Universal Scaling near Band-Tuned Metal-Insulator Phase Transitions

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We present a theory for band-tuned metal-insulator transitions based on the Kubo formalism. Such a transition exhibits scaling of the resistivity curves in the regime where $T\tau > 1$ or $\mu\tau > 1$, where τ is the scattering time and μ the chemical potential. At the critical value of the chemical potential, the resistivity diverges as a power law, $R_c \sim 1/T$. Consequently, on the metallic side there is a regime with negative dR/dT, which is often misinterpreted as insulating. We show that scaling and this "fake insulator" regime are observed in a wide range of experimental systems. In particular, we show that Mooij correlations in high-temperature metals with negative dR/dT can be quantitatively understood with our scaling theory in the presence of T-linear scattering.

Thanks to the advent of highly tunable "twisted" Van der Waals heterostructures [1–3], the field of quantum matter physics is in a position to study continuous zero-temperature phase transitions with an unprecedented accuracy. Detailed (and smooth) experimental results allow a systematic comparison between different theoretical predictions, which is particularly true for continuous metal-to-insulator transitions (MITs).

Interaction-induced MITs, such as the Mott transitions, display quantum critical behavior, including scaling of the resistivity [4,5]. A full theoretical understanding of Mott criticality, which would include a precise calculation of the scaling exponents, is still lacking [6]. One of the main challenges lies in the fact that an MIT is, in general, *not* a transition described by symmetry breaking, which makes it challenging to identify the source of scaling.

Recently, scaling has been observed in a simple *band-tuned* MIT in a $MoTe_2/WSe_2$ bilayer at full filling of the first valence flat band [7]. By tuning the displacement field, one can open a band gap to the second valence band. The scaling behavior there has been analyzed using a model with disorder and a bosonic field [8], inspired by earlier work on "Mooij" correlations [9,10]. However, the observed scaling can also be interpreted in a much simpler perspective.

From a theoretical viewpoint, calculating the conductivity is notoriously difficult. An exception is the classical Drude formula, $\sigma = (ne^2\tau/m)$, which can also be derived with fully quantum-mechanical advanced methods such as the Kubo formula [11,12]. A natural question is whether the observed scaling at a metal-insulator transition can be explained with the same set of assumptions that is used to derive Drude theory.

Indeed, in this Letter we show that only a small number of very natural assumptions lead to scaling behavior near a band-tuned MIT. The only assumptions are that the scattering time τ is large, parametrized by $T\tau > 1$ or $\mu\tau > 1$ (with μ the chemical potential measured from the band edges on the metallic side), and that the electron self-energy is local and proportional to the electron density of states. These quantitative conditions are relevant for weakly correlated, weakly disordered materials. Under these assumptions, the critical resistivity at the MIT is diverging as $R_c(T) \sim 1/T$, in contrast to the oft-cited picture that the critical resistivity curve is independent of temperature. We derive an explicit scaling form, showing that in the scaling regime the resistivity is given by a universal $R(T, \mu) = R_c(T)f(\mu/T)$. Contrary to the physics of universality at continuous phase transitions, the scaling of the resistivity breaks down very close to the MIT.

