Thermal Transport across a Continuous Metal-Insulator Transition

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The celebrated Wiedemann-Franz (WF) law is believed to be robust in metals as long as interactions between electrons preserve their fermion-quasiparticle character. We study thermal transport and the fate of the WF law close to a continuous metal-insulator transition (MIT) in the Falicov-Kimball model (FKM) using cluster-dynamical mean-field theory (CDMFT). Surprisingly, as for electrical transport, we find robust and novel quantum critical scaling in thermal transport across the MIT. We unearth the deeper reasons for these novel findings in terms of (i) the specific structure of energy-current correlations for the FKM and (ii) the microscopic electronic processes which facilitate energy transport while simultaneously blocking charge transport close to the MIT. However, within (C)DMFT, we also find that the WF law survives at $T \to 0$ in the incoherent metal right up to the MIT, even in absence of Landau quasiparticles.

I. INTRODUCTION

In recent years, there have been lots of studies on thermo-electric properties of the strongly correlated materials such as $\text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3$, $\text{LaFe}_3\text{CoSb}_{12}$ and $\text{CeFe}_3\text{CoSb}_{12}$ which have myriad applications [1] in designing new devices. There are different theoretical investigations of the thermo-electric materials [2–4]. The Boltzmann theory which is applicable in weakly coupled system where Landau quasiparticle picture remains valid. But this theory will not work in the strongly correlated materials as the perturbation theory breaks down in this regime. Kubo formalism has been used in both weak and strong coupling regime. But the drawback of Kubo formalism is that its dynamical nature (frequency dependence) makes difficult to calculate some experimentally accessible quantities such as the thermopower or Seebeck coefficient, Lorenz number and thermal conductivity. Another approach proposed by Shastry [5], where he formulated the computation of the thermal response to dynamical temperature gradients by neglecting the intricacy of the full dynamics of the Kubo formalism.

It is interesting to study the effect of disorder in materials along with interaction [6]. Transport properties (electric, thermal) with the controlled disorder can play a vital role in designing new materials. One of the most prominent kind of disorder systems is binary disordered alloy where disorder is induced by creating vacancies in the crystalline order for materials like $A_xN$, with $A=$Ta, Nb, etc. Here, the disorder strength can be controlled in normal metals at low temperature $T$, the celebrated Wiedemann-Franz (WF) law [9] relates the electrical and thermal conductivities via a universal Lorenz number, $L_0 = \frac{\kappa_d(T)}{T\sigma_i(T)} = \frac{\pi^2 k_B^2}{3e^2}$, the Sommerfeld value. Even in strongly correlated metals [10], the WF law still holds as $T \to 0$ as long as the metallic state is a Landau Fermi Liquid (LFL), presumably due to a Ward identity [11]. Explicit counter-examples are $D = 1$ Luttinger liquids [12], cuprates [13] and $f$-electron systems [14] near quantum phase transitions, where Landau quasiparticle views break down. It is well known that Landau quasiparticle picture also naturally breaks down at interaction- or disorder-driven metal-insulator transitions (MIT) (at $T = 0$). However, the former are generically first-order, and are accompanied by instabilities to more conventional symmetry-broken states at lower $T$, preventing clean study of the breakdown of the WF law. Thus, continuous MITs at $T = 0$ turn out to be an ideal playground to study this issue.

Quite generally, quantum critical fluctuations at a continuous MIT affect critical features in conductivity. This has been studied in the context of the finite-but low $T$ critical end-point in the $d = \infty$ Hubbard model [15], and recent CDMFT work for the FKM also shows that conductivity [16] and magneto-transport [17] exhibit remarkable quantum-critical scaling at a “Mott” QCP. Whether and how such novel QC features show up in thermal transport is a very interesting, albeit scarcely studied, issue. Thermal transport primarily measures energy current correlations in solids [7, 18]. Most generally, the electronic contribution to the thermopower, $S_{el}(T)$, is best interpreted as the entropy of an electric current [19]. In weakly correlated metals, $S_{el}(T) \approx J_1T$ is small at low $T$. In strongly correlated Landau Fermi Liquid (LFL) metals, in contrast, $S_{el}(T) = AT$ is sizably enhanced at low $T$, passes through a broad maximum at intermediate $T$ before asymptoting to the Heikes law [20] at high $T \gg T_{LFL} \approx t_{eff} = z_{FL}t$, where $t_{eff}$ is the correlation-induced reduction of the bare kinetic energy ($t$) and $z_{FL}$ is the Landau quasiparticle residue. In the Mott insula-
tor, one expects $S_{el}(T \rightarrow 0)$ to diverge owing to the loss of carriers upon gap opening. It is then natural to expect that soft quantum-critical fluctuations at a QCP associated with a continuous MIT should also reflect in thermal transport. Moreover, such studies also permit one to analyze Thomson effects using the Kelvin relations [19]. In fact, the Thomson co-efficient, which is just heat per unit current and unit temperature gradient, is simply related to the thermopower via $\tau_{th}(T) = T(dS_{el}(T)/dT)$: thus, this quantifies the "specific heat of electricity" [19]. That the $\gamma$-co-efficient of the usual constant-volume specific heat diverges at a continuous MIT is well known. Does the "specific heat of electricity" also show a critical divergence at such a MIT?

