Bad metallic transport in a modified Hubbard model

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Introduction to the Mott Ioffe Regel limit

- The Mott-Ioffe-Regel (MIR) limit [cf. Ioffe & Regel 60] upper bounds the scattering rate:

$$\text{Mean free path lower bound: } l_{mfp} > a \tag{1}$$

$$\text{Scattering rate upper bound: } \Gamma_{scatt}(l_{mfp}) < \Gamma_{scatt}(a) \tag{2}$$

where l_{mfp} is the the mean free path.

- Therefore, the MIR limit upper bounds the resistivity $\rho \sim \Gamma_{scatt}$!

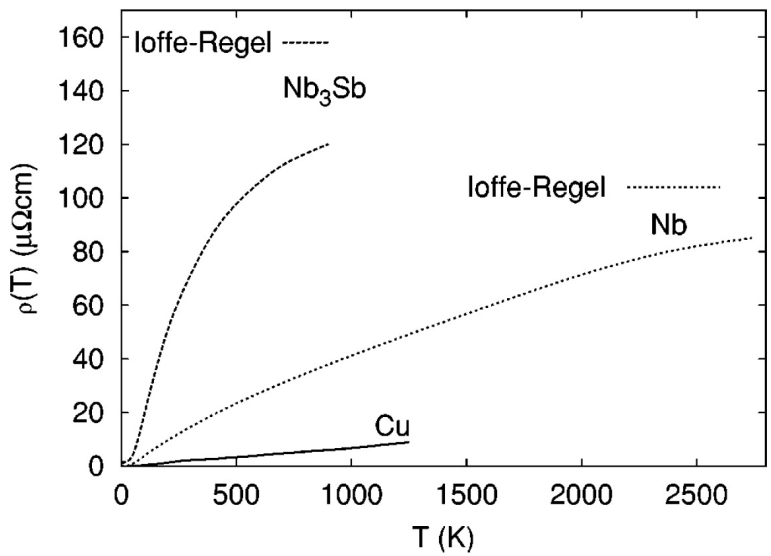


Figure: Conventional metals have a resistivity ρ that saturates below the MIR limit [cf. Gunnarsson et al. 05]

Introduction to bad metals

- Bad metals have resistivities which increase with temperature above the MIR limit.
- Bad metals are frequently found in strongly correlated systems (ex. normal state of high-T_c superconductors)

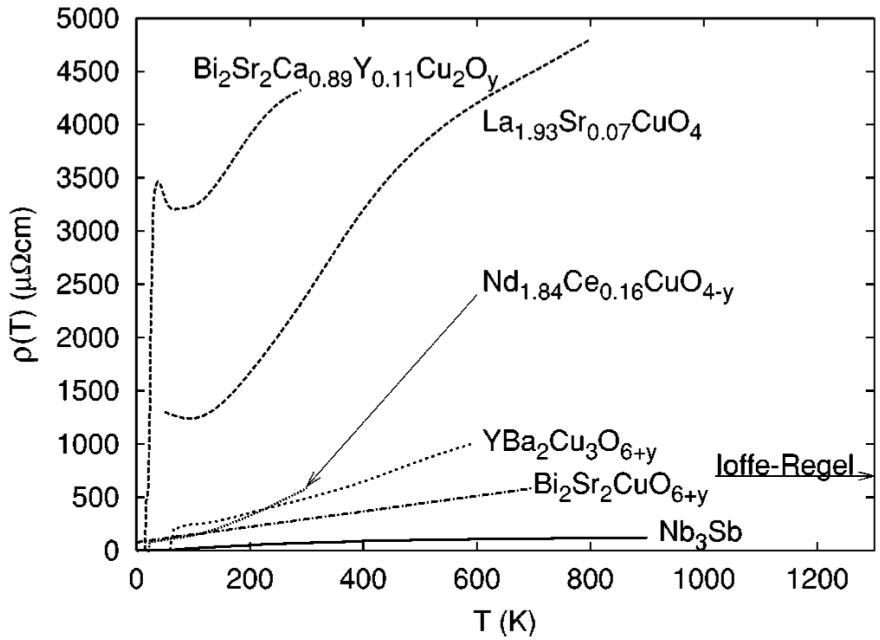


Figure: Bad metals have resistivity ρ increase well above the MIR limit. [cf. Gunnarsson et al. 05]

