Quantum critical scaling of the conductivity tensor at the metal-insulator transition in $Nb_{1-x}Ti_xN$

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In contrast to the Landau paradigm, a metal-insulator transition (MIT), driven purely by competition between itinerance and localization and unaccompanied by any conventional (e.g, magnetic) order-disorder instabilities, admits no obvious local order parameter. Here, we present a detailed analysis of the quantum criticality in magneto-transport data on the alloy $Nb_{1-x}Ti_xN$ across a Ti-doping-driven a MIT. We demonstrate, for the first time, clear and novel quantum criticality reflected in the *full* conductivity tensor across the MIT. Wide ranging, comprehensive accord with recent theoretical predictions strongly suggests that these unanticipated findings are representative of a *continuous* MIT of the band-splitting type, rather than a conventional Anderson disorder or a "pure" correlation-driven first-order Mott type.

Quantum phase transitions (QPT) between different phases, driven by tuning non-thermal parameter(s) at zero temperature ($T = 0$), continue to underpin novel developments in quantum matter [1]. Among QPTs, the fundamental example of a metal-insulator transition (MIT), driven either dominantly by electron correlations [2], disorder [3, 4], or both [5, 6], is distinguished by lack of a Landauesque, local order parameter. Such novel QPTs, believed to lie outside the conventional Landau-Ginzburg-Wilson (LGW) paradigm of critical phenomena, solely involve competition between kinetic energy-induced delocalization and correlation-and/or disorder-induced localization of carriers. Careful work [7] increasingly shows that such QPTs may underlie "strange" metallicity involving partial localization of carriers. Thus, investigation of "Mott quantum criticality" is a timely issue of great relevance to emergence of unusual electronic behavior in quantum matter.

In contrast to pure correlation-driven (first-order) cases, (strong or weak) disorder-driven MITs show genuine quantum criticality [8, 9]. Notwithstanding complications due to interplay of itinerance and interaction-and/or disorder-driven localization, unveiling quantum critical dynamics is facilitated by diverging spatio-temporal dynamical fluctuations as $T \to 0$ near the quantum critical point (QCP), permitting use of scaling relations to characterize finite T, ω (here, ω is the excitation energy) responses. Near a QPT, both, the spatial correlation length, ξ_x and correlation time, τ, diverge like $\xi_x \propto |x - x_c|^{-\nu}$ and $\tau \propto \xi_x^z \propto |x - x_c|^{-z\nu}$, with x a tuning parameter, x_c its critical value at the QCP, ν the correlation length exponent and z the dynamical critical exponent. A new thermal timescale, $t_{th} \simeq \hbar/k_BT$, viewable as the system size in the temporal direction, appears at finite T. Thus, finite-T data can be finite-size-scaled in terms of the ratio t_{th}/τ to track the growth of critical fluctuations as a system enters the quantum critical fan above a QCP at finite T. Specifically, singular parts of physical response functions in the quantum critical region must be universal functions of $\tau/t_{th} \propto T/|x - x_c|^{z\nu}$.

At a continuous phase transition (here, achieved by Ti-substitution in NbN) MIT, the control parameter, related to the doping (here, x), is its deviation from the critical doping, x_c, and physical responses must scale as $T/|x - x_c|^{z\nu}$ in the quantum critical regime of the MIT. Moreover, one also expects deeper manifestations of quantum criticality: (i) in a wide x-regime around x_c, $\tilde{\rho}_{xx}(T, \delta x) = 1/\tilde{\rho}_{xx}(T, -\delta x)$, with $\tilde{\rho}_{xx} = \rho_{xx}(T)/\rho_c(T)$ the scaled dc longitudinal resistivity, ρ_c is the resistivity at $x = x_c$ and $\delta x = (x - x_c)/x_c$ the distance from the QCP. This property, first seen in pioneering studies for the 2D electron gas in MOSFETS [10], implies that the M- and I-phases are mapped into each other by a simple reflection, exposing a novel *duality* between them. The upshot thereof is that the β- (or Gell-Mann Low function, $\beta = \frac{d\ln(\tilde{\rho}_{xx}^{-1})}{d\ln(L)}$, L is the length scale) has precisely the same form on both sides of the QCP [9], (ii) quantum critical scaling, *i.e*, the $\tilde{\rho}_{xx}(T)$ curves for both, insulator (I) and metal (M) phases *separately* collapse onto two universal curves when plotted versus a "scaling variable", $(T/T_0)^{1/z\nu}$. Here, $T_0(\delta x) = c|\delta x|^{z\nu} \propto \xi_x^{-z}$ (with c is a constant) vanishes at the QCP, reflect-

