_{-D}^0 d\omega \frac{(r+1)e^{-\omega\tau} |\omega|^r}{2D^{r+1}(1+e^{-\beta\omega})} \\ &\quad - \int_0^D d\omega \frac{(r+1)e^{-\omega\tau} |\omega|^r}{2D^{r+1}(1+e^{-\beta\omega})} \\ &= G^{(1)} + G^{(2)}. \end{aligned} \quad (\text{C4})$$

Now consider $G^{(1)}$, and taking the limit $\beta \rightarrow \infty$, we get

$$\begin{aligned} G^{(1)} &= - \int_{-D}^0 d\omega \frac{(r+1)e^{-\omega\tau} |\omega|^r}{2D^{r+1}(1+e^{-\beta\omega})} \\ &\simeq \int_0^D d\omega \frac{(r+1)e^{-\beta\omega} e^{\omega\tau} \omega^r}{2D^{r+1}}. \end{aligned}$$

The above integral will have a contribution around $(2/\beta)^{r+1}$ for $\tau \rightarrow \beta/2$, and it will vanish for $\beta \rightarrow \infty$, implying $G^{(1)} \rightarrow 0$ in the zero-temperature limit. Now, taking $x = \omega\tau$ with $\beta \rightarrow \infty$, we get

$$G_f(\tau) = G^{(2)} = -\tau^{-(r+1)} \int_0^\infty dx \frac{(r+1)e^{-x} |x|^r}{2D^{r+1}} \quad (\text{C5})$$

$$\propto -\tau^{-(r+1)} \Gamma(r). \quad (\text{C6})$$

Thus, $G_f(\tau)$ depends on r as given in Eq. (C6). We calculate $G_f(\tau)$ from Eq. (C4) directly by calculating the integral numerically without making the approximations involved in arriving at Eq. (C6). The results for varying r and D are plotted in Figs. 12 and 13. The figures show that the exponent r has its effect only for $\tau \gg 1$, which is easily noticeable from Fig. 12. We emphasize that these (Figs. 12 and 13) are not CTQMC results, but are obtained from Eq. (C4).

In Fig. 14 we demonstrate sample fits of $G_f(\tau)$ obtained from CTQMC calculations with the power law form, $\tau^{-(1+r)}$ for $t_\perp = 0.5$ (Kondo screened phase) and for $t_\perp = 1.5$ (Mott insulator phase) (top and bottom panel, respectively), where Eq. (C4) does not fit the data at all, as should be expected far away from criticality. This is contrary to the middle panel of

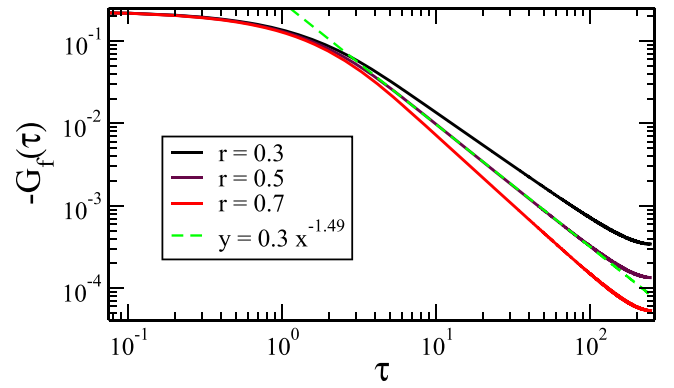


FIG. 12. Numerically calculated $G_f(\tau)$ from the ansatz $\rho_f(\omega) = A|\omega|^r \Theta(D - |\omega|)$ with $D = 1.0$, $\beta = 500.0$ using Eq. (C4). The r is found to have its effect on $G_f(\tau)$ for $\tau \gg 1$.

Fig. 14, representing the QCP, where the agreement is found to be the best, and a soft-gap power law form is seen over more than two decades (see Fig. 6).