Past theoretical and numerical approaches to bad metals

- Most work to understand bad metals fall under the categories of:

$\rightarrow$ large-N expansions,

$\rightarrow$ dynamical mean field theory (DMFT),

$\rightarrow$ quantum Monte Carlo (QMC)

- *Our objective:* We want a realistic, yet solvable, model for bad metals that avoids introducing artificial control parameters.

Perturbative treatment of the Hubbard model, $t \ll U$ [cf. Mukerjee et al. 05]

- Quasiparticles are ill-defined, so working with itinerant electrons in momentum space is unnatural.
- *Let's work with the polar opposite of Fermi liquid theory*, where e-e interaction energies are much larger than the hopping:

$$H = H_t + H_U, \tag{3}$$

$$H_t = t \sum_{\langle i,j \rangle s} c_{is}^\dagger c_{js}, \tag{4}$$

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{5}$$

$$\text{limit: } t \ll U, kT \tag{6}$$

- Can we do perturbation theory in the hopping t?

Hubbard model at low-t [cf. Mukerjee et al. 07, Beni et al 74]

- Perturbation theory in t is trivially tractable:

$\rightarrow$ The thermal ensemble lies in the occupation number basis

$$e^{-\beta H} \approx e^{-\beta H_U} \tag{7}$$

$\rightarrow$ All sites are uncorrelated

$$\mathcal{Z} = z^N \tag{8}$$

where z is the single site partition function.

- An analytically tractable model for a strongly correlated electron system is *rare*. What can we calculate?

Hubbard model at low-t: transport and thermodynamics

- All conductivities diverge:

$$\sigma(\omega) = D_0\delta(\omega) + \sum_{\pm} D_{\pm}\delta(\omega \pm U), \tag{9}$$

$$D_0(n, T) \propto \frac{t^2}{T} n(2-n) \text{ for } T \gg U \tag{10}$$

- Thermodynamics show symptoms of massive energy degeneracy:

$$\text{Schottky anomaly: } c_n = (\beta U)^2 e^{-\beta U}, \tag{11}$$

$$\text{Compressibility diverges: } \chi \to \infty \text{ for } T \to 0 \tag{12}$$

- H_U is hugely degenerate! The perturbation theory is sick.
- Can we resolve the degeneracy while keeping the model solvable?

Introduce interactions between different sites

- Add an interaction term that can resolve the degeneracies:

$$H = H_t + H_U + H_V, \tag{13}$$

$$H_V \equiv \sum_{\langle i,j \rangle} V(|i-j|) n_i n_j, \tag{14}$$

$$t \ll T, U, V \tag{15}$$

- The thermal ensemble lives in the occupation number basis $\{n_{is}\}$:

$$\text{Thermal probability distribution: } \frac{e^{-\beta H}}{\mathcal{Z}} \approx \frac{e^{-\beta(H_U+H_V)}}{\mathcal{Z}} \tag{16}$$

- Classical Monte Carlo can easily generate a representative thermal ensemble for us!

A typical configuration in the thermal ensemble

- In numerical simulations: $V(r) = Ve^{-r/l}$, $l = 2a$ and $V = 0.1U$
- The single-particle energy due to interactions is

$$\epsilon_{is} = Un_{i,-s} + \sum_{j \neq i} V(|i-j|)n_j. \tag{17}$$

- The massive degeneracy has been lifted. We can now safely work perturbatively in $\frac{t}{T}$.