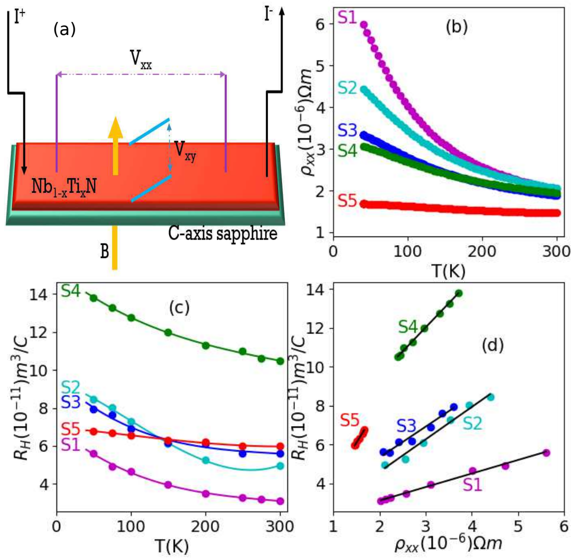

Figure 1. (a) **Schematic measurement geometry of $Nb_{1-x}Ti_xN$:** ρ_{xx} and ρ_{xy} are determined by measuring the longitudinal (V_{xx}) and Hall (V_{xy}) voltages, respectively, at a fixed d.c. bias current I. The magnetic field B is applied perpendicular to the sample. (b) The temperature variation of longitudinal resistivity of all five samples at $B = 0$. $\rho_{xx}(T)$ decreases for all five samples with increasing T, affirming the "Mooij correlation" in the metallic phase. (c) Variation of Hall coefficient $R_H(T)$ as a function of temperature T. The solid lines are cubic polynomial fits. (d) Variation of Hall coefficient R_H as a function of longitudinal resistivity ρ_{xx}. The solid lines are straight line fits.

ing a divergent localization length. Thus, we expect that the scaled *dc* resistivity will exhibit a scaling law: $\tilde{\rho}_{xx}(T, \delta x) = F_{\pm}(T/|\delta x|^{z\nu})$, with $F_{\pm}$ being a scaling functions in the M (+) and I (−) phases, and $F_{\pm}$ constrained by the reflection symmetry. The exponents z and ν, extracted from such analysis, help identify whether the MIT belongs to the Mott, Anderson, or of an other, unconventional type.

Experiments and results – Armed with these preliminaries, we now present our experimental results for the alloy $Nb_{1-x}Ti_xN$ relegating the details in the **SI1**. Five samples of $Nb_{1-x}Ti_xN$ films of thickness ~ 10 nm, with different x, were grown on c-axis sapphire by high temperature chemical vapour deposition. All the films grow epitaxially as was evident from high resolution transmission electron microscopy (HRTEM) and x-ray diffraction studies (the detailed have been published elsewhere [11, 12]). The relative composition of Ti and Nb were controlled by the gas flow rates. Fig. 1(a) shows a schematic to measure the longitudinal (V_{xx}) and Hall (V_{xy}) voltage, respectively, at a fixed d.c. bias current I in presence of a magnetic field B, applied perpendicular to the sample. The measurements were carried out in a commercial Physical Property Measurement System (Quantum Design's). In Fig. 1(b), we show that $\rho_{xx}(T)$ at zero magnetic field decreases with T, clearly revealing the "Mooij correlation" well into the metallic phase, and up to room temperature. ρ_{xy} is determined by sweeping the magnetic field from 0 to 8 Tesla. At a fixed temperature, ρ_{xy} varies linearly with the magnetic field, the slope gives Hall coefficient, R_H. In Fig. 1(c), we show that $R_H(T)$ decreases with temperature similar to $\rho_{xx}(T)$, also found in an earlier work on NbN [13]. More importantly, as shown in Fig. 1(d), $R_H(T) = C + C'(x)\rho_{xx}(T)$ with the ratio $r = \frac{\Delta R_H/R_H}{\Delta\rho_{xx}/\rho_{xx}}$ lying between 0.7 and 0.9. The disorder of our samples is characterized by Ioffe-Regel parameter $k_F\ell$ which is determined at 50 K (where the electron-phonon interaction is small) from the following formula, assuming free electron model: $k_F\ell = \frac{\hbar(3\pi^2)^{2/3}}{n^{1/3}\rho_{xx}e^2}$, here, k_F is the Fermi wave-vector,ℓ the elastic mean free path and n the free electron density, determined from $R_H(= 1/ne)$. We note that with increasing x, $k_F\ell$ increases i.e., the disorder decreases. In the following, instead of x, we analyze our data in terms of $k_F\ell$— a more common measure of disorder.