APPENDIX D: DETAILED ANALYSIS ON THE HYBRIDIZATION FUNCTION

1. $T \rightarrow 0$ behavior of the moments

Now, let us try to understand the $T \rightarrow 0$ behavior of M_1 (recall $M_k = \int d\epsilon \rho_0(\epsilon) f_n^k(\epsilon)$, where $f_n(\epsilon) = V^2 [i\omega_n - \epsilon - t_\perp^2 / (i\omega_n - \epsilon)]^{-1}$) and M_2 for $t_\perp = t_{\perp,c}$. We have

$$\begin{aligned} M_1 &= V^2 \int_{-\infty}^{\infty} d\epsilon \frac{\rho_0(\epsilon)}{i\omega_n - \epsilon - \frac{t_{\perp,c}^2}{i\omega_n - \epsilon}} \\ &= V^2 \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \frac{i\omega_n - \epsilon}{(i\omega_n - \epsilon)^2 - t_{\perp,c}^2} \\ &= \frac{V^2}{2} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \left(\frac{1}{i\omega_n - \epsilon - t_{\perp,c}} + \frac{1}{i\omega_n - \epsilon + t_{\perp,c}} \right), \end{aligned}$$

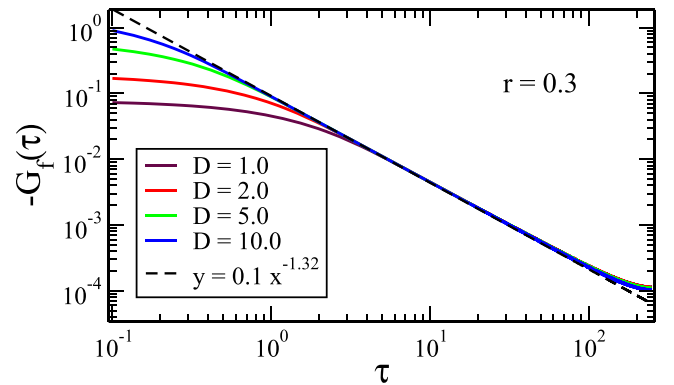


FIG. 13. Numerically calculated $G_f(\tau)$ from the ansatz $\rho_f(\omega) = A|\omega|^r \Theta(D - |\omega|)$ with $r = 0.3$ and $\beta = 500.0$ using Eq. (C4). $G_f(\tau) \propto \tau^{-(1+r)}$, with $r \approx 0.3$, is independent of the cutoff D .

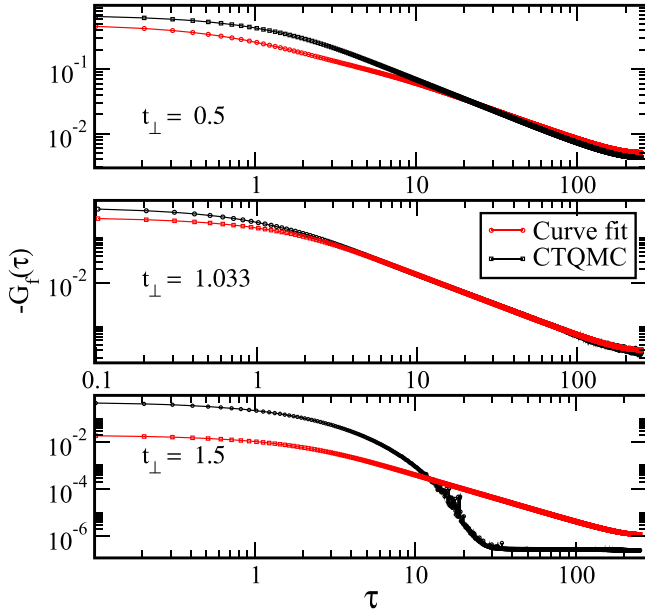


FIG. 14. The Matsubara time Green's function $-G_f(\tau)$ obtained from CTQMC for $T/D = 2.0 \times 10^{-3}$ is fitted to the integral Eq. (C4), using r and D as fitting parameters. The top and bottom panels represent the FL and MI regimes where the integral equation does not fit the data. There is a clear fit only at the QCP ($t_\perp = 1.033$, middle panel) with $r \approx 0.3$, and the fit is independent of D in the large- τ limit. This indicates that the DOS away from the QCP does not have a power law form.

where, in the limit of $\omega_n \rightarrow 0^+$, the real part of M_1 becomes [using $1/(x + i0^+) = \mathcal{P}(1/x) - i\pi\delta(x)$]

$$\text{Re}M_1 = \frac{V^2}{2} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \left[P\left(\frac{1}{-\epsilon - t_{\perp,c}}\right) + P\left(\frac{1}{-\epsilon + t_{\perp,c}}\right) \right].$$

