Transport and spectra in the half-filled Hubbard model

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Promises

1. Hubbard model and half-filling
2. Dynamical mean-field theory (DMFT) + iterated perturbation theory (IPT)
3. Benchmark: Mott transition
4. Resistivity: Comparison with expt. $NiS_{2-x}Se_x$
5. Resistivity: Thermal hysteresis Cr-doped V_2O_3
6. Why thermal hysteresis?
7. Further investigation: Avalanches
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Hubbard model and half-filling

Minimal model to depict correlation effect: competition between kinetic/hopping (t_{ij}) and on-site (local) Coulomb repulsion U

Single-band Hubbard Hamiltonian:

$$\hat{H} = -\sum_{<ij>,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{h.}c.) + \epsilon_d \sum_{i\sigma} c^{\dagger}_{i\sigma}c_{i\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} \quad (1)$$

$\epsilon_d \Rightarrow$ Orbital energy
$c^{\dagger}_{i\sigma}(c_{i\sigma}) \Rightarrow$ creates (annihilates) an e^- of spin σ at site i

Half-filled when one electron per site: $< n_i >= 1 \Rightarrow \epsilon_d = -U/2$

Exact solution not available except in 1D (*Lieb and Wu, 1968*).

Dynamical mean-field theory (DMFT)

- Write an effective action in term of mean-field single-site Green's function $\mathcal{G}$ at site-0

$$S_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c^\dagger_{0\sigma}(\tau)\mathcal{G}_0{}^{-1}(\tau-\tau')c_{0\sigma}(\tau') + U\int_0^\beta d\tau\, n_{0\uparrow}(\tau)n_{0\downarrow}(\tau) \quad (2)$$

- Lattice problem maps on to a self-consistent single-impurity problem $\Rightarrow$ mean-field since spatial degrees of freedom integrated out.
- Dynamic since temporal information retained through τ, τ'.
- Exact mapping in the limit of ∞ coordination number z (or ∞ dimension) as the hopping amplitude t_{ij} is scaled as $t_*/\sqrt{z}$.
- Self-energy and vertex function becomes momentum $\mathbf{k}$ independent.

DMFT: Implementation

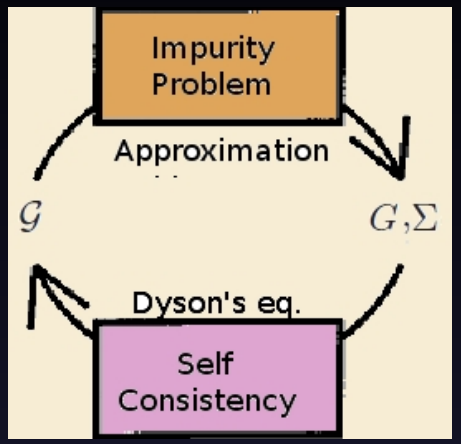
General

i) guess $\mathcal{G}$ or Σ

ii) impurity problem solver (IPS) $\Rightarrow \Sigma$ & G

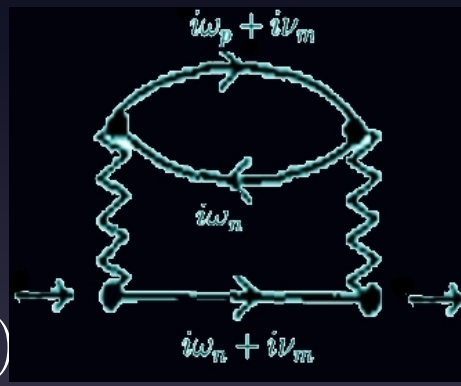
iii) Calc. $\mathcal{G}$ from Dyson's eq.

iv) Repeat ii)-iii) until self-consistency achieved.