Quantum critical scaling – We briefly provide the quantum critical scaling procedure of $\rho_{xx}(T)$ and Hall conductivity, $\sigma_{xy}(T)(\sim R_H(T)/\rho^2_{xx}(T))$ (see the **SI2** for details). First, using the data for five samples, we obtained $\rho_{xx}(T)$ on all points of T vs k_Fl plane by polynomial fitting of order 3 with T in the range $40 - 120$ K and k_Fl in the range $1.4 - 3.0$. At a given temperature (T), we determine the metal-insulator critical value of k_Fl, $(k_Fl)_c$, as the inflection point of ρ_{xx} vs k_Fl curve. The line $\delta k_Fl = k_Fl - (k_Fl)_c = 0$ separates the metallic ($\delta k_Fl > 0$) and the insulating ($\delta k_Fl < 0$) phases at different temperatures. As shown in Fig. 2(a), the scaled longitudinal resistivity, $\tilde{\rho}_{xx}(T, \delta k_Fl) = \rho_{xx}(T, \delta k_Fl)/\rho_c(T)$), (here $\rho_c(T)$ is the resistivity at $(k_Fl)_c$), changes continuously from the metallic ($\delta k_Fl > 0$) to the insulating ($\delta k_Fl < 0$) phase. The horizontal axis is scaled to $|\ \delta k_Fl\ |/t_{xx}(T)$ such that all the metallic (M) and insulating (I) curves corresponding to different T fall on one metallic and one insulating master curve, respectively. From the plot of $t_{xx}(T)(\sim T^{1/(z\nu)_{xx}})$ vs T we get the exponent $(z\nu)_{xx}$. For the scaling of $\sigma_{xy}(T)$ we use a protocol similar to the one used above for $\rho_{xx}(T)$.

Our results expose *all* the characteristic signatures of quantum-critical behavior expected at a continuous MIT. In particular, in Fig. 2(b), we show that $\rho_{xx}(T, \delta k_Fl)$ exhibits a clean crossing point at $\delta k_Fl = 0$ when plotted as a function of δk_Fl. Moreover, as shown in Fig. 2(c), clear quantum-critical scaling is obtained upon plotting $\log(\rho_{xx}(T, \delta k_Fl)/\rho_c)$ versus $T/T_0^{xx}(\delta k_Fl)$, with $T_0^{xx} = c\ |\ \delta k_Fl\ |^{(z\nu)_{xx}}$ affirming the quantum critical character of the MIT. We extract $(z\nu)_{xx} = 1.5$, a value that sub-