Since $\rho_0(\epsilon) \neq 0 \forall \epsilon \in [-D, D]$ and $\rho_0(\epsilon) = 0 \forall |\epsilon| > D$, while $t_{\perp,c} > D$ for all the quantum critical points in the phase diagram, we get

$$\begin{aligned} \text{Re}M_1 &= \frac{V^2}{2} \int_{-D}^D d\epsilon \rho_0(\epsilon) \left[\frac{1}{-\epsilon - t_{\perp,c}} + \frac{1}{-\epsilon + t_{\perp,c}} \right] \\ &= \frac{V^2}{2} \int_{-D}^D d\epsilon \rho_0(\epsilon) \left[\frac{-2\epsilon}{\epsilon^2 - t_{\perp}^2} \right] = 0 \end{aligned}$$

for a p - h symmetric $\rho_0(\epsilon)$. The imaginary part of M_1 becomes

$$\text{Im}M_1 = \frac{V^2}{2} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \{-\pi[\delta(-\epsilon - t_{\perp,c}) + \delta(-\epsilon + t_{\perp,c})]\}.$$

With the same argument as we made earlier, since $|\epsilon| \leq D < t_{\perp,c}$ always, we get $\text{Im}M_1 = 0$. Thus, in the limit of $T \rightarrow 0$, we have shown that $M_1 \rightarrow 0$.

Now let us evaluate M_2 in the limit $i\omega_n \rightarrow i0^+ = i\eta$, where $\eta \rightarrow 0^+$,

$$M_2 = \frac{V^4}{4} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \frac{(i\eta - \epsilon)^2}{[(i\eta - \epsilon)^2 - t_{\perp,c}^2]^2}$$

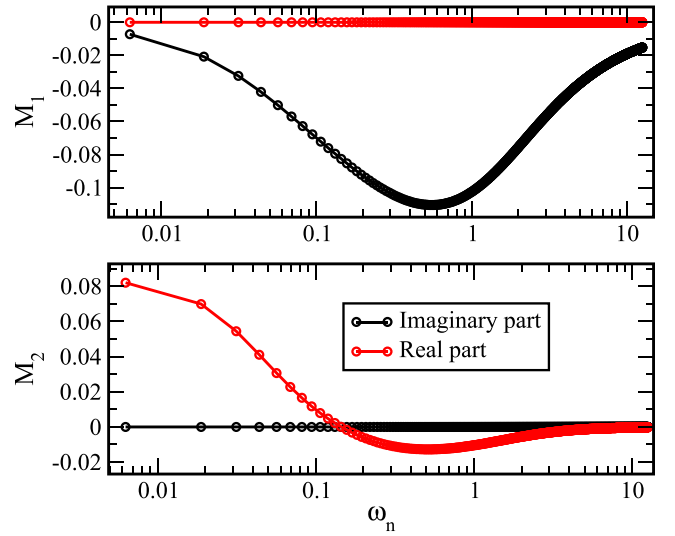


FIG. 15. Plot of the real and imaginary part of the moments M_1 and M_2 as a function of ω_n for $\beta = 500$ and calculated at $t_\perp = t_{\perp,c}$, $V = 0.44D$, $U = 1.75D$.

$$\begin{aligned} &= \frac{V^4}{4} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \frac{\epsilon^2 - 2i\eta\epsilon}{(\epsilon^2 - t_{\perp,c}^2)^2 - 4i\eta\epsilon(\epsilon^2 - t_{\perp,c}^2)} \\ &= \frac{V^4}{4} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \epsilon^2 \left[P\left(\frac{1}{(\epsilon^2 - t_{\perp,c}^2)^2}\right) + i4\pi\delta(\epsilon^2 - t_{\perp,c}^2) \text{sgn}[\epsilon(\epsilon^2 - t_{\perp,c}^2)] \right]. \end{aligned}$$

From the same argument that we made earlier that $|\epsilon| < D$ and $t_{\perp,c} > D$, the imaginary part goes to zero. Hence only the real part of M_2 survives,

$$\begin{aligned} \text{Re}M_2 &= \frac{V^4}{4} \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) \epsilon^2 P\left(\frac{1}{[\epsilon^2 - t_{\perp,c}^2]^2}\right) \\ &= \frac{V^4}{4} \int_{-D}^D d\epsilon \rho_0(\epsilon) \frac{\epsilon^2}{[\epsilon^2 - t_{\perp,c}^2]^2}. \end{aligned}$$

From the above expression, it is easy to see that $\text{Re}M_2$ is positive-definite and finite, since the integrand is positive-definite, and $t_{\perp,c} > D$ for all the quantum critical points in the phase diagram.