Motivated hereby, we study thermal transport in the simplest lattice model of interacting fermions, the Falicov-Kimball model (FKM) in detail within a two-site cluster-DMFT [8] within the alloy-analogy formalism. Specifically, we (i) unearth quantum-critical scaling in thermal transport and correlate it with electrical transport, and (ii) examine the microscopic origin of the electronic processes involving energy current which distinguish thermal from electrical transport. The FKM is ideal since it shows a continuous "Mott" MIT within both DMFT [21], CDMFT [8] and also within Coherent Potential Approximation (CPA) with Dynamical Cluster Approximation (DCA) [22]. We focus on quantum critical features in thermal transport in the strong-scattering regime where $k_{F}l \approx 1$ invalidates quasiclassical Boltzmann approaches, since the very concept of well-defined LFL quasiparticles breaks down.

FKM can be solved exactly within DMFT [21] in infinite dimensional systems. As an advanced mean field type technique DMFT is more reliable method for studying materials properties in three or higher dimension [23]. As for the conductivity tensor $\sigma_{ij}$, it turns out that thermal transport co-efficients can be precisely evaluated within our two-site CDMFT [8]. This is because the irreducible cluster resolved particle-hole vertex corrections rigorously drop out from the Bethe-Salpeter equations (BSE) for all current-current correlation functions [24]. Further, having explicit closed-form analytical expressions for the cluster propagators, $G(K, \omega)$, minimizes the computational cost, even within CDMFT.

The plan of the paper is as follows: In Sec. II we describe in details of our model within cluster-DMFT formalism and the calculation of thermal transport (thermopower, thermal conductivity, Lorentz number and Thomson coefficient) using Cluster DMFT formalism. In Sec. III we report numerical result for the thermal transport using CDMFT and Quantum criticality of thermal transport across the MIT. In Sec. IV we compare our result with single site DMFT result. We present discussion and conclusions in Sec. V.

II. GENERAL FORMULATION FOR THERMAL TRANSPORT WITHIN CLUSTER DMFT

The Hamiltonian for spinless FKM [21] or equivalent binary-alloy disorder model is

$$H_{FK} = -t \sum_{\langle i,j \rangle} (c_{i}^{\dagger}c_{j} + h.c.) + U \sum_{i} c_{i}^{\dagger}c_{i} + \mu \sum_{i} c_{i}^{\dagger}c_{i} \tag{1}$$

on a Bethe lattice with semicircular band density of states (DOS) as an approximation to a three dimensional lattice. Where, $c_{i}^{\dagger}(c_{i})$ is the electron creation (annihilation) operator for spinless electron at site $i$, $x_{i}$ is variable that can take either 0 or 1 value, $v_{i} = Ux_{i}$ is viewed as a static disorder potential for the c-fermions.

In our recent work [8] we use our recent exact-to-O(1/D) extension of DMFT to solve FKM applying equation of motion. The local Green’s function in two-site cluster DMFT is,

$$\hat{G} = \begin{pmatrix} G_{00}(\omega) & G_{0a}(\omega) \\ G_{a0}(\omega) & G_{aa}(\omega) \end{pmatrix}$$

where, the matrix element $G_{ij}(\omega)$

$$G_{ij}(\omega) = \left[ \frac{1 - \langle x_{0} \rangle - \langle x_{a} \rangle}{\xi_{2}(\omega)} + \frac{\langle x_{0} \rangle - \langle x_{a} \rangle}{\xi_{2}(\omega) - U} \right] \left[ \delta_{ij} - \frac{F_{2}(\omega)}{(t - \Delta_{a0}(\omega))(1 - \delta_{ij})} \right]$$

$$+ \left[ \frac{\langle x_{0} \rangle - \langle x_{a} \rangle}{\xi_{1}(\omega)} + \frac{\langle x_{0} \rangle - \langle x_{a} \rangle}{\xi_{1}(\omega) - U} \right] \left[ \delta_{ij} - \frac{F_{1}(\omega)}{(t - \Delta_{a0}(\omega))(1 - \delta_{ij})} \right] \tag{2}$$

where the bath function $\Delta(\omega)$ is related with the local Green’s function through suitable self-consistency condition. The self energy is given as,

$$\Sigma(\omega) = \hat{G}_{0}^{-1}(\omega) - \hat{G}^{-1}(\omega) \tag{3}$$

with $\hat{G}_{0}(\omega)$ is the Wiess Green’s function, $\hat{G}_{0}(\omega) = (\omega + i\delta)^{-1}$, $\mu \mathbb{I} - \hat{\Delta}(\omega)$. We use the algorithm described in paper [8] to find the local Green’s function and self energy. In symmetric basis (cluster momentum basis), we can write $G_{S} = (G_{00} + G_{aa})$ and $G_{P} = (G_{00} - G_{aa})$ with $S = (0,0,...)$ and $P = (\pi, \pi, ...)$.

Now, using Kubo-Greenwood formula we calculate
the transport properties. In contrast to the electrical conductivity which involves the particle current, \(J_{q} = \sum_{q} q_{q} c_{q}^{+} c_{q}\) with \(q_{q} = \nabla q_{q}\) for an unperturbed band structure \(\epsilon_{q}\), the heat current required for thermal transport is more complicated [21]

\[
J_{q} = \sum_{q} (\epsilon_{q} - \mu) q_{q} c_{q}^{+} c_{q} + \frac{U}{2} \sum_{q, q'} W(q - q')(q_{q} + q_{q'}) c_{q}^{+} c_{q'}
\]

with \(W(q) = \frac{1}{\pi} \sum_{j} e^{-q_{j} R_{j} d_{j}}\), and thus the heat current contains both “kinetic” and “potential” terms. Quite generally, in terms of the Onsager co-efficients, \(L_{lm}(l, m = 1, 2)\) with \(L_{12} = L_{21}\), one finds

\[
\sigma_{dc}(T) = e^{2} L_{11}
\]