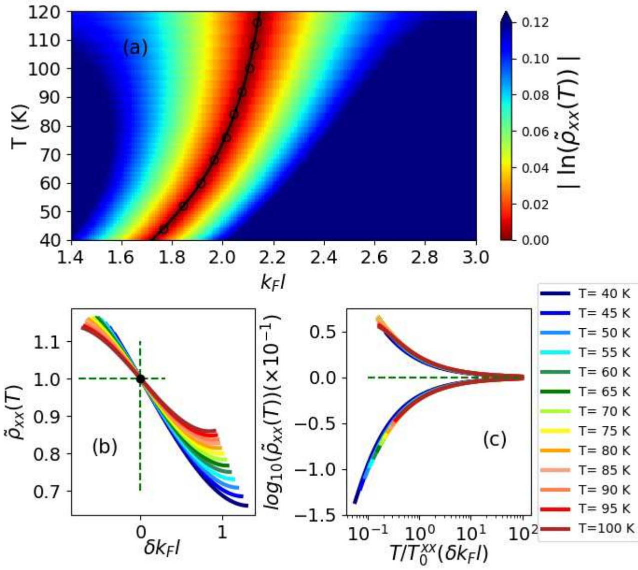

Figure 2. Color plot of the T-dependent scaled dc resistivity as a function of $k_F l$ (upper panel (a)). The "fan-like" form expected for quantum criticality is clearly seen. Black empty circles represent the "quantum Widom line", defined as the crossover scale that describes the increasingly rapid crossover between a metal and an insulator as $T \to 0$. In $Nb_{1-x}Ti_xN$, the metallic side of the QPT is pre-empted by a low-T transition to superconductivity [12]. In the lower panels, “Duality” between the metal and insulator revealed in the dc longitudinal resisitivity: (a) Crossing point in the scaled resistivity $\tilde{\rho}_{xx}(T) = \rho_{xx}(T)/\rho_c(T)$ showing a clear MI “transition” at $\delta k_F l = k_F l - (k_F l)_c = 0$, (b) $\tilde{\rho}_{xx}(T)$ vs $T/T_0^{xx} = T/c \mid \delta k_F l \mid^{(z\nu)_{xx}}$ exhibits clear quantum critical scaling, and mirror-symmetry, with $(z\nu)_{xx} \approx 1.51$.

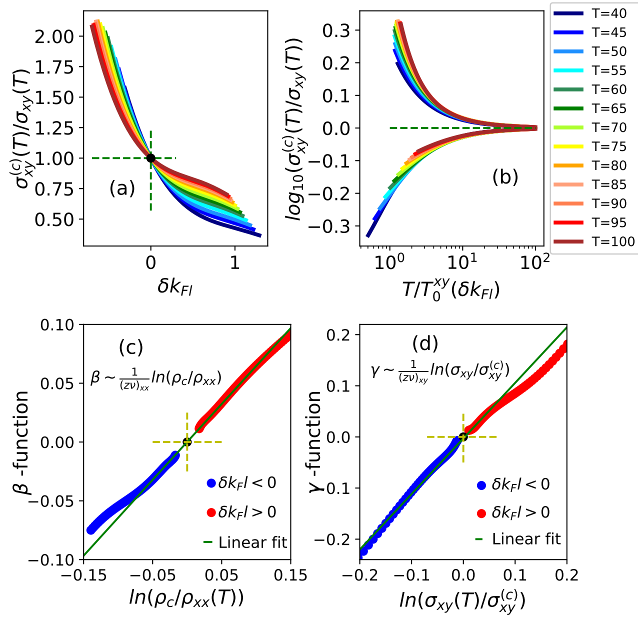

Figure 3. (a) Crossing point in (scaled) Hall conductivity $\sigma_{xy}^{(c)}(T)/\sigma_{xy}(T)$ is further proof of the MIT at $\delta k_F l = k_F l - k_F l_c = 0$, (b) Remarkably, $\sigma_{xy}^{(c)}(T)/\sigma_{xy}(T)$ vs $T/T_0^{xy} = T/c \mid \delta k_F l \mid^{(z\nu)_{xy}}$ shows quantum critical scaling and mirror-like symmetry with $(z\nu)_{xy} = 0.97$, (c) β- (or Gell-Mann-Low) function for the full dc conductivity tensor: In the left panel, β-function vs $ln(g_{xx})$ and (d) in the right panel, γ-function vs $ln(g_{xy})$. Both β and γ-functions show clear $ln(g)$ dependence, even quite well into the metallic phase, testifying to a very unusual manifestation of Mott-like quantum criticality.

stantially differs from $z\nu = 0.67$ for a purely correlation driven Mott MIT, but in the range observed earlier for MOSFETs [10] ($z\nu = 1.6$). More remarkably, we unearth clear signatures of “mirror symmetry” between metallic and insulating branch in Fig. 2(c).