Our IPS:

Iterated perturbation theory (IPT) approx: (2nd order about Hartree term).



$$\Sigma_2(\omega) = \lim_{i\omega\to\omega^+} \frac{U^2}{\beta^2} \sum_{m,p} \mathcal{G}(i\omega+i\nu_m)\mathcal{G}(i\omega_p+i\nu_m)\mathcal{G}(i\omega_p)$$

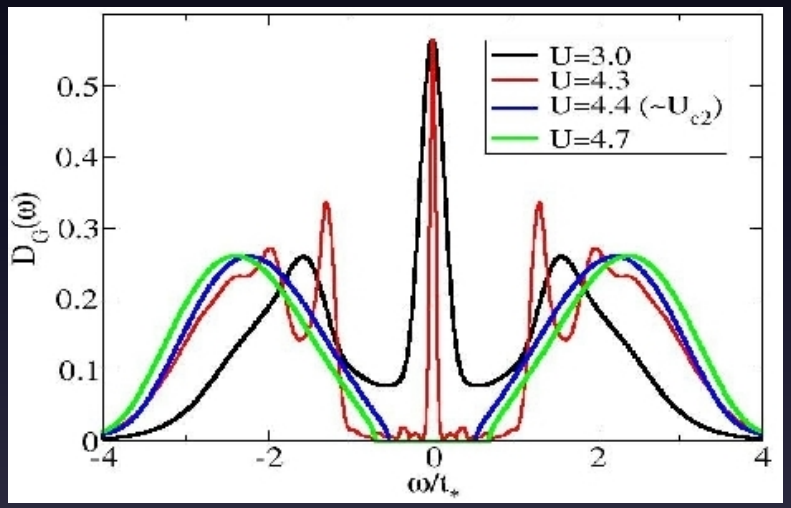
Specific

- Real freq. approach in contrast to conventional Matsubara freq. approach
- Major advantages: can capture $T = 0$ features and avoid rigor of analytical continuation