(5)

\[
S_{cl}(T) = -\frac{k_{B} L_{12}}{e L_{11}}
\]

(6)

and

\[
K_{cl}(T) = \frac{k_{B}^{2} L_{11} L_{22} - L_{12}^{2}}{T L_{11}}
\]

(7)

The \(L_{lm}\) can themselves be expressed in terms of the cluster propagators by noticing that these are the zero-frequency limit of the analytically continued “polarization” operators. Explicitly, \(L_{lm} = \lim_{\omega \rightarrow 0} R e^{\frac{i l m}{2} (\omega)}\), with

\[
L_{11}(i \omega_{n}) = \int_{0}^{\beta} d \tau e^{i \omega_{n} \tau} Tr \langle T_{\tau} e^{-H_{J_{c}}(\tau) J_{c}(0)} \rangle Z
\]

(8)

\[
L_{12}(i \omega_{n}) = L_{21}(i \omega_{n}) = \int_{0}^{\beta} d \tau e^{i \omega_{n} \tau} Tr \langle T_{\tau} e^{-H_{J_{c}}(\tau) J_{q}(0)} \rangle Z
\]

(9)

and

\[
L_{22}(i \omega_{n}) = \int_{0}^{\beta} d \tau e^{i \omega_{n} \tau} Tr \langle T_{\tau} e^{-H_{J_{q}}(\tau) J_{q}(0)} \rangle Z
\]

(10)

In absence of vertex corrections to transport co-efficients, the \(L_{lm}\) can finally be expressed in terms of the cluster propagators, \(G(K, \omega)\). \(L_{11}\) is the same as the one derived for the dc conductivity \(\sigma_{xx}(T)\) earlier [16]:

\[
L_{11} = \sum_{a = S, P} \frac{T \sigma_{0}}{e^{2}} \int dc \rho_{a}(\epsilon) \int d\omega (-\frac{d f(\omega)}{d \omega}) A_{a}^{2}(\epsilon, \omega)
\]

(11)

The Onsager co-efficient relevant for heat transport is most conveniently given in the two-site cluster bonding-anti-bonding basis \((S, P\) channels [8]) as the sum of the “kinetic” and “potential” contributions as sketched above, \(L_{12} = L_{12}^{K} + L_{12}^{P}\) and following Freericks et al. [18] for our two-site CDMFT, this reads

\[
L_{12} = \sum_{a = S, P} \frac{T \sigma_{0}}{e^{2}} \int dc \rho_{a}(\epsilon) \int d\omega (-\frac{d f(\omega)}{d \omega}) A_{a}^{2}(\epsilon, \omega)
\]

(12)

while \(L_{22}\) is given by

\[
L_{22} = \sum_{a = S, P} \frac{T \sigma_{0}}{e^{2}} \int dc \rho_{a}(\epsilon) \int d\omega (-\frac{d f(\omega)}{d \omega}) \omega A_{a}^{2}(\epsilon, \omega)
\]

(13)

As for the conductivity tensor [17], it turns out that thermal transport co-efficients can be precisely evaluated within our two-site CDMFT [8].

### III. RESULT WITHIN CLUSTER DMFT

In this section, we show the result of the thermal transport with two site CDMFT approach. For convenience consider non-interacting electrons half-bandwidth as unity i.e. 2t=1. Since we aim to correlate specific features in electrical and thermal transport with each other, we start by recapitulating dc resistivity.

In Fig. 1(a), we exhibit the dc resistivity, \(\rho_{dc}(U, T)\) as a function of \(U\) as the system is driven through a continuous MIT at \(U_{c} = 1.8\) [16]. It is clear that at intermediate \(0.95 < U < 1.8\), clear pseudogap signatures appear in \(\rho_{dc}(T)\) over a progressively wider \(T\)-range, between the high-\(T\) incoherent metal and a low-\(T\) bad metal, before the MIT occurs for \(U \geq 1.8\). This feature is associated with proximity to the “Mott” quantum critical point (QCP) occurring between a \(T = 0\) very bad metal and a “Mott” insulator at \(U_{c}\). We are interested in how this Mott quantum criticality manifests in thermal transport.

In Fig. 1(b), we show how the electronic contribution to the thermopower varies across the continuous MIT. Several features stand out: (i) for weak-to-intermediate \(U < 0.9\), \(S_{cl}(T) \approx AT\) at low \(T < 0.025t\) is small (not shown), as expected for a weakly correlated metal, and goes hand-in-hand with \(\rho_{dc}(T) \approx const\) at low \(T\). (ii) In the intermediate-to-strong coupling \((0.9 < U < 1.7)\) regime, where one is in the increasingly bad-metallic low-\(T\) regime, \(S_{cl}(T)\) is still linear-in-\(T\) but is significantly enhanced by factors of \(O(50 - 100)\) over its weakly correlated values. \(S_{cl}(T)\) also exhibits a broad peak around \(T^{*} \approx 0.04t\), before continuously falling off to achieve the Heikes value [20, 25] at very high \(T\). It is very interesting that \(S_{cl}(U, T) \approx A(U)T\) with \(A(U)\) increasing with \(U\) holds throughout this very bad metallic regime, even as \(\rho_{dc}(T \rightarrow 0) \approx 100h/e^{2}\). This is the regime in which no quasiclassical Boltzmann view of transport is tenable, since application of Drude-Boltzmann ideas would nec-
essarily yield $k_{F}l < 1$ (where no $1/k_{F}l$-expansion is possible). Since thermopower features result solely from a non-Landau quasiparticle cluster propagator within CDMFT, this implies that this low-$T$ enhancement in $S_{el}(T)$ involves non-Landau-FL quasiparticle (branch-cut continuum) excitations. Just before the MIT, $S_{el}(T \to 0)$ is still linear in $T$, but is enhanced by a factor of about 100 relative to its small $U$ value. (iii) Finally, precisely at the QCP $U = 1.8$, clear anomalies obtain: $S_{el}(T)$ increases with decreasing $T$ right down to $T \to 0$, but achieves a finite value. For $U > 1.8$, opening of the “Mott” gap in the one-electron density-of-states [8] produces a divergent $S_{el}(T \to 0)$. This is not a violation of the Nernst theorem, since $\rho_{dc}(T \to 0)$ simultaneously diverges.