Remarkably, the off-diagonal conductivity $\sigma_{xy}(T, \delta k_F l)$, also exhibits a similar and anomalous quantum critical scaling (see Fig. 3(a)). While well known for the longitudinal resistivity [6], such a clear signature of a MIT in the off-diagonal has never been seen to our best knowledge, though recent work on disordered TaN films [14] hints such a possibility. Specifically, the scaled (by the critical $\sigma_{xy}^{(c)}$ at the MIT) Hall conductivity curves $\log(\sigma_{xy}^{(c)}/\sigma_{xy}(T, \delta k_F l))$, for the M- and I-phases, separately coalesce onto two universal functions of $T/T_0^{xy}(\delta k_F l)$, precisely as for the dc resistivity. Moreover, in Fig. 3(b), we show that mirror symmetry is obeyed in this case as well. Thus, the duality between the M- and I-phases also manifests in Hall conductivity.

Even more manifestations of the unusual quantum criticality are visible upon extracting the β-function, defined as $\beta = \frac{d\ln(\rho_c/\rho_{xx}(T))}{d\ln(T)}$ with $L = T^{-1/z}$, with z the dynamical exponent. We calculate β-function numerically from the Fig. 2(c). In Fig. 3(c), we show that $\beta(\rho_c/\rho_{xx}(T)) \simeq \log(\rho_c/\rho_{xx}(T))$ and is continuous across the MIT: while one expects $\rho_{xx}(T) \simeq \exp[(T/T_0)^{-1/(z\nu)_{xx}}]$ in an insulating phase, it is remarkable that this behavior continues to hold quite deep in the metallic phase as well. A truly surprising finding of ours is that the γ-function (the Gell-Mann Low function for σ_{xy}, $\gamma = \frac{d\ln(\sigma_{xy}(T)/\sigma_{xy}^{(c)})}{d\ln(T)}$) also shows a completely unanticipated Mott-like scaling: in Fig. 3(d), we show that $\gamma(\sigma_{xy}/\sigma_{xy}^{c}) \simeq \log(\sigma_{xy}/\sigma_{xy}^{c})$ as well, even deep in the M-phase. We can directly extract the exponent $z\nu$ from these, and find that $(z\nu)_{xx} = 1.51$ and thus, $T_0^{(xx)} \simeq \mid \delta k_F l \mid^{1.51}$, while $(z\nu)_{xy} = 0.97 \simeq 1.0$, implying that $T_0^{(xy)} \simeq \mid \delta k_F l \mid^{1.0}$. These distinct $(z\nu)$ values suggests that the decay of longitudinal and Hall currents maybe controlled by distinct relaxation rates. Indeed, this holds near the MIT : while $\rho_{xx}(T) = [\sigma_0 + AT^{0.7}]^{-1}$ between 50 K and 300 K (shown in Fig. SI3), it is obvious that the Hall angle (θ_H) defined by $B\cot\theta_H(T) = \rho_{xx}(T)/R_H(T)$, exhibits a different T-dependence (shown in Fig. SI5). It immediately follows that the transverse relaxation rate, $\tau_H^{-1} \simeq \cot\theta_H$, is distinct from the longitudinal relaxation rate, $\tau^{-1}(T) \simeq \rho_{xx}(T)$, manifesting the two-relaxation rates scenario. This is exciting because such a feature is widely appreciated to be one of the tell-tale signatures of a "strange" metal [15]. But it arises whenever $R_H(T)$ is sizably T-dependent, as in our case. Ultimately, this points to a novel manifestation of the non-perturbative breakdown of Landau fermion-like quasiparticles in the quantum critical region associated with a continuous MIT. It is clearly *not* related to proximity to a $T = 0$ melting of any quasiclassical order, nor to any vagaries of a Fermi surface reconstruction, since no Fermi surface can possibly exist in the very bad metallic state close to the MIT (see the resistivity data in Fig. 2). It is truly remarkable that the full conductivity tensor nevertheless exhibits a novel, Mott-like quantum critical scaling at the MIT in $Nb_{1-x}Ti_xN$: this has a range of deeper implications, detailed below.

