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Bad-metal behavior reveals Mott quantum criticality in doped Hubbard models

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"Bad-Metal" (BM) behavior featuring linear temperature dependence of the resistivity extending to well above the Mott-Ioffe-Regel (MIR) limit is often viewed as one of the key unresolved signatures of strong correlation. Here we associate the BM behavior with the Mott quantum criticality by examining a fully frustrated Hubbard model where all long-range magnetic orders are suppressed, and the Mott problem can be rigorously solved through Dynamical Mean-Field Theory. We show that for the doped Mott insulator regime, the coexistence dome and the associated first-order Mott metal-insulator transition are confined to extremely low temperatures, while clear signatures of Mott quantum criticality emerge across much of the phase diagram. Remarkable scaling behavior is identified for the entire family of resistivity curves, with a quantum critical region covering the entire BM regime, providing not only new insight, but also quantitative understanding around the MIR limit, in agreement with the available experiments.

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also be destroyed by adding electrons to the system, i.e., the Mott insulating state [16]. The Mott insulator opens a spectral gap at the Fermi level and produces a lattice with random hopping amplitudes [16].

dimensional Bethe lattice, as well as the fully connected bare density of states and set the half-bandwidth $D = 1$ as the unit of energy. This corresponds to the infinitely-dimensional Bethe lattice, as well as the fully connected lattice with random hopping amplitudes [16].

At half-filling, strong enough on-site interaction $U$ opens a spectral gap at the Fermi level and produces the Mott insulating state [16]. The Mott insulator can also be destroyed by adding electrons to the system, i.e., raising the chemical potential $\mu$. When $\mu$ reaches the upper Hubbard band, the system is once again conducting [20]. In both cases, at low-temperature the transition is of the first order, and features a pronounced jump in the upper Hubbard band, the system is once again conducting [20]. In both cases, at low-temperature the transition is of the first order, and features a pronounced jump in

$\lambda$,[9] of the free energy functional $F\left[\left(\omega_n\right)\right]$ near its global minimum; this can be numerically determined by monitoring the convergence rate in the DMFT self-consistency loop [17]. Having in mind the analogy of this definition with the standard Widom crossover line for classical liquid-gas transitions [33], we refer to the instability line as the "quantum Widom line" (QWL) [18].

We carried out a careful $\lambda$-analysis for the doped Mott insulator (see Supplementary Section III [28]), and we
display the resulting QWL trajectory $\mu^*(T)$ as an orange line in all plots (throughout this Letter, an asterisk in the superscript indicates physical quantities evaluated along the QWL; e.g. $\rho^*(T)$ is resistivity calculated at temperature $T$ at $\mu = \mu^*(T)$). The QC region (green) spreads above the critical end-point (red points and dotted line) and quickly extends to much lower temperatures as $T_c$ is reduced (Fig. 1b). The QWL, separating the metallic-like and the insulating-like behavior, marks the center of the corresponding QC region, where the resistivity curves are expected to display the scaling behavior of the form

$$\rho(\mu, T) = \rho^*(T) F(T/T_0(\delta \mu)).$$

(1)

Here the parameter $T_0$ should assume power-law dependence on the deviation from the QWL: $T_0(\delta \mu) \sim d \mu^{\nu \gamma}$, with $d \mu = \mu - \mu^*(T)$.

To check validity of the scaling hypothesis Eq. (1), we calculate the resistivity along the lines parallel to the QWL, as shown in Fig. 2a. We find that, for the doped Mott insulator, the resistivity shows very weak temperature dependence along the QWL. In particular, above $T = 0.08$ it follows the line of constant resistivity which coincides with the MIR limit, $\rho^*(T > 0.08) = \rho_{\text{MIR}}$ (in contrast to the behavior previously established at half-filling [17, 18] where $\rho \gg \rho_{\text{MIR}}$ along the QWL). In fact, all curves converge precisely to the MIR limit at high temperatures, suggesting its fundamental role in characterizing the metal-insulator crossover for doped Mott insulators. The curves also display the characteristic “bifurcation” upon reducing temperature, and a clear change in trend upon crossing the QWL. The scaling analysis confirms that all the curves indeed display fundamentally the same functional dependence on temperature, and that they all can be collapsed onto two distinct branches of the corresponding scaling function (Fig. 2b). The scaling exponent has been estimated to be $\nu \approx 1.35 \pm 0.1$ for both branches of the scaling function, which display mirror-symmetry [17, 19] over almost two decades in $T/T_0$, and the scaling covers more than three orders of magnitude in resistivity.