It is clear from Fig. 1(b) that $S_{el}(U, T \to 0)$ curves fan out to either metallic or insulating values, except at the “Mott” QCP, where $S_{el}$ is finite. This suggests that, like electrical transport [16], thermal transport should also exhibit characteristic quantum critical features. To unravel this novel possibility, we repeat earlier procedure [16] for thermopower by making the metallic and insulating curves fall on to two “universal” curves by scaling both with a $U$-dependent scale, $T_{0}^{th}(U)$. In the left panel of Fig. 2, we exhibit $\log(S_{el}(T)/S_{el}^{(c)})$ versus $T$. Remarkably, this bares clear signatures of “mirror” symmetry, exactly as in electrical transport. This strongly presages novel “Mott” quantum critical features in thermal transport as well. More clinching support for such criticality is seen in right panel of Fig. 2, where we show $\log(S_{el}(T)/S_{el}^{(c)})$ versus $T/T_{0}^{th}(U)$ as done earlier [16]. Remarkably, we find (i) clear “mirror” symmetry between metallic and insulating curves around the critical $S_{el}(U_{c})$, and (ii) $T_{0}^{th}(\delta U) = c_{th}|\delta U|^{\eta}$ with $\eta = 1$ (in Fig. 3 left panel). To further cement this unusual idea, we also show in the right panel of Fig. 3 the “beta”-function (or the Gell-Mann Low function) for thermopower, $\beta_{th}(s) = d[\log(s)]/d[\log(T)]$ versus $s$, with $s = (S_{el}(T)/S_{el}(T_{0}))$ and $S_{el}(T)$ being the critical thermopower right at the MIT (red circled curve in Fig. 1(b)). Remarkably, we find $\beta_{th}(s) \simeq \log(s)$ near the MIT, exactly as found before for the $dc$ conductivity. This conclusively establishes novel quantum-critical scaling of the thermopower at the “strong localization” MIT as well.

Appearance of such quantum-critical scaling in thermopower at the MIT is very surprising, and calls for us to look more closely at this term. The energy current, in contrast to the electrical current, involves three sites, and reads [26]

$$j_{i, Q} = i\hbar/(4c_{i+\delta}c_{i-\delta} + h.c) - \frac{U}{2}(j_{i-\delta} + j_{i+\delta})(n_{i,d} - \frac{1}{2})$$

where we have relabelled $c \to c_{\uparrow}, d \to c_{\downarrow}, \delta$ denotes nearest neighbors of site $i$, and $j_{i,\pm\delta}$ is the electrical current.
operator. For the FKM, we have \([n_{i,d}, H] = 0\) for all \(i\), and thus \(n_{i,d} = 0, 1\) only. The expression for \(j_{i,Q}\) now simplifies to a revealing form

\[
    j_{i,Q} = t^2 \left( i c_{i−d}^\dagger c_{i+δ} + h.c. \right) \pm \frac{U}{4} (j_{i−δ,i} + j_{i,i+δ})
\]

for (+, −) corresponding to \(n_{i,d} = 0, 1\). Thus, for the FKM, we find that \(j_{i,Q}\) is directly related to the electrical current operator, providing direct insight into the underlying reason for emergence of very similar quantum critical scaling responses in \(\rho_{dc}(T)\) [16] and \(S_{cl}(T)\) above. Simply put, energy current correlations mirror those of the electrical current.

Armed with these positive features, we now study the electronic contribution to the thermal conductivity, \(K_{el}(T)\), in Fig. 1(c). In the small \(U\) regime, \(K_{el}(T) \approx A_2 T\) is linear in \(T\), as would be expected for a weakly correlated metal, with transport being determined by a LFL. This is the regime where \(\rho_{dc}(T \rightarrow 0) \approx const\), and formally corresponds to the weak scattering regime where \(k_F l > 1\) holds (this is thus the regime where self-consistent Born approximation (SCBA) applies). As we enter the intermediate-to-strong scattering regime with \(0.95 < U < 1.8\), progressive bad metallicity in resistivity goes hand-in-hand with emergence of a low-energy scale in \(K_{el}(T)\), where its power-law-in-\(T\) \((K_{el}(T) \sim T^n, n > 1)\) behaviour at intermediate-\(T\) crosses over to a linear-in-\(T\) variation as \(T \rightarrow 0\). Precisely at \(U_c = 1.8\), we find \(K_{el}(T) \approx T^{1+\nu}\). This behavior is characteristic of heat conductivity arising from non-fermionic excitations. In our case, such collective modes can only be of electronic origin: these are the low-energy particle-hole fluctuations, which remain low-energy excitations in the insulator when charge degrees of freedom are frozen out at low energies. Upon closer inspection, we see that the linear-in-\(T\) contribution gives way to a power-law behavior \((K_{el}(T) \approx T^{1+\nu}, 0 < \nu < 1)\) right down to \(T = 0\) for \(U = 1.8\) within our numeric, precisely where the MIT occurs. This finding is completely consistent with breakdown of the LFL quasiparticle description in the quantum critical region associated with the MIT.