Band-tuned MIT.—Consider a weakly interacting electron system described by a band structure. The system is metallic if there is a nonzero density of charge carriers, characterized by a nonzero chemical potential μ. The system is an insulator if there is a gap toward exciting charge carriers. By continuously changing the band structure we can induce a band-tuned MIT. This can be achieved with pressure, displacement field, or even due to spontaneous symmetry breaking such as ferromagnetic polarization. Without loss of generality, the dispersion at a band edge is parabolic, with the dispersion set by $\xi_{\mathbf{k}} = (k^2/2m) - \mu$, where m is the effective mass. With this notation, $\mu > 0$ corresponds to the metal, $\mu < 0$ to an insulator, and $\mu = 0$ is the critical point. The chemical potential μ is thus the tuning parameter of the MIT, as shown in Fig. 1.
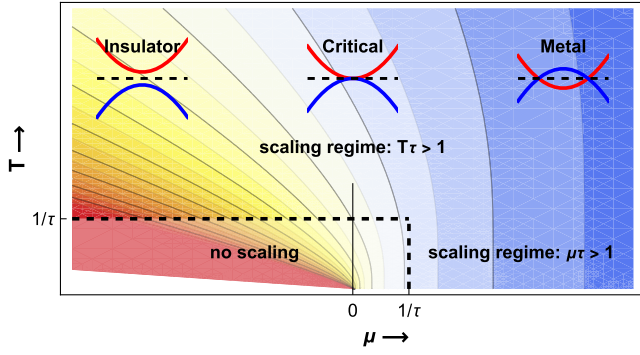
FIG. 1. In a band-tuned metal-insulator transition (MIT), the system changes from having overlapping valence (blue) and conduction (red) bands in the metallic side (right) to having a gap on the insulating side (left). The tuning parameter is the chemical potential μ. When either $T\tau > 1$ or $\mu\tau > 1$, the resistivity (in shades on the background) can be described by a scaling form, as shown in Fig. 2. This scaling relation breaks down very close to the transition, where localization and interaction effects will change the picture.

In general, the conductivity is determined by disorder, electron-electron interactions, and electron-phonon coupling. Nonzero resistivity from electron-electron interactions requires umklapp scattering, which becomes asymptotically irrelevant at low carrier densities (though there might be nontrivial vertex corrections) [13]. Similarly, at zero temperature there is no thermal occupation of phonons, and therefore no electron-phonon contribution to the resistivity. The zero-temperature behavior of a band-tuned MIT is therefore completely dominated by disorder. In principle, strong disorder might push the system into Anderson insulation. However, in $d = 2, 3$ it is considered that the combination of weak disorder and weak interactions generally precludes true localization [14–17]. Moreover, even in the absence of interactions, quantum corrections to the conductivity are not relevant in the regimes $\mu\tau > 1$ and $T\tau > 1$ considered here, and will therefore be neglected throughout this work.

Conductivity.—With these natural assumptions, the conductivity close to the MIT is calculated using the Kubo formula for local self-energies [11,18], which reads

$$\sigma_{xx} = \pi \sum_n^{N_b} \int d\xi \Phi_{x,n}(\xi) \int dz A_n^2(\xi, z)[-f'(z)], \quad (1)$$

where $A_n(\xi, z)$ is the one-particle spectral function for the nth band, and f is the Fermi function. The details of the following derivation are presented in Ref. [19]. The entire momentum dependence is contained in the *transport function* $\Phi_{x,n}(\xi) = \int (d^d p/(2\pi)^d)\delta(\xi - \xi_{\mathbf{p}})j_x^2(\mathbf{p})$. The transport function itself displays universal behavior in the vicinity of a band-tuned MIT: given a parabolic band dispersion for either holelike or electronlike bands, the

current operator equals $\mathbf{j}(\mathbf{p}) = (e/m)\mathbf{p}$. Consequently the transport function for each band is proportional to the density of states $N(\xi) = \int (d^d p/(2\pi)^d)\delta(\xi - \xi_{\mathbf{p}})$ times a linear function:

$$\Phi_x(\xi) = \frac{2e^2}{dm}(\xi + \mu)N(\xi). \quad (2)$$

This universal shape stems from the fact that the current squared is proportional to the dispersion, $j^2 \propto \xi$. Focusing for now on $d = 2$, we assume a constant, energy-independent scattering rate τ, so that the imaginary part of the self-energy is $\mathrm{Im}\Sigma(z) = -\Theta(z + \mu)(2\tau)^{-1}$. This scattering time is typically of the order $\tau \sim 10^{-12}$–10^{-14} s ~ 10–10^3 eV^{-1}. When $\mu\tau > 1$ or $T\tau > 1$, the Kubo formula radically simplifies, and we find the conductivity,