**Bad-Metal behavior.** We demonstrated the emergence of clearly defined quantum critical behavior thorough an analysis of the $(\mu, T)$ phase diagram, with $d \mu = \mu - \mu^*$ as the scaling parameter. From the experimental point of view it is, however, crucial to identify the corresponding QC region in the $(\delta, T)$ plane and understand its implications for the form of the resistivity curves for fixed level of doping $\rho(T)|_{\delta}$. By performing a careful calculation of the $\delta(\mu, T)$ dependence (see Supplementary Fig. 4 [28]), it is straightforward to re-plot our phase diagram and resistivity curves in the $(\delta, T)$ plane. Remarkably, we find that the quantum critical scaling region covers a broad range of temperatures and dopings, and almost perfectly matches the region of the well-known bad metal transport [21, 22], characterized by the absence of long-lived quasiparticles and linear $\rho(T)|_{\delta}$ curves. We first analyze the $(\delta, T)$ phase diagram in detail, and then establish a connection between the slope of $\rho(T)|_{\delta}$ curves in the bad metal regime and the QC scaling exponent $\nu \gamma$.

In Fig. 3a we show the phase diagram of the doped Mott insulator. At $T = 0$, the Mott insulator phase is found exclusively at zero doping. At low enough temperature and finite doping, characteristic Fermi liquid behavior is always observed. Here, the resistivity is quadratic in temperature, while a clear Drude peak is observed at low frequencies in optical conductivity and density of states (see Supplementary Fig. 5 [28]). The coherence temperature $T_{\text{FL}}$ is found to be proportional to the amount of doping $\delta$, however with a small pre-factor of about 0.1, in agreement with Refs. [20, 21]. In a certain temperature range above $T_{\text{FL}}$, a Drude peak is still present as well as the quasiparticle resonance in the single-particle density of states, but the resistivity no longer follows the FL $T^2$ dependence. This corresponds to the “Resilient Quasiparticle” (RQP) transport regime, which was carefully examined in Ref. [21]. At even higher temperatures, the temperature-dependent resistivity at fixed doping $\rho(T)|_{\delta}$ enters a prolonged linear regime (see Fig. 3a) [35], which is accompanied by the eventual disappearance of the Drude peak around the MIR limit. This behavior is usually referred to as the Bad Metal regime [21]. The resistivity is comparable to the MIR limit throughout the BM region, and the QWL (as determined from our thermodynamic analysis) passes through its middle.

The region of linear $\rho(T)|_{\delta}$ dependence is found to be completely encompassed by the QC scaling region between the dashed lines on Fig. 3a (see Supplementary...
Here we observe that the charge compressibility is nearly constant along the QWL, $\chi^*(\delta) \approx 0.33$, which may be interpreted as another manifestation of the quantum critical behavior we identified. $T^*(\delta)$ is approximately a linear function $T^*(\delta) \approx K_0 + K\delta$, where $K \approx 2$ and $K_0$ is small. In Fig. [3], we compare the approximation stated in Eq. (2) with the DMFT result and find excellent agreement.

Finally, noting that for $\delta > 5\%$, $\rho^*(\delta) = \rho_{\text{MIR}}$, we arrive at the central result of this Letter:

$$\rho_{\text{QCBM}}(T)|_\delta \approx \rho_{\text{MIR}} \left( 1 + C \delta^{-1/\nu} (T - K\delta) \right).$$

In the quantum critical bad metal regime, the resistivity has a linear temperature dependence with the slope decreasing as a power $-1/\nu$ of doping. This demonstrates a direct connection of the universal high temperature behavior in the Bad Metal regime with the (zero-temperature) quantum phase transition. The MIR limit of the resistivity is reached at temperature roughly proportional to the amount of doping, $T^*(\delta) \propto \delta$, since the doping level sets the main energy scale in the problem. The result of this simplified scaling formula is color-plotted in Fig. 4a (with $C = 0.69$, $K = 1.97$ and $\nu = 1.35$) and shown to capture the features of the full DMFT solution at high temperatures.