Even more insight into the breakdown of the LFL quasiparticle description close to the MIT is provided by examination of the \(T\)-dependent Lorenz number, \(L_0(T) = K_{el}(T)/T \sigma_{xx}(T)\), as a function of \(U\). In Fig. 1(d), we exhibit \(L_0(U, T)\) across the MIT. Throughout the metallic phase, including the very bad metal, \(L_0(T \rightarrow 0) = \frac{4}{5}\) (in units of \(k_B = 1 = e\), even though \(L_0(T)\) exhibits significant \(T\)-dependence up to the lowest \(T\), especially for \(U > 1.4\), implying no breakdown of the WF law in the metallic phase. Precisely at the MIT, however, \(L_0(T \rightarrow 0) \approx 10\), indicating breakdown of the WF law exactly at the MIT. In the insulator \((U > 1.8)\), \(L_0(T \rightarrow 0)\) diverges, as it must, since \(K_{el}(T) \approx T^4\) while \(\rho_{dc}(T) \approx \exp(E_g/k_BT)\). Our finding is remarkable be-
Figure 4. (Color online) Quantum critical scaling in scaled electrical conductivity $T^{-\nu}\sigma_{el}(T)$ (panel (a)), thermopower $S_{el}(T)$ (panel (b)), scaled thermal conductivity, $T^{-1-\nu}K_{el}(T)$ (panel (c)) and Lorenz number (panel (d)) when plotted as functions of the “scaling variable” $y(U,T)=|U-U_c|/U_cT$, demonstrating clean quantum critical scaling in electrical as well as thermal transport at the Mott QCP.

Figure 5. (Color online) Thomson Co-efficient $\tau_{th}(T)$ for FKM as a function of $U/t$

Because, whilst the resistivity shows clear precursor features of impending proximity to the MIT via progressive enhancement of bad-insulating and very bad metallic regimes beginning from $U = 0.95$, both $S_{el}(T)$ and $K_{el}(T)$ continue to display apparently conventional behavior right up to the MIT. Further, spectral responses clearly show non-Landau-FL metallicty [8], and while one may argue for a non-WF behavior at any $T \neq 0$, our results indicate no breakdown of the WF law at $T = 0$.

Remarkably, upon proper rescaling, it now turns out that $\sigma_{xx}(T), S_{el}(T), K_{el}(T)$ and $L_0(T)$ all exhibit clear quantum-critical scaling features. At the QCP, we find (not shown) that $K_{el}(T) \approx T^{-1/3} = T^{-1+\nu}$ with $\nu = 4/3$. Recalling that $\nu = 4/3$ is precisely the correlation length exponent we find for the dc conductivity [16], this suggests an alternative way to exhibit quantum critical scaling that bares the link between electrical and thermal transport.

In Fig. 4, we find that $T^{-4/3}\sigma_{xx}(T)/\sigma_0, S_{el}(T), T^{-7/3}K_{el}(T)$ and $L_0(T)$ exhibit clear collapse of the metallic and insulating curves onto two clear branches when plotted as a function of the "scaling variable" $y = |U-U_c|/U_cT$, i.e., as a function of the distance from the "Mott" QCP. Since $\sigma_{xx}(U) \approx (U_c-U)^{4/3}$ as found earlier [16], $\nu = 4/3$ and $z = 1$, as expected for the FKM. Further, $z\nu = 4/3 > (2/d)$ implies that the Harris criterion holds, implying a genuinely clean QCP. Again, these features reflect the finding above, where energy current correlations simply mirror the electrical current correlations for the FKM, providing direct microscopic rationale for closely related quantum-critical transport in both. We are aware of only one previous study [27, 28] where
this issue was studied phenomenologically, by using the experimental conductivity as an input into the Kubo formula for the $L_{\text{imp}}$. In contrast, our results emerge from a truly microscopic CDMFT formulation for the FKM, and our finding of $z = 1$ is very different from $z = 3$ and $\nu = 1$ (latter taken from experimental conductivity data). It is also different from $z = d$ found [29, 30] for scaling in the non-interacting disorder model. Together with Mott-like criticality in transport [16], these differences reflect the qualitatively distinct “strong coupling” nature of the QCP in the FKM.

Finally, using the Kelvin formula, we now show the Thomson co-efficient as a function of $U/t$ across the MIT. In Fig. 5, we show $\tau_{th}(U/t, T)$. In the metallic phase, right up to $(U/t) = 1.7$, the Thomson co-efficient exhibits a weak $T$-dependence at high $T$, changes sign at a low-to-intermediate $T_1 \approx O(0.08t)$, passes through a maximum around $0.5T_1$ before vanishing linearly at lowest $T$. Exactly at the MIT, qualitative changes occur: $\tau_{th}(U > U_c, T)$ now exhibits two distinct regimes where $d\tau_{th}(T)/dT$ changes sign (around $1.13t$ and $0.05t$) before asymptoting to a finite negative value in the insulator. Remarkably, much alike the way in which the $\gamma$-co-efficient of the usual specific heat at constant volume diverges upon approach to the MIT, we find that the $\gamma$-co-efficient of the “specific heat of electricity”, defined as $\gamma_e = (dS_{el}(T))/dT$, progressively increases with $U/t$ right up to the MIT, diverging at the “Mott” QCP.