$$\sigma(T, \mu) = \frac{e^2}{h}\tau T \log[1 + e^{\mu/T}], \quad (3)$$

per conduction or valence band. This is our central result for the conductivity close to the band-tuned MIT. Surprisingly, it contrasts a few commonly held convictions on metal-insulator transitions. First, at the critical point, the conductivity is *linear* in temperature, $\sigma_c(T) \equiv \sigma(0, T) = (e^2/h)\tau T \log 2$, rather than temperature independent. Furthermore, on the metallic side of the transition ($\mu > 0$), the temperature derivative of the resistivity can be negative: a "fake insulator" regime that is commonly misinterpreted as insulating. Furthermore, Eq. (3) satisfies a universal scaling form,

$$\sigma(\mu, T) = \sigma_c(T)F(\mu/T), \quad (4)$$

which allows the collapse of many resistivity curves onto a simple scaling function $F(x) = \log_2[1 + e^x]$. The theoretical resistance curves near the band-tuned MIT, including the scaling properties, are shown in Fig. 2.

Hidden in plain view is the fact that Eq. (3) is, at zero temperature on the metallic side, equivalent to Drude theory. Explicitly, its low-temperature limit for $\mu = E_F > 0$ yields $\sigma = \Phi(E_F)\tau$, with $\Phi(E_F) = ne^2/m$ in any dimension d yielding $\sigma = ne^2\tau/m$.

At finite temperature the scaling regime persists, even with a temperature-dependent scattering time $\tau(T)$, provided that τ^{-1} is still proportional to the density of states. When τ is temperature independent, in fact, *all* resistivity curves on the metallic side are fake insulators with $d\rho/dT \leq 0$ (cf. Fig. 2). Only when the scattering rate increases with temperature, for example, from electron-phonon interactions shown in Fig. 2(b) or from umklapp scattering, we find traditional metallic behavior with $d\rho/dT > 0$. In this case, inside the metallic regime there exists a point where the temperature derivative of the resistivity $d\rho/dT$ changes sign. We will discuss universal
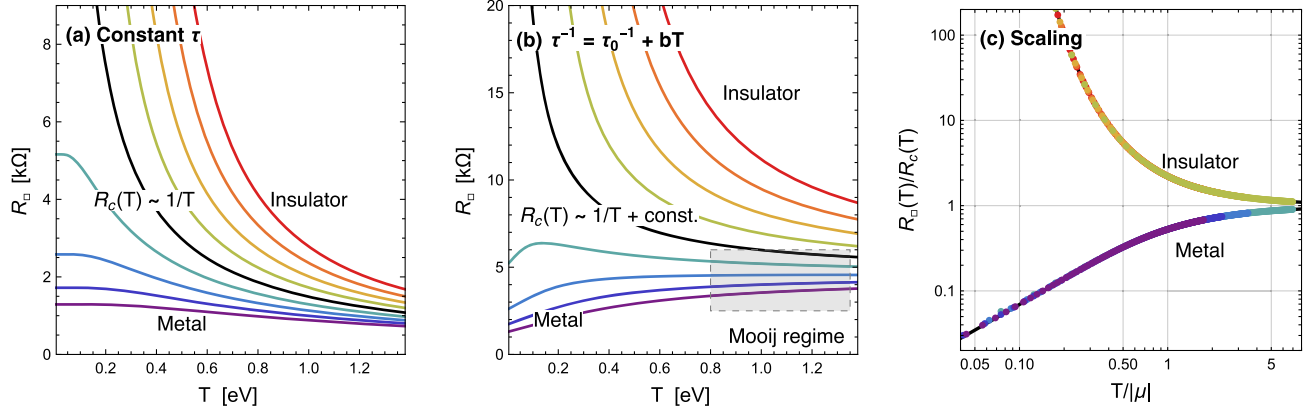
FIG. 2. Theoretical resistance curves close to a band-tuned metal-insulator transition. (a) Resistance calculated using Eq. (3), for a constant scattering time $\tau = 25$ eV^{-1}, and chemical potential μ ranging from -0.8 to $+0.8$ eV. The resistance at the critical point $\mu = 0$ diverges as $R_c(T) \sim 1/T$. On the metallic side, the resistance decreases as a function of temperature (a "fake" insulator), whereas on the insulating side the resistance is activated. (b) Resistance for a temperature-dependent scattering rate $\tau^{-1} = \tau_0^{-1} + bT$ with $\tau_0 = 25$ eV^{-1} and $b = 0.1$. On the metallic side, a resistivity maximum arises at a temperature dependent on the distance from the transition. At high temperatures, this gives rise to Mooij correlations (see Fig. 4). (c) When $T\tau > 1$ or $\mu\tau > 1$, the resistance curves follow a simple scaling law, $R(T, \mu) = R_c(T)f(\mu/T)$. This can be verified by plotting R/R_c versus $T/|\mu|$. All data points collapse onto one of the two curves, associated with either metallic or insulating behavior.