Discussions and Conclusions – To appreciate the novelty of our findings, we emphasize that our results contradict expectations from both, the weak localization (WL) view of an Anderson MIT as well as the correlation-driven Mott MIT. In the first scenario, while scaling of σ_{xy} is long known, semiclassical arguments in that case dictate that both, $\beta(\rho_c/\rho_{xx}(T))$ and $\gamma(\sigma_{xy}/\sigma_{xy}^c)$ scale like $\beta(\rho_c/\rho_{xx}(T)) \sim (D-2)-(\rho_{xx}/\rho_c)$, resulting in the quantum correction for σ_{xy} being twice that for $1/\rho_{xx}$. It turns out that this holds only as long as the inverse Hall constant, related to $h(L) \simeq L^{D-2}/R_H B$ [16], scales *classically* as L^{D-2} for small B. Given our finding of a sizably T-dependent R_H, especially near the MIT, this assumption obviously breaks down in our case. Additionally, we find $0.7 < r = \frac{\Delta R_H/R_H}{\Delta\rho_{xx}/\rho_{xx}} < 0.9$ (thus, it seems that no particular "universal" meaning may be associated with $r = 0.69$ seen earlier for NbN [13]), in stark contrast to the prediction of a universal value $r = 2.0$ in WL theory. Thus, there is no reason to expect conventional scaling to hold. On the other hand, our results are also irreconcilable in a pure correlation driven Mott scenario: apart from the fact that the MIT would have to be first order at low T with a bad-metallic, linear-in-T resistivity at the finite-T critical point [17, 18], the low-T correlated metallic phase away from the critical point would be a heavy Landau Fermi liquid giving, for example, $\rho_{xx}(T) \simeq \rho_0 + aT^2$. Both of these are clearly in conflict with our finding of $(d\rho_{xx}/dT) < 0$ (Mooij correlation) over a wide T-scale, $T_c < T < 300$ K, well into the metallic side of the MIT. Moreover, in our finding the value $(z\nu)_{xx} = 1.5$ substantially differs from $(z\nu)_{xx} = 0.67$ [17] for a purely correlation driven Mott MIT.

Our findings raise the following fundamental issues: (i) what is the nature of this novel QCP? and (ii) what are the nature of the M- and I-phases? Since the QCP we find is closer in nature to that seen in MOSFETs [10], where $z\nu \simeq 1.6$, strong disorder (induced by Ti-doping) is dominant but interactions will also be important, especially near the MIT. At a minimalist level, we propose an effective, random Falicov-Kimball model (FKM) as a simplest model of the real (random) alloy. The FKM is isomorphic to the binary alloy Anderson disorder problem, wherein conduction c-fermions scatter off a random binary (since $Un_{id} = 0, U$) disorder potential created by the localized d-fermions. Within binary alloy analogy the model shows a continuous MIT of the band-splitting type [19] as the the disorder strength (U) crosses a critical value U_c. The FKM possesses a *local* Z_2 gauge symmetry, arising from the fact that the d-fermions number at *each* site is conserved: $[n_{i,d}, H_{FK}] = 0$ for each i. In the quantum disordered phase, the ground state is thus macroscopically degenerate in the thermodynamic limit, breaking Landau's first postulate (non-degeneracy of the ground state) and invalidating Fermi liquidity from the outset. In the regime $k_F l \simeq O(1)$ of relevance here, DMFT and cluster-DMFT approaches yield a metallic state composed of a superposition of lower- and upper Hubbard bands, with progressive deepening of the charge pseudogap near the MIT [19, 20]. The rigorous absence of d-fermion hopping implies no $c-d$ hybridization and total wipe-out of lattice Kondo screening, precluding low-T Landau Fermi liquidity. In this situation, transport is incoherent, and the high-T bad-metal behavior now persists down to $T = 0$ (in fact, the only scale, as in local quantum critical scenarios, is the temperature itself). The CDMFT studies of the FKM [21, 22] show clean quantum critical scaling of magneto-transport, with $(z\nu)_{xx} = 1.31 \simeq 4/3$ and $(z\nu)_{xy} = 3/4$, comparing very favorably with $(z\nu)_{xx} = 1.51$ and $(z\nu)_{xy} = 0.97$ found here. Furthermore, both $\rho_{xx}(T)$ and $R_H(T)$ were predicted to increase with decreasing T and roughly follow each other, precisely as seen here. Even more importantly, theoretical prediction of $0.6 < r < 0.8$ is also in very good accord with results here, where we find $0.7 < r < 0.9$. This wide accord strongly support a band-coalescing MIT of the "simplified Hubbard" or "binary alloy" model type in our system. Moreover, finding of $(z)_{xx} = 1, (\nu)_{xx} \simeq 4/3$ in CDMFT [21] versus $(z\nu)_{xx} = 1.51$ in $Nb_{1-x}Ti_xN$ accords with expectations from a percolation-driven, continuous MIT expected in the strong-disorder limit of a binary-alloy disorder problem [23]. Further, nanoscale electronic phase separation (EPS) is rigorously expected [24] on theoretical grounds in FKM or binary-alloy models. Our findings suggest that carrier dynamics occurs along percolative paths in a strongly inhomogeneous background (set by disorder).