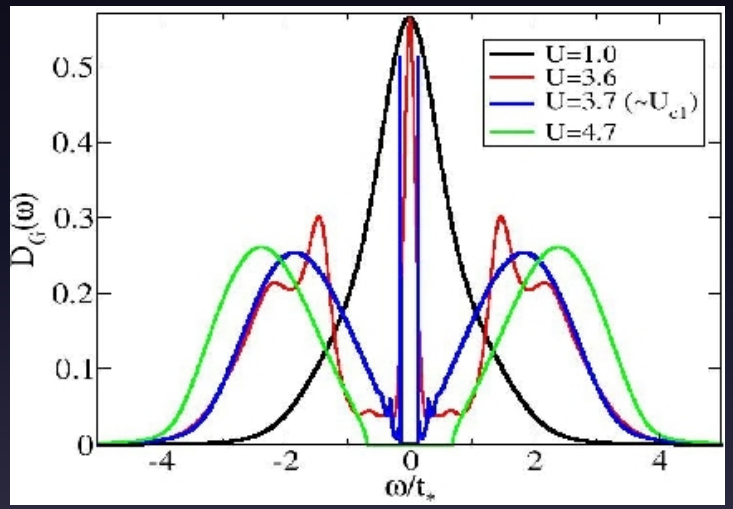
3 Benchmark: Mott transition at $T = 0$

Spectral function=$-\frac{1}{\pi}\mathrm{Im}G(\omega)$

U increasing



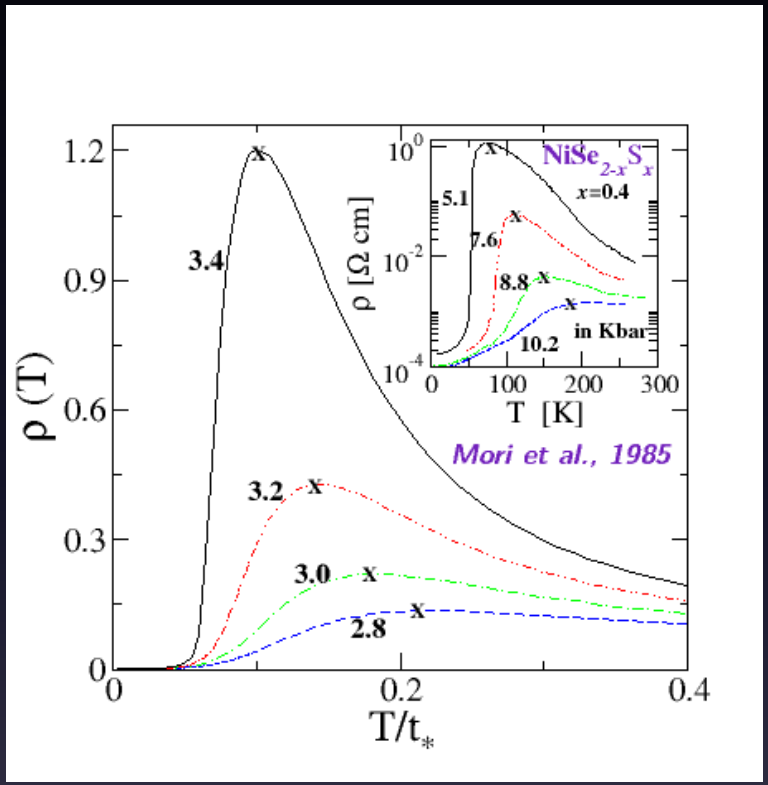
U decreasing

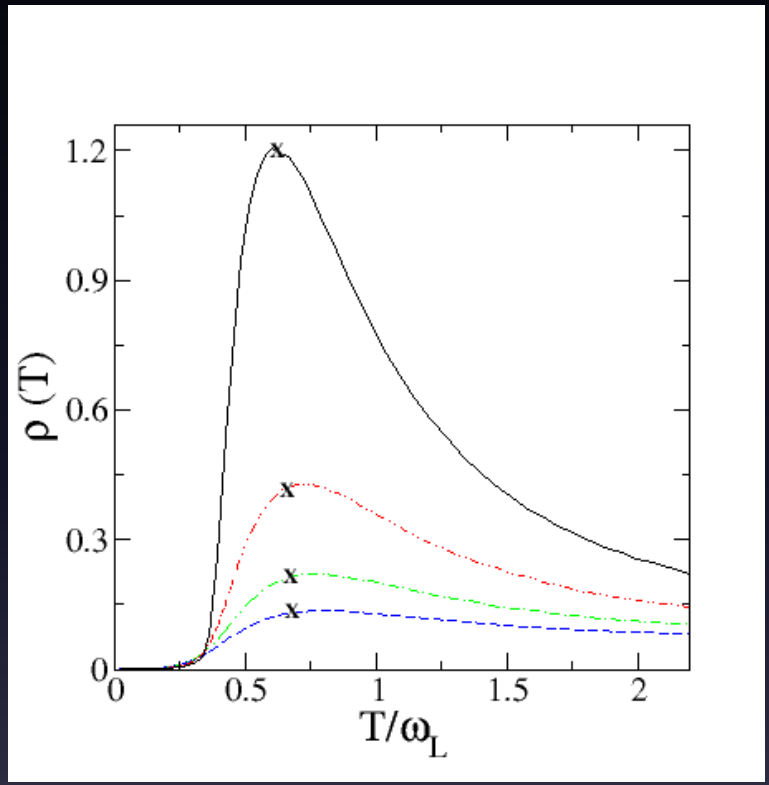


Expected Mott metal-insulator transition observed.