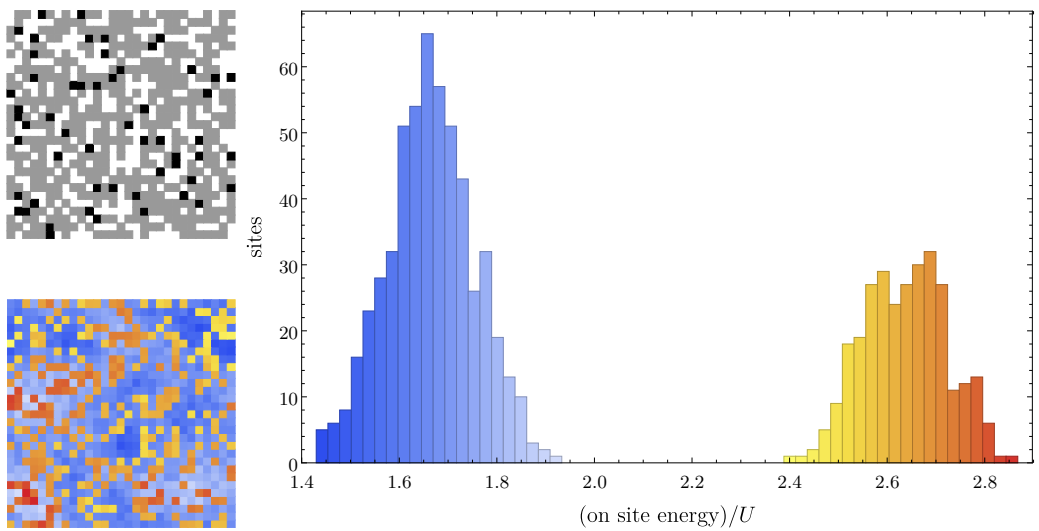


Figure: *Upper left*: state configuration (n=0.62, kT=0.5). *Lower left*: on-site potentials $\epsilon_{i\uparrow}$. *Right*: histogram of $\epsilon_{i\uparrow}$

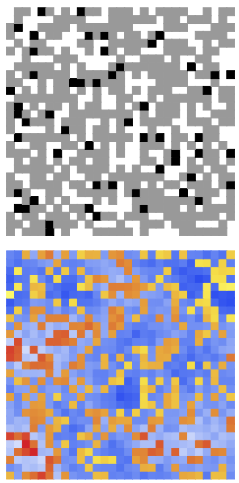
Transport equations

- The Kubo formula in our perturbative-in-t model reduces to:

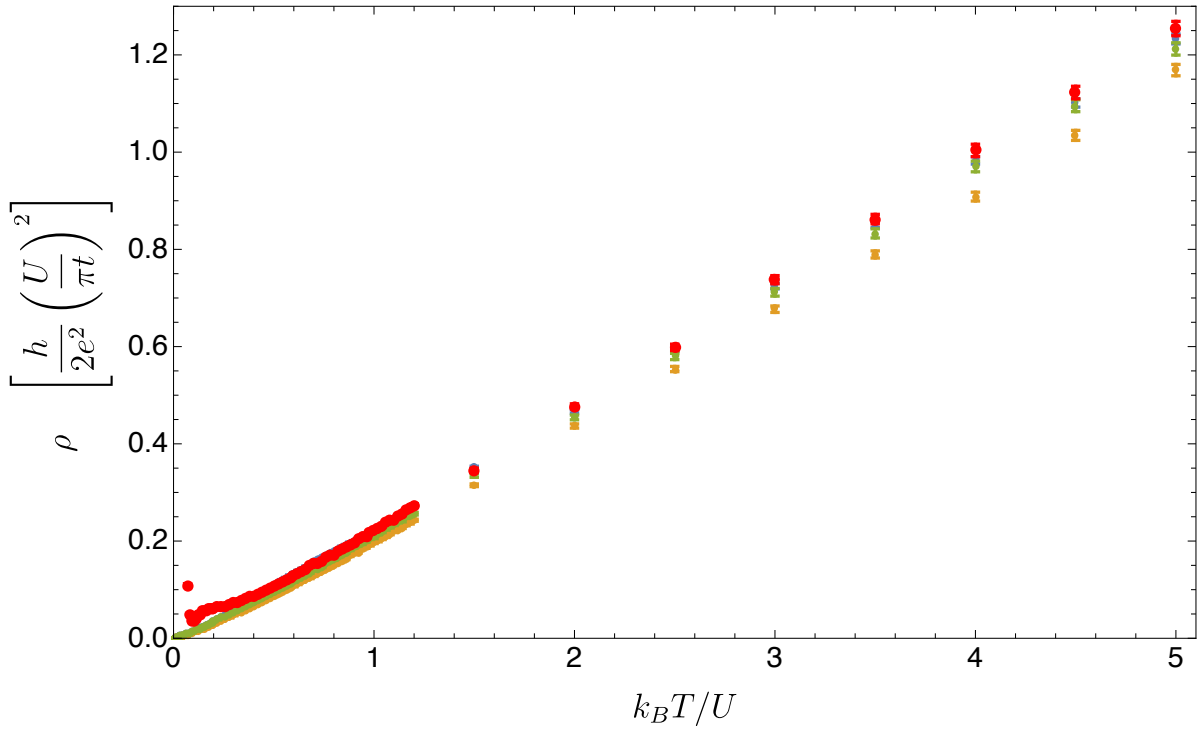
$$\mathrm{Re}\sigma(\omega) \sim e^2 t^2 \sum_{\{n\}} \frac{e^{-\beta(E_{\{n\}}-\mu N)}}{\mathcal{Z}} \sum_{i,s} \Delta_{is}(\omega) + \mathcal{O}(t^4), \tag{18}$$