In $Nb_{1-x}Ti_xN$, as in NbN, a transition to superconductivity (SC) at very low T prevents the observation of the QPT as $T \to 0$. Thus, it is not possible to monitor $\sigma_{xx}(\delta k_F l, T \to 0) = Ce^2/\hbar\xi_x \simeq (\delta k_F l)^{(\nu)_{xx}}$, to extract $(\nu)_{xx}$ (and hence $(z)_{xx}$) separately (see, however, Fig. **SI8**, where an analysis based on data for $T > 20$ K gives $(\nu)_{xx} = 1.17$ and $(z)_{xx} = 1.2$. We cannot exclude that these values will change if the SC could be destroyed by a magnetic field). Studying the electric-field (E)-driven MIT [25] should resolve this issue: this is because, at low T, $\rho_{xx}(E, \delta k_F l)$ would depend only on $\frac{\delta k_F l}{E^{1/(z+1)\nu}}$, since the electric field introduces a new length scale, $L_E \simeq E^{-1/(z+1)}$, and as long as this is smaller than $L_T \simeq T^{-1/z}$, E-field scaling will be obtained even in presence of heating effects [25]. Used together with our results here it would allow an estimation of $(z)_{xx}$ and $(\nu)_{xx}$ separately: this is clearly a direction for future experiments.

Our findings strongly link the superconductor-insulator transition (SIT) in $Nb_{1-x}Ti_xN$ to an underlying QCP associated with a *fermionic* MIT. This has deeper implications for the nature of the SC instability, implying the need to go beyond purely bosonic descriptions of the SIT by incorporating critical fermionic dynamics at a fermionic MIT seen here. Since the very bad metal is associated with a finite residual entropy ($O(\ln 2)$ per site in the FKM or binary alloy model), at least in quasi-local approaches, it seems that SC emerges as the *only* coherence-restoring instability (since competing instabilities to Wigner crystal/charge-density-wave, etc. will be inhibited by strong disorder-induced nanoscale inhomogeneity) that can quench this entropy as $T \to 0$. In the critical regime ($k_F l \simeq 1.0$), such a SC must have a short pair-coherence length, $\xi_{pair} \simeq l \simeq O(a)$, a the lattice spacing and, in fact, percolative dynamics in a nanoscale EPS state also imply a strong phase fluctuation dominated SIT. This fully accords with earlier work [26]. Our work suggests that the non-trivial interplay between such critical dynamical fluctuations near the MIT with onset of two-particle pair coherence in the SC phase is a crucial controlling factor influencing the nature of the SIT itself in such systems, and mandates incorporating this link into extant theories of the SIT, at least for such systems.

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