IV. SINGLE-SITE DMFT RESULTS FOR THERMAL TRANSPORT

Here, we compare our result with single site DMFT [7] result. For single site DMFT on Bethe lattice local self energy $\Sigma(\omega)$ reads,

$$\Sigma(\omega) = U\langle x_i \rangle + \frac{U^2\langle x_i(1 - \langle x_i \rangle)\rangle}{\omega - U(1 - \langle x_i \rangle) - i^2G_{\text{loc}}(\omega)}$$ (16)

The spectral function, $A(k, \omega) = -\frac{1}{\pi} \text{Im}G(k, \omega)$ with $G(k, \omega)^{-1} = \omega - \epsilon_k - \Sigma(\omega)$. Inserting $A(k, \omega)$ in Kubo-Greenwood formula we calculate current-current correlation function [18, 21]. It is well known that for single-site DMFT irreducible vertex correction vanishes in the Bethe-Salpeter equation, so only the bare bubble contributes.

We now show single-site DMFT results for electrical and thermal transport. In dc resistivity across the MIT, shown in Fig. 6 (which now occurs at a $(U/t)_{\text{C-DMFT}} = 1.1$), we see features very similar to those found in CDMFT. However, (i) $\rho_{dc}(T)$ at $U_c$ now attains values $O(40)c^2$, much smaller than the $O(200)c^2$ found in CDMFT. Correspondingly, $S_{el}(T)$, $K_{el}(T)$ and $L_0(T)$ exhibit very similar behavior to that found in CDMFT, as shown in Fig. 6. At first sight, one may thus conclude that no qualitative difference exists between DMFT and CDMFT results.

However, closer inspection of DMFT results, obtained by performing the same scaling analysis as the one done in the main text, reveals crucial differences between DMFT and CDMFT results. Comparing scaling for
V. DISCUSSION AND CONCLUSION

What is the microscopic origin of boson-like collective modes that can provide a distinct channel for heat conduction which simultaneously blocks charge transport? It is most instructive to invoke the analogy with the Hubbard model, where one-electron excitations in the Mott insulator are frozen out at low energies \( \omega < \Delta_{MH} \), the Mott-Hubbard gap in the one-electron DOS. Were one to consider the Hubbard model, dynamical bosonic spin fluctuations, originating from second-order-in-(\( t/U \)) virtual one-electron hopping processes, would be the natural low-energy excitations. However, in the FKM-like binary alloy model we consider, identifying \( c \rightarrow c_1, d \rightarrow c_1 \) leads to an Ising super-exchange to second order in a \( (t/U) \) expansion when \( U >> t \) in the “Mott” insulator. It is important, exactly as in the Hubbard case, that it is the virtual hopping of a \( c \)-fermion between neighboring sites (from \( 0 \) to \( \alpha \) and back in our two-site cluster [8]) that is necessary to generate such a boson-like mode. Since this is not a real low energy charge fluctuation, it cannot cause real charge transport. But it does lead to a gain \( O(-t^2/U) \) in super-exchange energy; \( i.e. \) energy is not conserved, and so these virtual charge fluctuations indeed cause energy transport. Physically, this n.n hopping in a gapped “Mott” insulator involves creation of a particle-hole pair (a holon-doublon composite on neighboring sites). At low energy, this local “exciton” is effectively a bosonic mode that disperses on the scale of \( J \approx t^2/U \). These bosons are thus not necessarily linked to any broken symmetry, but naturally emerge in a “Mott” insulator. In our CDMFT, the dynamical effects of such “excitonic” inter-site correlations on the cluster length scale are fed back into the cluster self-energy, and thus the basic process leading to energy transport but not charge transport is included in CDMFT. This is also the reason why CDMFT performs much better than single site DMFT when we study quantum critical scaling in thermal transport. The underlying reason for this inability of DMFT results to properly describe quantum critical scaling of thermal transport can be understood heuristically as follows: in CDMFT approach, we have argued that thermal transport involves microscopic electronic processes associated with virtual hopping between a given site to its neighbors and back. Such second-order-in-hopping processes block charge transport, but allow energy transport, since such processes involve a gain of “super-exchange” (of Ising form for the FKM) energy. In single site DMFT, this process is \( O(1/d) \), and so is not adequately captured. But precisely such a process is captured in our CDMFT, since the dynamical effects of inter-site (intracluster) correlations are fed back into CDMFT self-energies by construction [8]. These “bosons” are thus natural candidates that can account for our finding of \( K_{el}(T) \approx T^{1+\nu} \) in the proximity of the MIT.

\[ S_{el}(T) \text{ within DMFT in Fig. 7 to those obtained from CDMFT in Fig. 2 and Fig. 3 in the previous section reveals that (i) scaling holds over a much narrower window in DMFT compared with CDMFT, and (ii) } \mu_{th}^{\text{DMFT}} = 1.2, \text{ compared to } \mu_{th} = 1 \text{ in CDMFT. It is thus more difficult to discern clean extended scaling behavior from DMFT results, and CDMFT clearly performs better in this respect.} \]

Moreover, repeating the analysis leading to Fig. 4, we exhibit the results in Fig. 8. It is now clear that the scaling features in \( S_{el}(T), L_0(T), T^{-\nu} \sigma_{xx}(T) \) and \( T^{-1-\nu} K_{el}(T) \) are of much poorer quality than those obtained from two-site CDMFT results.

Comparing with CDMFT results, several features stand out. These reveal very interesting differences between DMFT and CDMFT results, and we use these to propose that extensions of DMFT to include short-range spatial correlations seem to be necessary to discuss novel quantum critical scaling in thermal transport at the MIT.