Different transition points U_{c1} and U_{c2}: Hysteresis

Resistivity: expt. on $NiS_{2-x}Se_x$

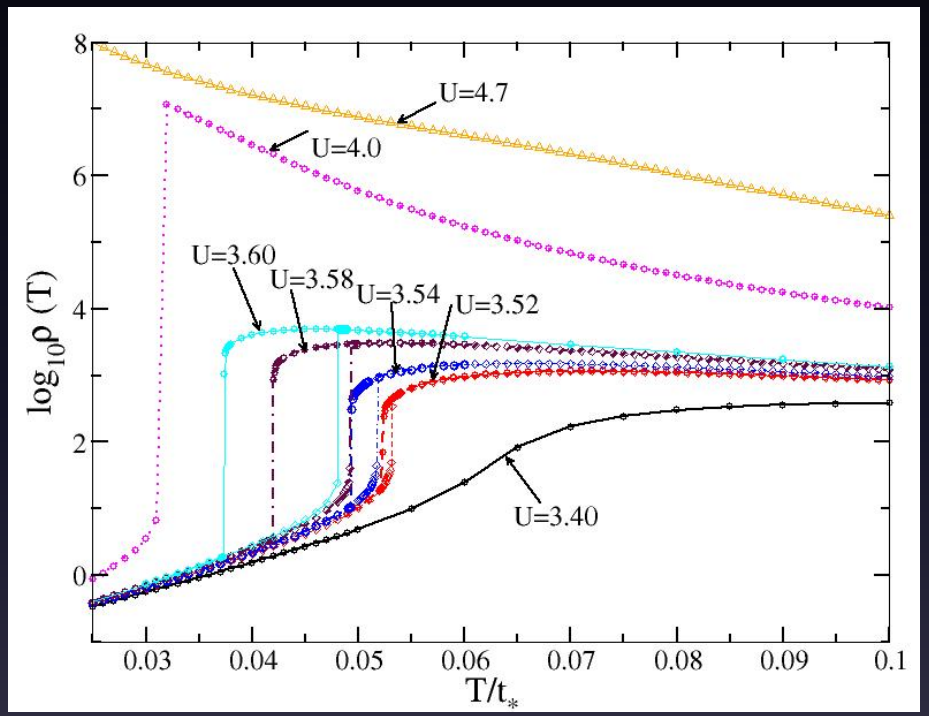


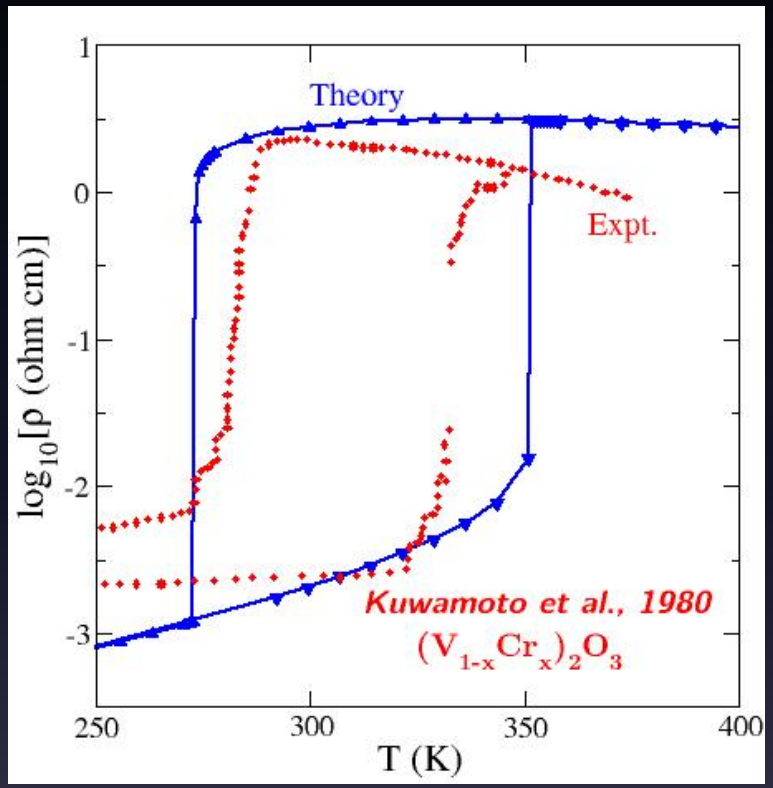


$\omega_L = Zt_*$, Z=quasiparticle residue

'Coherent' peak features governed by the associated low-E scale.