$$\Delta_{is}(\omega) = \delta(\omega - (\epsilon_{i,s} - \epsilon_{i-1,s}))n_{i-1,s}(1 - n_{i,s}) + \cdots \tag{19}$$

- $\Delta_{is}(\omega)$ can be calculated from ϵ_{is} and n_{is} in classical MC!
- Transport is controlled by local hops! DC conductivity comes from hops at resonant spots where $\epsilon_{i,s} - \epsilon_{i-1,s} \to 0$



A bad metal with linear-in-T resistivity



- *Why does $\rho \sim T$? Why is this a bad metal? Is this just classical, infinite temperature physics?*
- A simple model allows us to answer these questions!

Two bad metallic phases [cf. Perepelitsky et al. 16]

- Charge undergoes diffusive transport.

$$\rho \approx \frac{1}{D_{ch}} \cdot \frac{1}{\chi}. \tag{20}$$

- There is an infinite temperature ($T > U$) and an intermediate temperature ($t < T < U$) bad metallic phase!

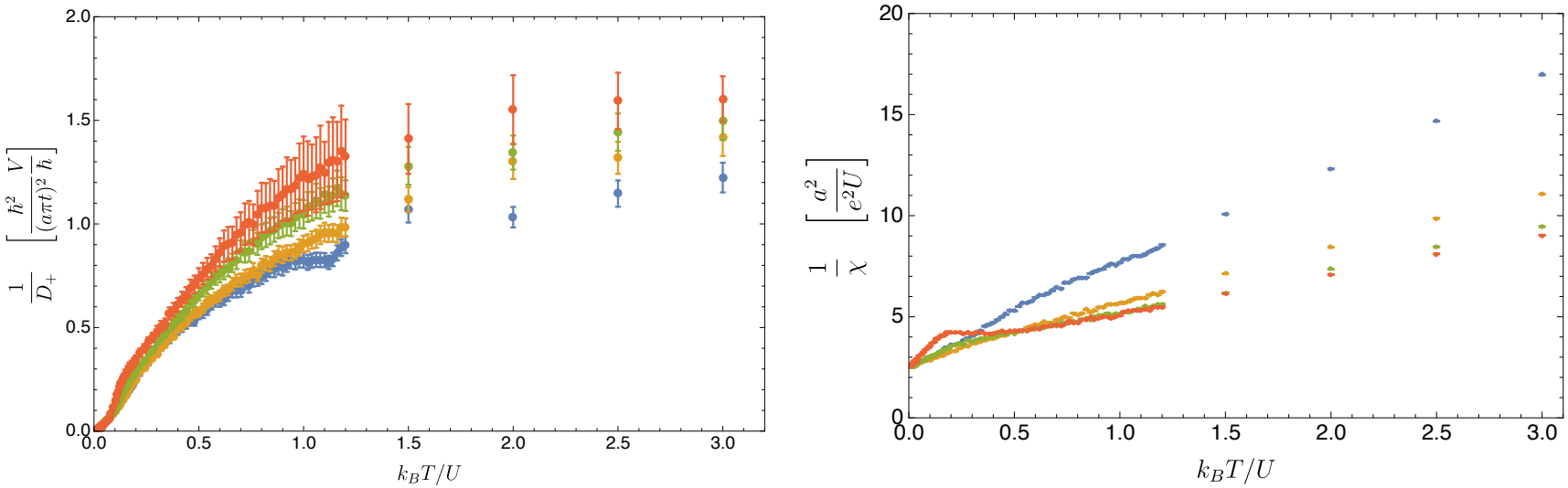


Figure: *Left*: Inverse charge diffusion $D_{ch}^{-1}(T)$. *Right*: Inverse charge compressibility $\chi^{-1}(T)$ for fillings $n = 0.25, 0.5, 0.75, 0.9$.

Source of linear-in-T resistivity

- For temperatures $k_B T \gg t$, the kinetic energy $K.E. \sim \frac{t^2}{T}$.
- The resistivity

$$\rho = \frac{1}{\mathcal{D}} \cdot \frac{1}{\tau} \tag{21}$$

where $\mathcal{D} \sim$ K.E. is the "Drude weight" of the central conductance peak, and τ is the transport lifetime.

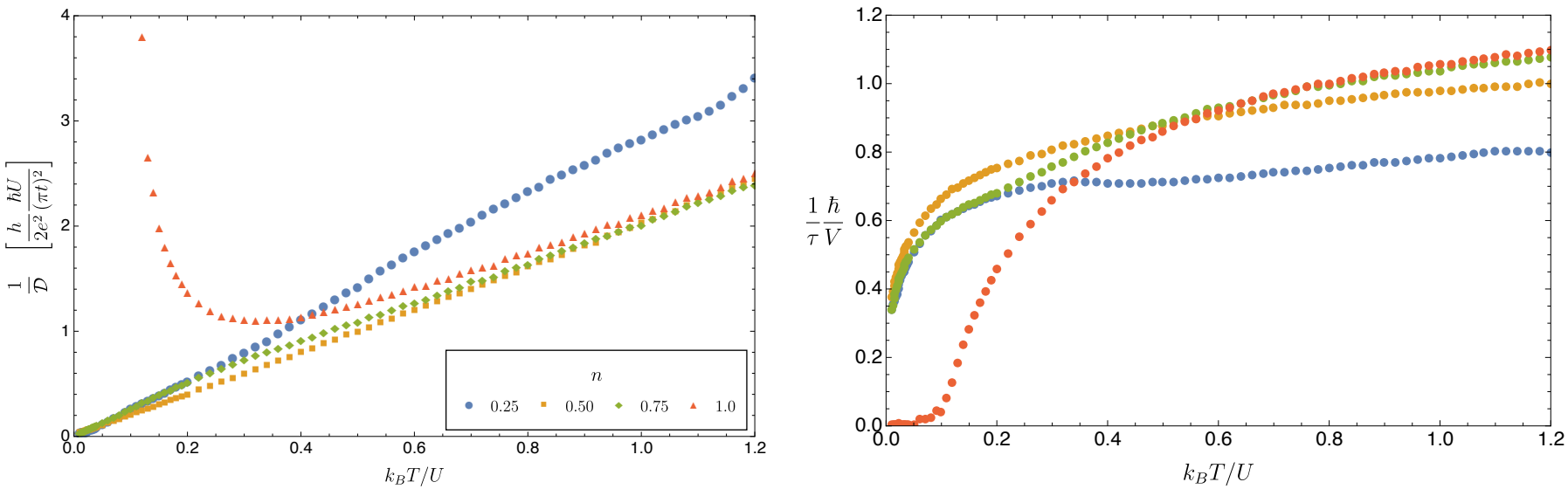
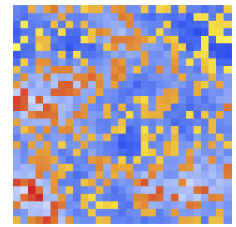