Thus, while critical features in electrical transport may be adequately captured by single-site DMFT as above (though the critical exponents \( z \) and \( \nu \) are, as expected, different), we find that description of energy transport, and, in particular, much better elucidation of quantum critical thermal transport, requires cluster extensions capable of properly distinguishing between non-local aspects entering the distinct microscopic processes which underlie energy transport, as opposed to charge transport.

![Figure 7.](image-url) (Color online) (a) In left panel, \( \log(S_{el}(T)/S_c) \) vs \( T/T_0 \) and (b) in right panel, \( T_0^{th}(\delta U) \) vs \( \delta U \) within single-site DMFT.
Figure 8. (Color online) Results similar to those obtained in Fig. 4, but now using single-site DMFT.

Very interestingly, a series of careful experiments on two-dimensional electron gases (2DEGs) show remarkable features [31]: (i) in the low-$n_x$ regime where $\rho >> h/e^2$, the activated $T$-dependence of $\rho_{dc}(T)$ shows a remarkable “slowing down” to an extremely bad metallic state, even as $\rho_{dc}(T \to 0) \approx 250h/e^2$, (ii) in the same $n_x$-regime, the thermopower shows hugely enhanced values (two orders of magnitude above the Mott value) and, perhaps even more remarkably, exhibits linear-in-$T$ behavior reminiscent of normal metals precisely below 1.0 K. It may be possible to apply our high-$D$ approach, which focuses on short-ranged correlations, to these mesoscopic systems if one could model the system as a 2DEG influenced by strong scattering from atomic-sized (strong) scattering charged centers. In light of our calculations, the dichotomy between the $T$-dependence of $\rho_{dc}(T)$ and $S_{el}(T)$ can be interpreted as follows: a real charge excitation is blocked in the “strong-disorder” limit of the FKM near the MIT due to blocking effects associated with Mottness, explaining the extraordinarily high $\rho_{dc}(T \to 0)$ below 1.0 K. But a collective particle-hole (or holon-doublon composite in Hubbard model lore) excitations are real low-energy electronic collective modes that naturally arise in this regime, and lead to a hugely enhanced $S_{el}$. It is interesting that our strong-coupling approach seems to rationalize the very unusual experimental observations in a single picture which emphasizes proximity to a (Mott-like) localization transition. That such observations may be subtle manifestations of novel phase fluctuation effects is not inconsistent with our view either, since it follows directly from the number-phase uncertainty principle that increasing proximity to electronic localization will necessarily generate large phase fluctuation-dominated state(s).

It is interesting to compare our CDMFT technique of studying thermal transport to the recent work on thermal transport by Finkel’stein and Schwiete [32, 33]. Based on perturbative renormalization group (RG) calculation they studied the quantum criticality using $2+\epsilon$ expansion and calculate the critical exponent corresponds to different universality classes. This theory describes the system with both disorder as well as interaction and treat the system as disordered Fermi liquid with disorder induced renormalized Landau parameter.

Despite the great success of this approach, there are certain limitations - (a) In perturbative RG, low temperature excitations are adiabatically connected to non-interacting (but disordered ) electrons. Hence, these excitations which are assumed to be fermionic in nature, play a leading role and collective excitations play a sub-leading role in low temperature region. While in CDMFT approach, fermionic like excitations are absent and the collective excitations play prominent roles. (b) Perturbative RG is unable to detect any metastable states (like glassy dynamics) arising due to the competition between disorder and interaction whereas our approach can easily capture those features.

To summarize, we have showed clear quantum-critical scaling features in $S_{el}(T)$, $K_{el}(T)$ and $L_0(T)$ at the MIT strongly testifies to robust quantum critical scaling of thermal transport at a continuous MIT. Ours is a truly microscopic approach, and is best valid in the strong lo-
calization regime \((k_F l \simeq 1)\), where a Hubbard-like band-splitting type of MIT obtains. This is the limit opposite to the well-studied weak localization (WL) case, where a perturbative-in-1\(k_F l\) expansion is possible: at strong localization, the criticality is better rationalized in terms of a locator expansion \([34]\), and exhibits signatures expected of a continuous “Mott” quantum criticality. Moreover, we are also able to connect these critical features in a very transparent way to those observed in electrical conductivity by analysing the structure of underlying correlations, thereby providing a direct rationalization for our findings. In view of the fact that the one-band Hubbard model exhibits “quantum critical” scaling in dc transport near the finite- but low \(T\) critical point \(\left(T_c \neq 0\right)\), it would also be interesting to study the possibility of related features in thermal transport for such cases in future if the finite-\(T\) critical point of the Mott transition could be driven to sufficiently low \(T\).