Thermal hysteresis, V_2O_3

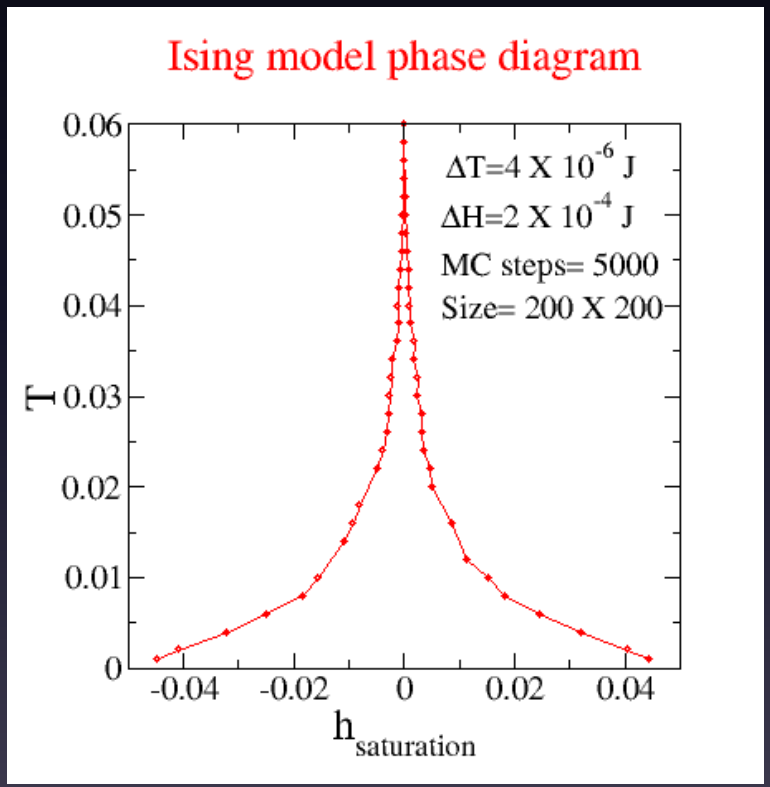


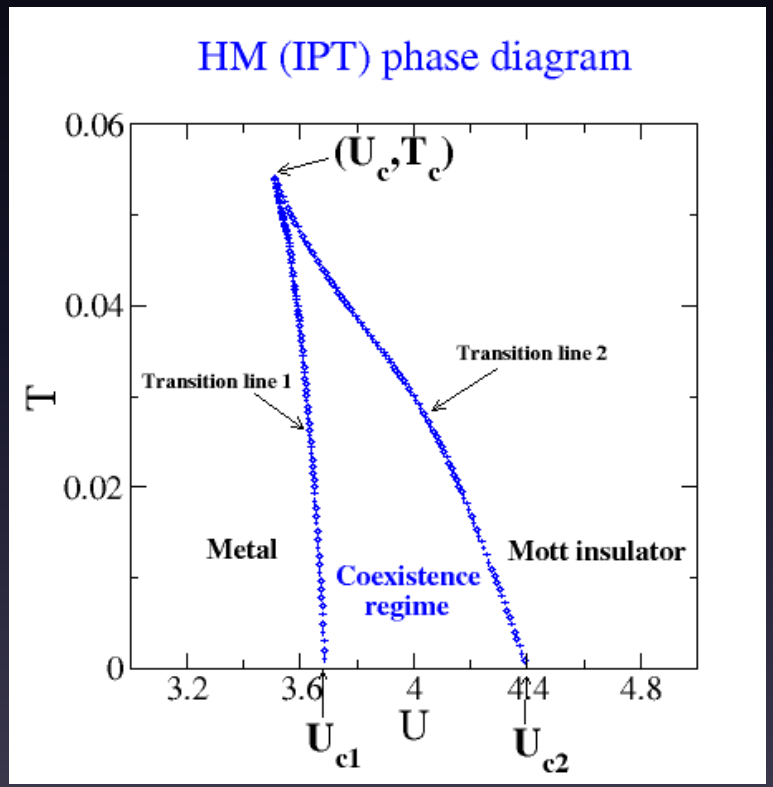


$U = 3.6t_*$ gives $t_* = 0.63$ eV ($\sim$ first-principle value)

Why thermal hysteresis?