Figure: *Left*: inverse Drude weight, *Right*: inverse current lifetime, Γ_{curr}

Transport through an effective disorder landscape

- A toy picture of transport will help us understand the bad metal
- Let's call this map an effective disorder landscape.



- The disorder landscape changes adiabatically slowly:

$$\text{time for an electron to hop:} \quad \sim \frac{\hbar}{t} \tag{22}$$

$$\text{time for current to decay:} \quad \sim \frac{\hbar}{U}, \tag{23}$$

$$\text{landscape changes very slowly:} \quad \frac{\hbar}{t} \gg \frac{\hbar}{U} \tag{24}$$

- Any local current decays rapidly.

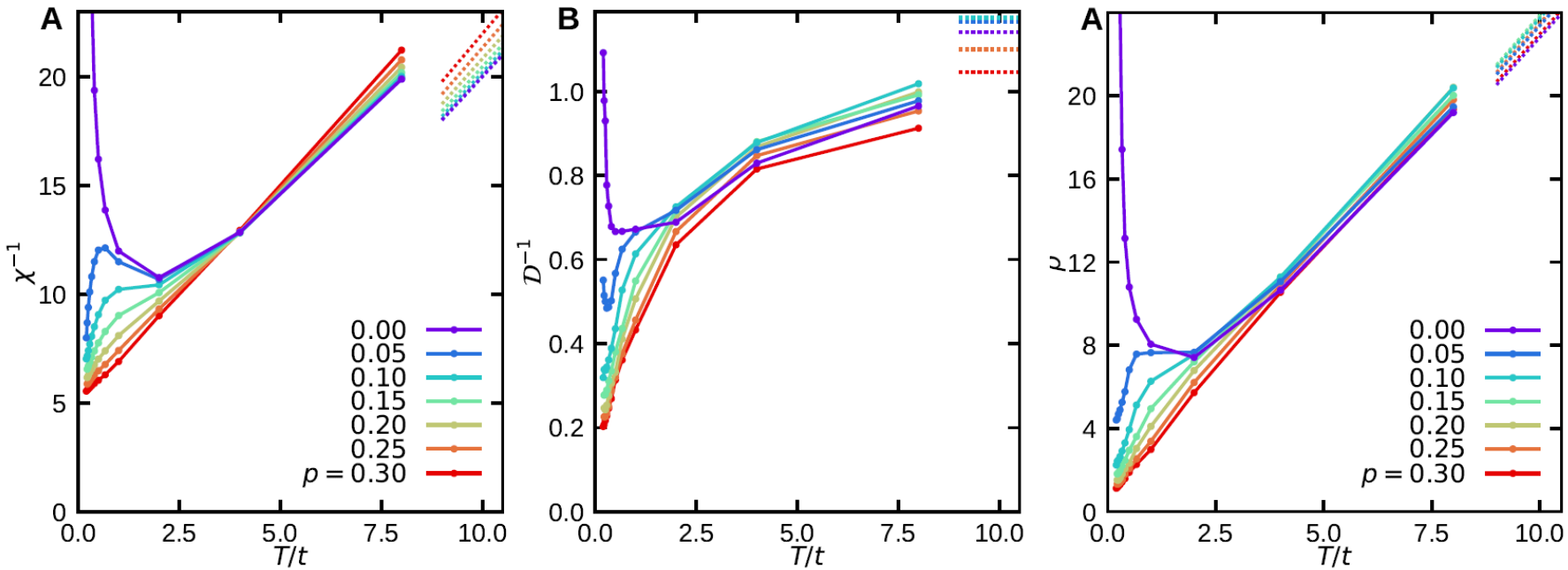
Non-quasiparticle transport and bad metals

• The MIR argument does not apply for non-QP transport. The theoretical challenge is understanding the physical source of this non-QP transport.