properties around this point later in the context of Mooij correlations [9,20].

It is important to emphasize that the scaling form of Eq. (4) is limited to regions *not too close* to the transition. This limitation is similar to the one proposed by Mott-Ioffe-Regel (MIR) [21]. A common formulation of the MIR limit in metals is $k_F\ell \sim 1$, where ℓ is the mean-free path. This can be rewritten as $\mu\tau \sim 1$; we therefore find that, upon approaching the transition from the metallic side, the scaling hypothesis breaks down precisely at the MIR boundary. What happens close to the transition is nonuniversal, and depending on model parameters one can find various different violations of scaling (see Ref. [19]).

Band-tuned MIT in moiré bilayers.—We are now in a position to verify our universal scaling result of Eq. (3) in experimental results on real physical systems. Inspired by the recent developments in moiré materials, let us first focus on the MIT in MoTe$_2$/WSe$_2$ at full filling of the first valence flat band ($f = 2$) [7]. By tuning the perpendicular displacement field, a gap is opened up, yielding a band-tuned MIT. In Fig. 3 we fit the observed resistance curves as a function of displacement field using our theory. Indeed, the critical resistance diverges as $R_c \sim 1/T$, and the resistance curves obey scaling. As shown in Fig. 3(a), the scaling curve itself quantitatively matches the analytical form derived in Eq. (3). A similar scaling plot for these data
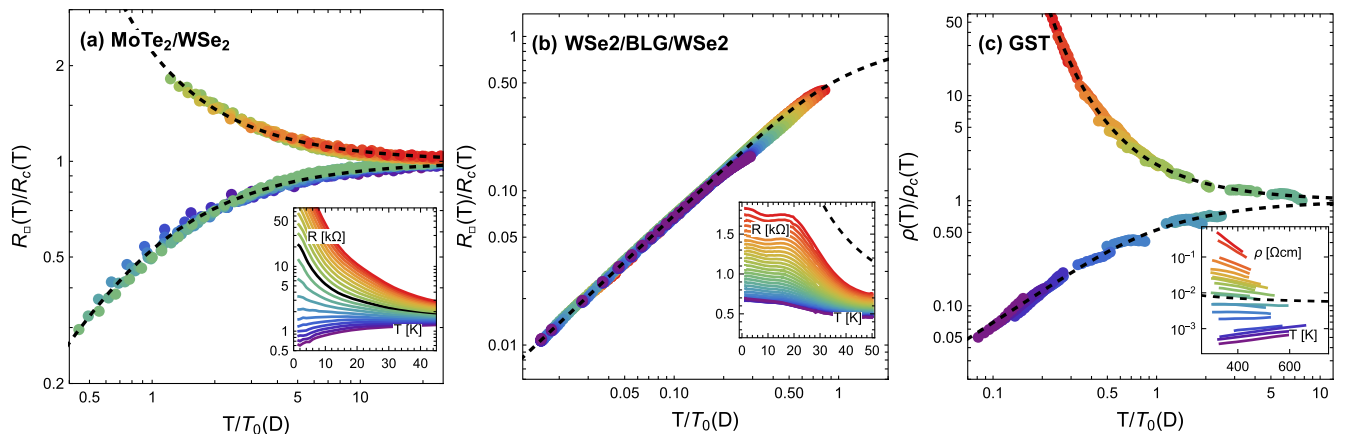