Phase diagram geometry plays a role.

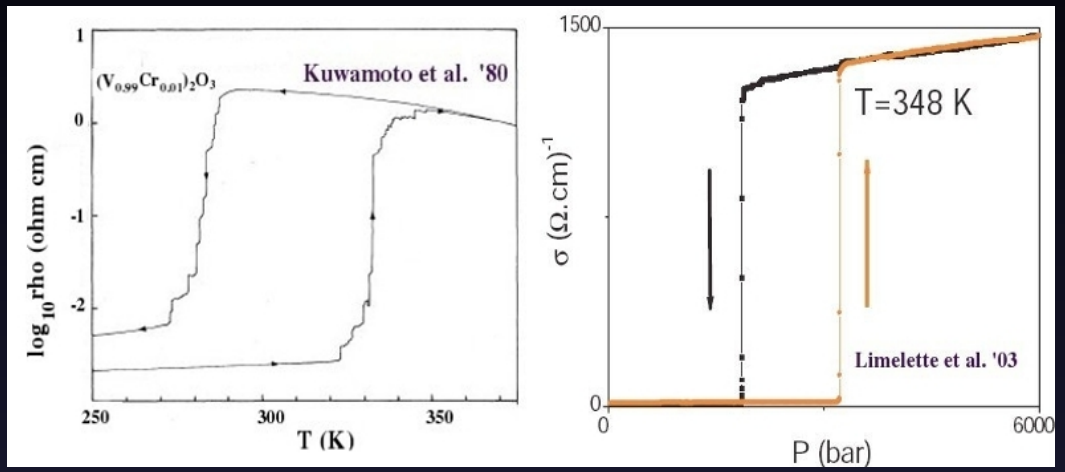


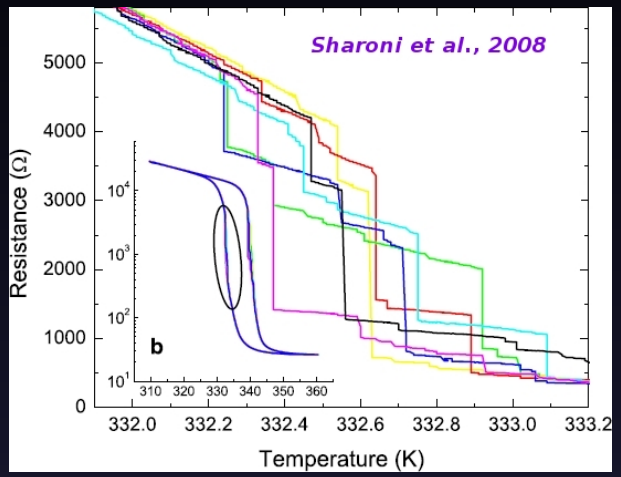


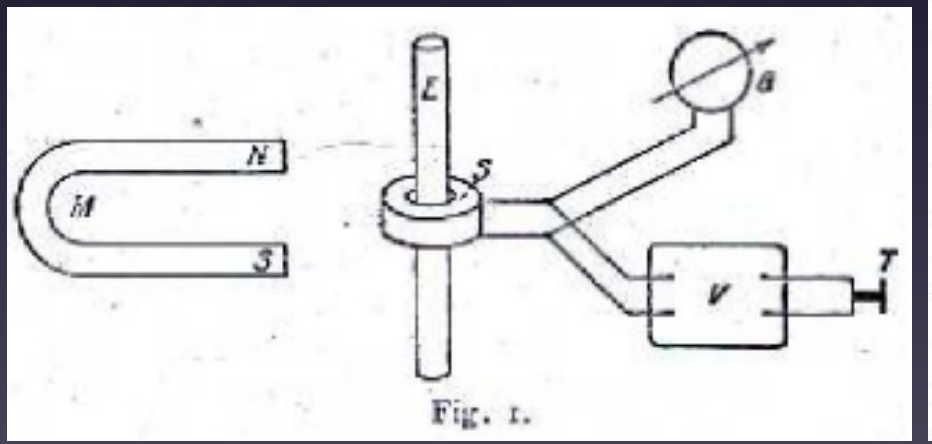
Hysteresis occurs only when both spinodal lines are crossed.