2. Finite frequency behavior of the moments

To understand the frequency behavior of the moments, M_1 and M_2 , at low enough temperatures, we calculate the respective moments as a function of ω_n for two different inverse temperatures, namely $\beta = 500$ (Fig. 15) and $\beta = 10^4$ (Fig. 16), using a power law form for the self-energy. Please note that our CTQMC calculations are limited to $\beta \leq 500$, so the $\beta = 10^4$ result shown in Fig. 16 assumes that the same power law form of the self-energy holds at this temperature, and the moments are computed using the equation given below Eq. (14). In Fig. 15, we show the moments M_1 and M_2 as a function of Matsubara frequency, as computed using

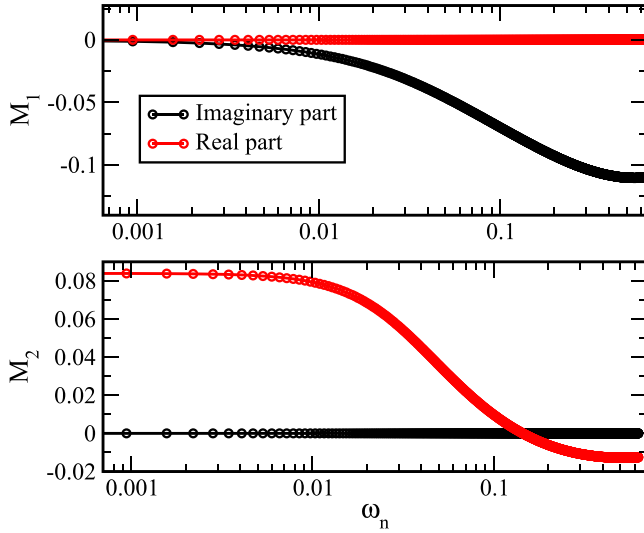


FIG. 16. Plot of the real and imaginary part of the moments M_1 and M_2 as a function of ω_n for $\beta = 10000$ and calculated at $t_\perp = t_{\perp,c}$, $V = 0.44D$, $U = 1.75D$.

the power law form of the self-energy at $\beta = 500$. We see that as $\omega_n \rightarrow 0^+$, M_1 approaches a finite value at the lowest Matsubara frequency, which will result in a deviation from a perfect power law form of the hybridization at the QCP. To consolidate this observation, we compute the moments at a much lower temperature, namely $\beta = 10^4$, and as may be seen in Fig. 16, $M_1 \rightarrow 0$.

Figure 16 clearly demonstrates that $M_1 \approx 0$ and M_2 is a real, positive-definite constant in the limit of $T \rightarrow 0$ that naturally implies $\omega_n \rightarrow 0$, and thereby it is only in this limit that the hybridization function is power-law vanishing with the form $\Delta(i\omega_n) \approx -\frac{iM_2|\omega_n|^r}{A}$, a genuine power-law. In fact, our analyses suggest that there would always exist a nonzero contribution from M_1 in the low-frequency behavior of $\Delta(i\omega_n)$ at all nonzero temperatures. However, the low-frequency contribution will progressively tend to zero as we approach zero temperature. We infer from our analyses and emphasize that one may need to go as low as $\beta = 10^4$ to demonstrate a true soft-gap hybridization at the QCP. Unfortunately, we do not have the resources required for accessing such low temperatures at present.

Another question that we address now is that of DMFT self-consistency. From our analytical calculations [see Eq. (16)], we see that the exponent appearing in the hybridization is the same as that of the spectrum and the self-energy [see Eq. (10)]. However, the CTQMC results shown in Fig. 7 paint a different picture. The figure shows that the critical $t_\perp$ data do not have a clear power law form, but if we do somehow fit a power law form to the low-frequency data, we see an exponent of 0.42, which differs from the self-energy exponent. Thus, a natural culprit for this mismatch may be identified as the absence of DMFT self-consistency. However, as we will show below, the real culprit is the limitation of our calculations to $\beta \leq 500$, due to the lack of resources, and not DMFT self-consistency.