• *In our model:* The electrons *want* to Anderson localize because they're in strong disorder! They can't because the disorder landscape is (slowly) dynamical.

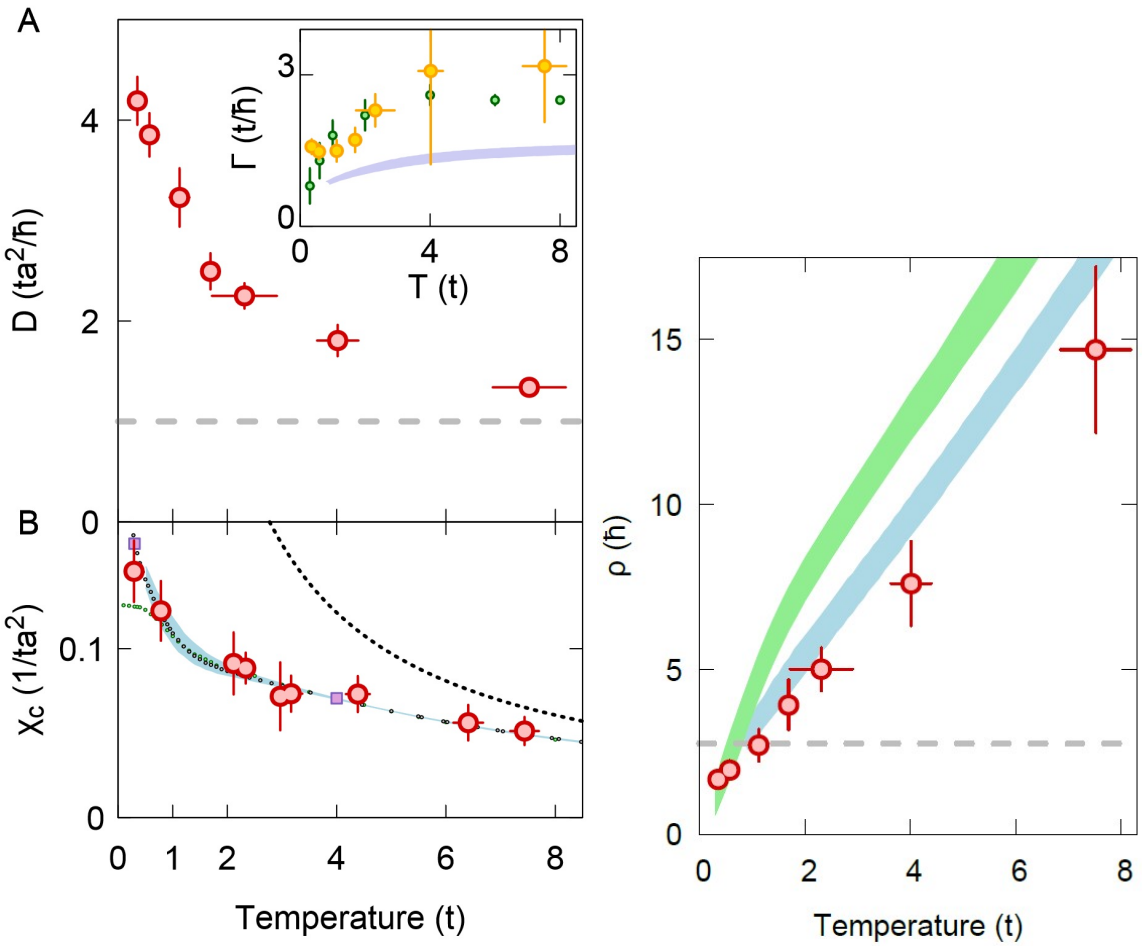
• *One possible direction* to look for more theoretical models for bad metals is to look for a "failed" insulator!