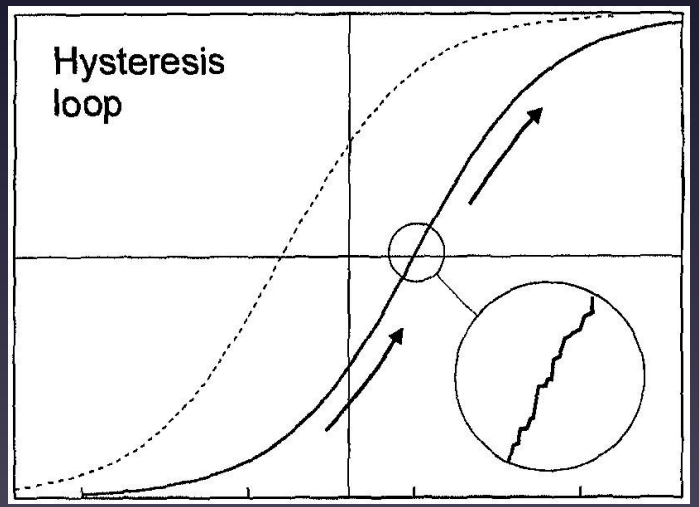
Further investigation

Avalanches, Barkhausen noise





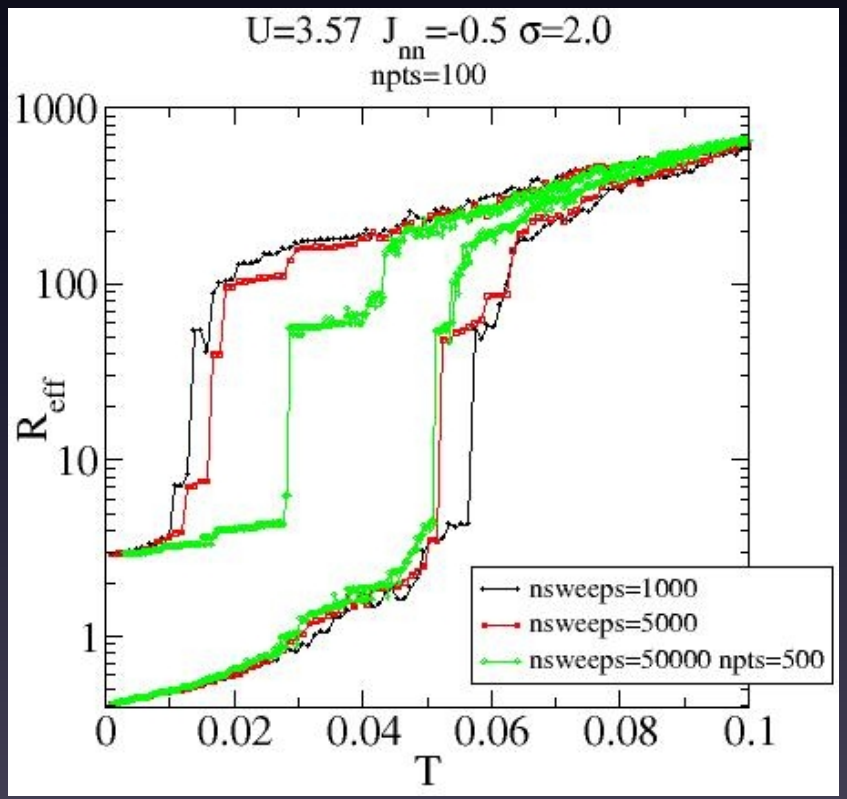


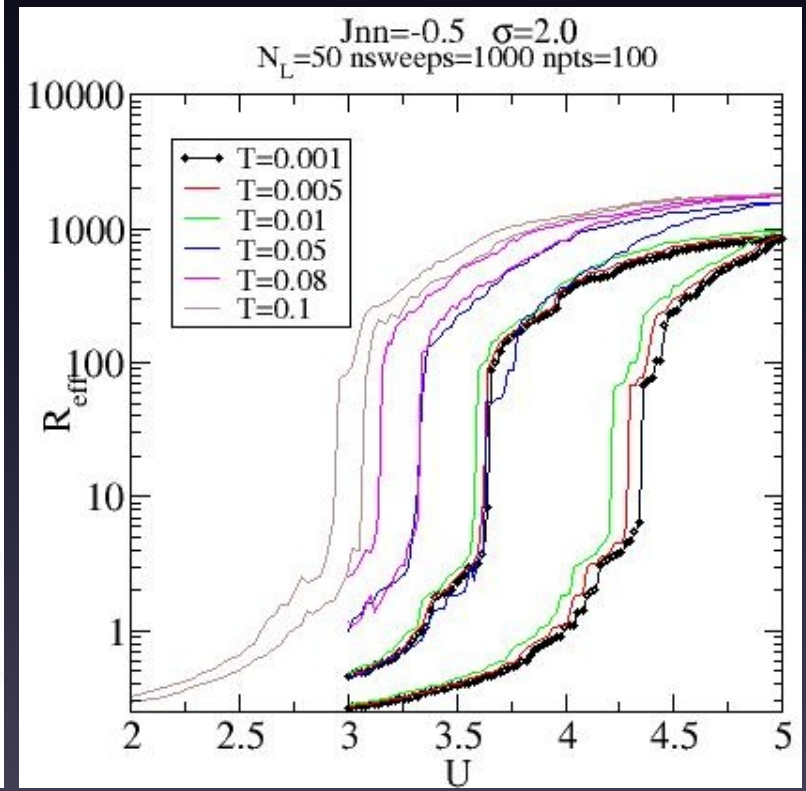


Further investigation