FIG. 3. Scaling near the band-tuned MIT is observed in a range of materials. Here, we apply our scaling analysis to three material systems [19]: (a) the moiré heterobilayer MoTe$_2$/WSe$_2$ [5], (b) the heterostructure WSe$_2$/bilayer graphene/WSe$_2$ [22], and (c) GST amorphous phase change materials [23]. The measured resistivities are shown in insets. In panels (a) and (c) we see a genuine MIT, with data collapse on both an insulating and conducting branch. The theoretical scaling curve of Eq. (4) is shown as a dashed black line, and shows remarkable agreement with the experimental results.

has been reported in Ref. [8], inspired by earlier work in Ref. [10], which describes disorder-induced polaron formation. While such polaronic effects have been shown to drive the MIT at large metallic densities, the scaling derived here analytically applies near band edges without the need of any polaronic effects.

There are many claims of MITs in graphene-based moiré materials that upon closer inspection seem to exhibit fake insulator behavior. Consider, for example, the WSe_2/bilayer graphene/WSe_2 heterostructure measured in Ref. [22]. At filling $\nu = 0$, the resistivity turns up at low temperatures reminiscent of an insulating gap. However, at around $T = 20$ K, the resistivity seems to saturate, to a displacement-field dependent value. The absence of a true diverging resistance at low temperature suggests that these systems retain a nonzero density of charge carriers, either from a band overlap or induced by potential inhomogeneities that are common in graphene systems. Indeed, when performing the scaling analysis, we can collapse all the curves of this system to the metallic branch of our scaling form, as shown in Fig. 3(b).

Disordered metallic alloys.—While Eq. (3) was derived for weak disorder scattering and $d = 2$, it is in fact far more universal. Often a momentum-independent self-energy arises even beyond perturbation theory and in any dimensions d. In realistic situations one can apply iterated schemes such as the self-consistent Born approximation for both disorder scattering and electron-phonon scattering in the adiabatic limit. This scheme obeys the equation $\Sigma(z) = s^2 G(z)$, with s a (possibly temperature-dependent) parameter quantifying the energy fluctuations involved in the scattering process. This implies that the inverse scattering time is proportional to the density of states $\mathrm{Im}\Sigma(z) \propto N(z) \sim \mathrm{Im}G(z)$, leading to a conductivity of the form $\sigma(T) = (e^2/d\pi m s^2)T \log[1 + e^{\mu/T}]$ in general dimensions d, consistent with Eq. (3) [19].

The universal scaling is indeed also observed in three-dimensional compounds away from the weak disorder limit, since the condition $\mathrm{Im}\Sigma(z) \sim N(z)$ implies that $\mu\tau > 1$ is always satisfied sufficiently close to the transition. In particular, we look at GST (GbSeTe compounds with varying composition) [23], a phase-change compound where the annealing history affects the effective number of charge carriers [24]. Here, in the high-temperature range $T = 300$–600 K, a smooth evolution from positive dR/dT to negative dR/dT is observed depending on the precise composition and history of the sample. Since the main effect of these compositional changes is in fact a shift of the chemical potential, we show in Fig. 3(c) that the experimental data on GST can be accurately described by our scaling theory.

Mooij correlations.—Universal scaling implies the existence of a fake insulator regime: a metal characterized by a (dimensionless) negative temperature coefficient of the resistance $\alpha = (T/R)dR/dT < 0$. Historically, the observation of a negative α in various disordered metals,

including binary alloys (Ni_xCr_{1-x}, Ti_xAl_{1-x}, Fe_xSi_{1-x}, etc.) [9,10], was considered a "high-temperature anomaly" [20]. In a seminal paper, Mooij [9] discovered a correlation between the temperature coefficient α and the resistivity ρ itself. There is currently no consensus on the origin of these Mooij correlations, though they have been interpreted in terms of quantum localization corrections to the conductivity [20,25] or the disorder-driven formation of polarons [10].