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[1] G. Mahan, B. Sales, and J. Sharp, “Thermoelectric materials: New approaches to an old problem,” Physics Today 50, 3, 42 50, 42 (1997).
[2] J.M. Ziman, Principles of the Theory of Solids (Cambridge University Press, 1972).
[3] Ryogo Kubo, “Statistical-mechanical theory of irreversible processes. i. general theory and simple applications to magnetic and conduction problems,” Journal of the Physical Society of Japan 12, 570–586 (1957).
[4] G.D. Mahan, Many-Particle Physics, Physics of Solids and Liquids (Springer, 2000).
[5] B. Srima Shastry, “Sum rule for thermal conductivity and dynamical thermal transport coefficients in condensed matter,” Phys. Rev. B 73, 085117 (2006).
[6] D. Belitz and T. R. Kirkpatrick, “The anderson-mott transition,” Rev. Mod. Phys. 66, 261–380 (1994).
[7] J. K. Freericks, D. O. Demchenko, A. V. Joura, and V. Zlatić, “Optimizing thermal transport in the falicov-kimball model: The binary-alloy picture,” Phys. Rev. B 68, 195120 (2003).
[8] P. Haldar, M. S. Laad, and S. R. Hassan, “Real-space cluster dynamical mean-field approach to the Falicov-Kimball model: An alloy-analogy approach,” Phys. Rev. B 95, 125116 (2017).
[9] R. Franz and G. Wiedemann, “Ueber die Wärme-Leitungsfähigkeit der Metalle,” Annalen der Physik 165, 497–531 (1853).
[10] Makariy A. Tanatar, Johnpierre Paglione, Cedomir Petrovic, and Louis Taillefer, “Anisotropic Violation of the Wiedemann-Franz Law at a Quantum Critical Point,” Science 316, 1320–1322 (2007).
[11] C. Castellani, C. Di Castro, G. Kotliar, P. A. Lee, and G. Strinati, “Heat-transport Ward identity and effective Landau Fermi-liquid parameters in disordered systems,” Phys. Rev. B 37, 9046–9048 (1988).
[12] C. L. Kane and Matthew P. A. Fisher, “Thermal Transport in a Luttinger Liquid,” Phys. Rev. Lett. 76, 3192–3195 (1996).
[13] R. W. Hill, Cyril Proust, Louis Taillefer, P. Fournier, and R. L. Greene, “Breakdown of Fermi-liquid theory in a copper-oxide superconductor,” Nature 414, 711–715 (2001).
[14] Frank Steglich, Christoph Geibel, Robert Modler, Michael Lang, Peter Hellmann, and Philipp Gegenwart, “Classification of strongly correlated f-electron systems,” Journal of Low Temperature Physics 99, 267–281 (1995).
[15] H. Terletska, J. Vučičević, D. Tanasković, and V. Dobrosavljević, “Quantum critical transport near the mott transition,” Phys. Rev. Lett. 107, 026401 (2011).
[16] P. Haldar, M. S. Laad, and S. R. Hassan, “Quantum critical transport at a continuous metal-insulator transition,” Phys. Rev. B 94, 081115 (2016).
[17] P. Haldar, M. S. Laad, S. R. Hassan, Chand Madhavi, and Raychaudhuri Pratap, “Quantum Critical Magnetotransport at a Continuous Metal-Insulator Transition,” arXiv:1603.00779 (2016).
[18] J. K. Freericks and V. Zlatić, “Thermal transport in the falicov-kimball model,” Phys. Rev. B 64, 245118 (2001).
[19] S. Maekawa, T. Tohyama, S.E. Barnes, S. Ishihara, W. Koshihara, and G. Khaliullin, “Physics of Transition Metal Oxides,” Springer Series in Solid-State Sciences (2004).
[20] R.R. Heikes and R.W. Ure, Thermoelectricity: science and engineering (Interscience Publishers, 1961).
[21] J. K. Freericks and V. Zlatić, “Exact dynamical mean-field theory of the falicov-kimball model,” Rev. Mod. Phys. 75, 1333–1382 (2003).
[22] M. Jarrell and H. R. Krishnamurthy, “Systematic and causal corrections to the coherent potential approximation,” Phys. Rev. B 63, 125102 (2001).
[23] Antoine Georges, Gabriel Kotliar, Werner Krauth, and Marcello J. Rozenberg, “Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions,” Rev. Mod. Phys. 68, 13–125 (1996).
[24] K. Haule and G. Kotliar, “Optical conductivity and kinetic energy of the superconducting state: A cluster dynamical mean field study,” EPL (Europhysics Letters) 77, 27007 (2007).
[25] PM Chaikin and G Beni, “Thermopower in the correlated hopping regime,” Physical Review B 13, 647 (1976).
[26] X. Zotos, F. Naef, and P. Prelovsek, “Transport and conservation laws,” Phys. Rev. B 55, 11029–11032 (1997).
[27] C. Villagonzalo, R.A. Römer, and M. Schreiber, “Transport properties near the anderson transition,” Ann. Phys. [Leipzig] 08, 269–272 (1999).
[28] Frank Milde, Rudolf A. Römer, and Michael Schreiber, “Energy-level statistics at the metal-insulator transition in anisotropic systems,” Phys. Rev. B 61, 6028–6035 (2000).
[29] Bernhard Kramer, Gerd Bergmann, and Yvan Bruynseraede, “Localization, interaction, and transport phenomena,”
[30] T. R. Kirkpatrick and D. Belitz, “Stable phase separation and heterogeneity away from the coexistence curve,” Phys. Rev. B 93, 144203 (2016).

[31] Vijay Narayan, Michael Pepper, and David A. Ritchie, “Thermoelectric and electrical transport in mesoscopic two-dimensional electron gases,” Comptes Rendus Physique 17, 1123 – 1129 (2016).

[32] G. Schwiete and A. M. Finkel’stein, “Thermal transport and wiedemann-franz law in the disordered fermi liquid,” Phys. Rev. B 90, 060201 (2014).

[33] G. Schwiete and A. M. Finkel’stein, “Renormalization group analysis of thermal transport in the disordered fermi liquid,” Phys. Rev. B 90, 155441 (2014).

[34] V. Dobrosavljević, Elihu Abrahams, E. Miranda, and Sudip Chakravarty, “Scaling theory of two-dimensional metal-insulator transitions,” Phys. Rev. Lett. 79, 455–458 (1997).