Comparison with Quantum Monte Carlo



- [E. Hwang and coworkers] ran QMC simulations of the Hubbard model with $U = 6t$ and $t' = -0.25t$.

Comparison with cold atoms experiment



- [P. Brown and coworkers] ran cold atom simulations of the Hubbard model with $U = 7.4t$.

Comparison with strongly correlated thermoelectrics

- Our model exhibits :

$\rightarrow$ large thermopower $|S| = \frac{\alpha}{\sigma} = \mathcal{O}(\frac{k_B}{e})$,

$\rightarrow$ small Lorenz ratio $L = \frac{\kappa}{\sigma T}$,

$\rightarrow$ large thermoelectric figure of merit $zT \equiv \frac{S^2}{L}$.

- Vanadium dioxide VO_2 [cf. Lee et al. 17] is a bad metal with linear-in-T resistivity and the same thermoelectric properties.

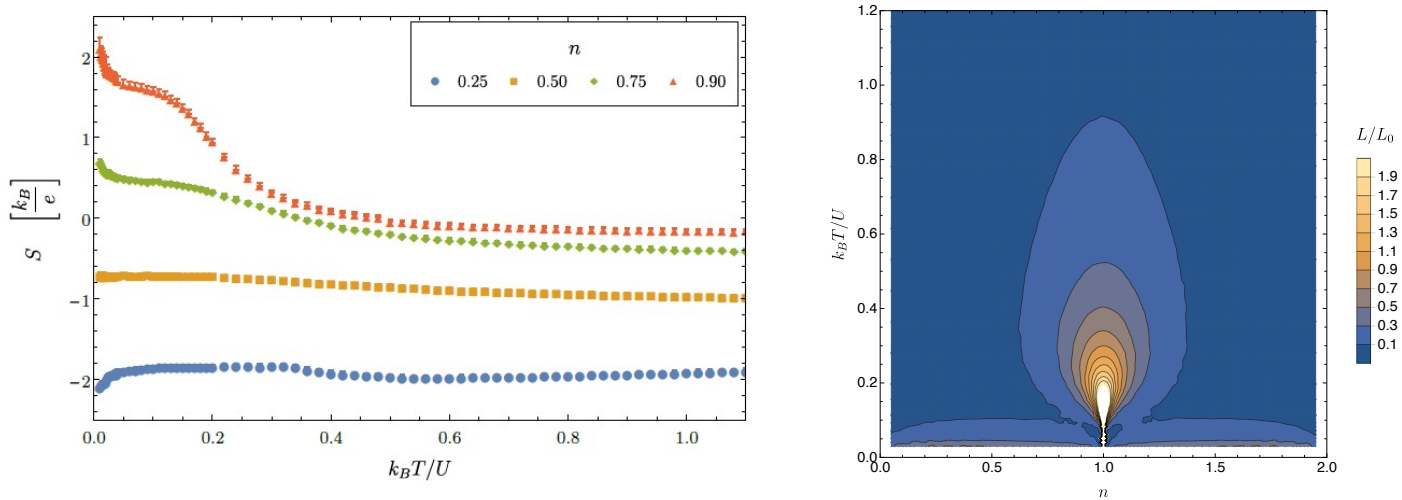


Figure: *Left:* Thermopower S vs $k_B T$, *Right:* contour plot of the Lorenz ratio L

Connection with other theoretical models

- Most theoretical work on bad metals utilizes a large-N approximation (ex. coupled SYK sites, electron-phonon models, DMFT).
- While large-N is a calculational tool, it also introduces an interesting physical feature – an inert bath to decay momentum rapidly.
- In our model, each electron interacts with a large number of nearby, nearly static electrons through H_V. These electrons act like an inert bath, forming a disorder landscape to rapidly degrade current.

Conclusions

• We have a simple, solvable model for a bad metal, with electrons hopping locally through an effective interaction-induced disorder landscape. It behaves like a "failed" insulator.
• Our theory agrees well with results from cold atom experiments, Quantum monte carlo simulations, and strongly correlated thermoelectrics like VO_2.