Interestingly, the scaling theory proposed in this Letter allows us to quantitatively describe Mooij correlations. To do so, we assume that at high temperature the scattering time τ is linear in T:

$$\tau^{-1} = \tau_0^{-1} + bT. \tag{5}$$

This form occurs in many metals, where b is either proportional to the electron-phonon coupling strength, or a more complex, "Planckian" quantum scattering [26]. With this assumption, the critical curve becomes flat at high temperature, $R_c(T) \to R^\infty \propto b$. This allows us to introduce a dimensionless resistivity R/R^∞. By taking the derivative of the scaling relation Eq. (3), and inverting it with respect to the tuning parameter μ at a fixed temperature T, we find that the temperature coefficient α only depends on R/R^∞:

$$\alpha(R) = \frac{R}{R^\infty}(1 - 2^{-R^\infty/R})\log_2[2^{R^\infty/R} - 1]. \tag{6}$$

In Fig. 4 we compare our analytical result with the original data presented by Mooij [9] and those collected in
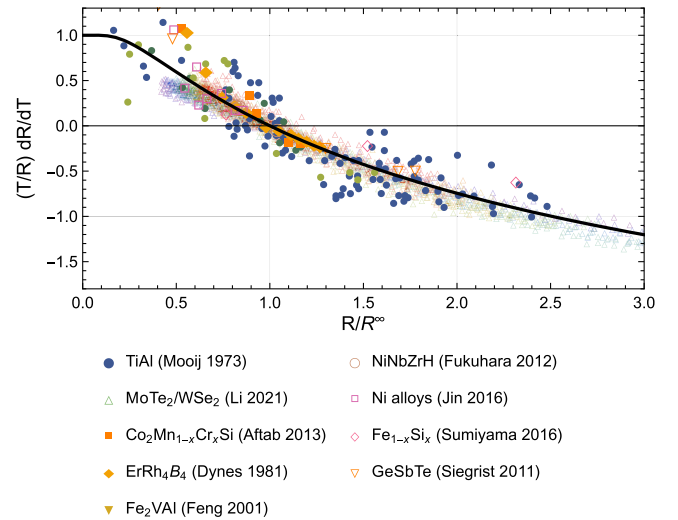

FIG. 4. The dimensionless temperature coefficient of the resistance versus the dimensionless resistance, for a variety of materials [5,9,23,27–32] (for details, see Ref. [19]), compared to our theoretical result of Eq. (6) (solid black line). For the experimental data the only fitting parameter is R^∞, the limit of the critical resistance at high temperature. We find an excellent agreement of the experimental Mooij correlations and our theory.

Ref. [10], finding a good agreement between the experimental results on binary alloys and Eq. (6). The recent data on moiré bilayers show an even more striking *quantitative* equivalence between the resistivity data in the high-temperature range $T = 26$–60 K: without a fitting parameter the experimental results of Ref. [5] match Eq. (6).

Outlook.—In this Letter we have shown that a simple theory of conductivity predicts universal scaling near band-tuned MITs consistent with experimental results in a wide range of materials, from recent moiré materials to decades-old data on binary alloys.

The predicted scaling regime does not extend arbitrarily close to the MIT: when $T\tau < 1$ and $\mu\tau < 1$ deviations from or a full breakdown of scaling can appear. Note that the difference between scaling close to and farther away from the transition has been discussed in Ref. [6]. The scaling described in this Letter is thus *not* due to the divergence of a length scale, and is *not* related to Landau order parameters, the renormalization group, or any other theory of universality in symmetry-breaking (quantum) phase transitions. The universal behavior of resistivity scaling near the MIT throughout many materials is just the consequence of generic weakly interacting electrons with weak disorder, in spirit similar to the stability of the Fermi liquid. The properties of Anderson and weak localization as well as Wigner crystallization and the Mott MIT [6] are phenomena that, on the other hand, are outside the scaling regime discussed here. It is an interesting open question whether the scaling described in this Letter can extend, under certain conditions, arbitrarily close to the MIT, thus connecting to the standard theoretical framework of continuous phase transitions [33].

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Correction: A missing minus sign in Eq. (6) has been inserted.