In Fig. 17, we show the imaginary part of the hybridization function as obtained through the DMFT Eqs. (13) and (15),

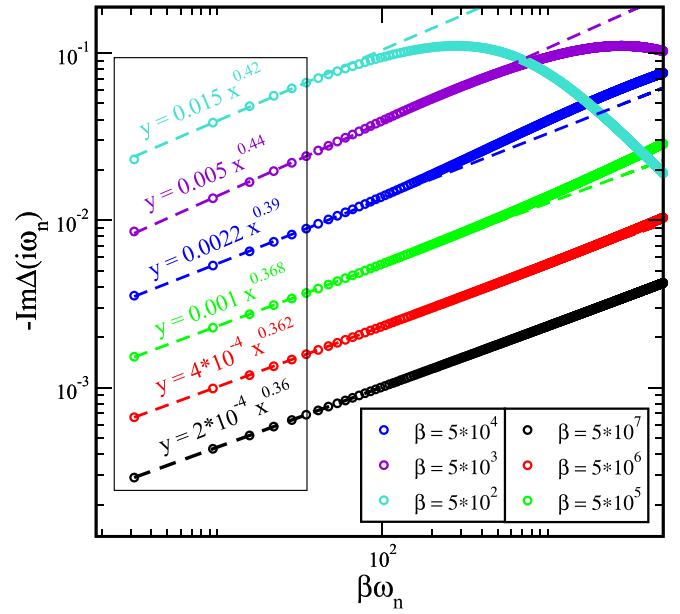


FIG. 17. The imaginary part of the hybridization function, $-\text{Im}\Delta(i\omega_n)$, calculated at $t_\perp = 1.033D$, $U = 1.75D$, $V = 0.44D$, is plotted as a function of the $\beta\omega_n$ for different inverse temperatures, and it is fitted with a power law. We assume a self-energy of the form $\Sigma(i\omega_n) \sim iA|\omega_n|^{-r}$ with $r = 0.36$, as an ansatz in Eq. (13) (justified as the self-energy manifests an isosbestic point in temperature, at $t_\perp = 1.033$). The important thing to note is that (i) the range of the power law form extends to higher frequencies as we go down in temperature, and (ii) the value of the exponent approaches the value $r = 0.36 = -\alpha_{\text{iso}}$, implying that a genuine soft-gap form with the expected soft-gap exponent, $-\alpha_{\text{iso}}$, in the hybridization function emerges as $T \rightarrow 0$.

using a power law form of the self-energy $\Sigma(i\omega_n) = iA\omega_n^{-r}$ with $r = 0.36$ plotted as a function of $\beta\omega_n$. Note that this gives us the freedom to choose a desired temperature, but we again iterate that our CTQMC calculations are restricted to $\beta \leq 500$. With this freedom, we obtain $-\text{Im}\Delta(i\omega_n)$ for increasingly lower temperatures, and as seen in Fig. 17, a power law form when fit to the low-frequency data matches the numerical results over an increasingly larger frequency range as the temperature is lowered. More importantly, the exponent of the power law decreases smoothly with decreasing temperature from 0.42 to the isosbestic exponent, 0.36. This shows that the DMFT self-consistency will not result in the same exponent in the hybridization at finite temperatures. And only at zero temperature will a perfect power law form with exactly the same exponent emerge in the hybridization at the quantum critical point.

APPENDIX E: ADDITIONAL NUMERICAL DETAILS

We use continuous-time quantum Monte Carlo as implemented in the TRIQS [45–50] open source package to study the finite-temperature behavior of the system. The Monte Carlo parameters used in the calculations were $n_{\text{cycle}} = 200\,000$, $n_{\text{warmup}} = 10\,000$, $n_{\text{length}} = 500$. The parameter, n_{cycles} , is increased to 1 000 000 for the final few DMFT iterations to reduce stochastic noise. Furthermore,

close to the transition point, we also increased the number of iterations for which $n_{\text{cycles}} = 1\,000\,000$ to get the converged data. The number of Legendre polynomials (n_l) considered is dependent on the temperature we choose. We used $n_l = 50$ – 100 for inverse temperature (β) ranging from 50 to 500. The number of processors (Dual Intel Xeon Cascadelake

8268) employed was 48. For carrying out the analytic continuation through the Padé approximation, we have used Beach's matrix formulation method, as implemented in the code [58], to find the Padé approximants. The maximum number of Padé approximant coefficients used for the analytic continuation is 80.

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