**Discussion.** Sufficiently systematic experimental studies of doped Mott insulators, covering an appreciable range of doping and temperature, remain relatively scarce. Still, approximately linear temperature dependence of the resistivity at high temperatures with the slope that decreases with doping has been observed, most notably in the seminal work of Takagi et al. [8] on La$_{2-x}$Sr$_x$CuO$_4$. To make a qualitative comparison with our theory and to highlight a universal link of Bad Metal behavior and quantum criticality associated with the Mott metal-insulator transition, in Fig. 4 we color code the reported experimental data; here the temperature is shown in the units of $T_{\text{MIR}}$ at 20% doping and the resistivity is given in units of $\rho_{\text{MIR}}$, which in this material is estimated as 1.7 m$\Omega$cm. The experimental results presented in Fig. 4 cover the temperature range

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**Figure 4:** Resistivity given by (a) the semi-analytical formula obtained from the scaling hypothesis, (b) DMFT result, and (c) the experimental result on cuprate La$_{2-x}$Sr$_x$CuO$_4$ samples from Ref. [8].

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**Figure 3:** (a) DMFT phase diagram of the doped Mott insulator on a frustrated lattice. The bad metal (green) region matches perfectly the region of quantum critical scaling. (b) The bad metal regime features linear temperature dependence of resistivity with the slope roughly proportional to an inverse power law of doping which we find to be a consequence of underlying quantum criticality.

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Section VI [28]. We therefore expect that the emergence of the linear-T dependence of the resistivity, as well as the doping dependence of its slope, should be directly related to the precise form of the corresponding scaling function. Indeed, at high temperature and close to the QWL, the argument of the scaling function $x = d\mu/T^{1/\nu}$ is always small, and the scaling function can be linearized, viz. $\tilde{F}(x) \approx 1 + Ax + \cdots$. We find that the coefficient $A$ has the numerical value $A \approx -0.74$. The functional form for $\rho(T)|_\delta$ close to the QWL is then directly determined by the behavior of the scaling parameter $x(T)|_\delta$. We find that $x(T)|_\delta$ is a linear function in a wide range of temperature around $T^*(\delta)$. Then, close to the QWL, the resistivity is well approximated by a linear function of the form

$$\rho(T)|_\delta \approx \rho^*(\delta) \left( 1 + A \frac{dx}{dT} \bigg|_{\delta,T=T^*(\delta)} (T - T^*(\delta)) \right).$$

(2)

Furthermore, the slope of the scaling argument at the QWL can be expressed as $\frac{dx}{dT}|_{\delta,T=T^*(\delta)} = \left( \chi^*(\delta) \frac{dT^*}{d\delta} (T^*(\delta))^{1/\nu} \right)^{-1},$ where $\chi^*(\delta) = \frac{d\delta}{d\mu}|_{\delta=T^*(\delta)}$. 

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**Figure 4:** Resistivity given by (a) the semi-analytical formula obtained from the scaling hypothesis, (b) DMFT result, and (c) the experimental result on cuprate La$_{2-x}$Sr$_x$CuO$_4$ samples from Ref. [8].
of 150 – 1000 K at 5 – 30% doping. Here one observes a striking similarity between DMFT theory and the experiment, as already noted in early studies [34-36]. We established this result by focusing on an exactly solvable model, where all ordering tendencies are suppressed, and single-site DMFT becomes exact. Real materials, of course, exist in finite (low) dimensions where systematic corrections to DMFT need to be included [37-40]. In many cases [11-13], these nonlocal corrections prove significant only at sufficiently low temperatures. Then our findings should be even quantitatively accurate in the high-temperature incoherent regime, as in the very recent experiments on organic materials [41] for the case of half-filling.

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[28] See Supplemental Material at [URL will be inserted by J_Pub] which includes Refs. [15][19].
[36] The high-temperature slope of the resistivity curves is estimated to be proportional to $\delta^{-1}$ in Ref. [35]. However, only four doping levels were considered and having in mind the uncertainty of the analytical continuation, it is difficult to distinguish this value from our slope $\delta^{-1/2}$. Our numerical data are in agreement with high precision CTQMC data from Ref. [21].