Random Resistor Network model to Random-field Ising model (RRNM+RFIM)

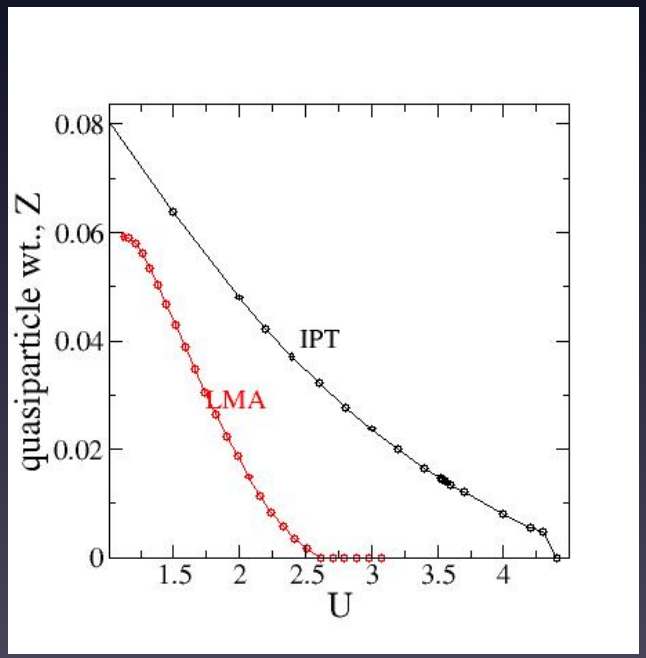
Reason for such mapping: Kotliar ’99, Kirkpatrick and Belitz ’95, Limelette et al. ’03, Papanikolaou et al. ’08 (Ising university class)

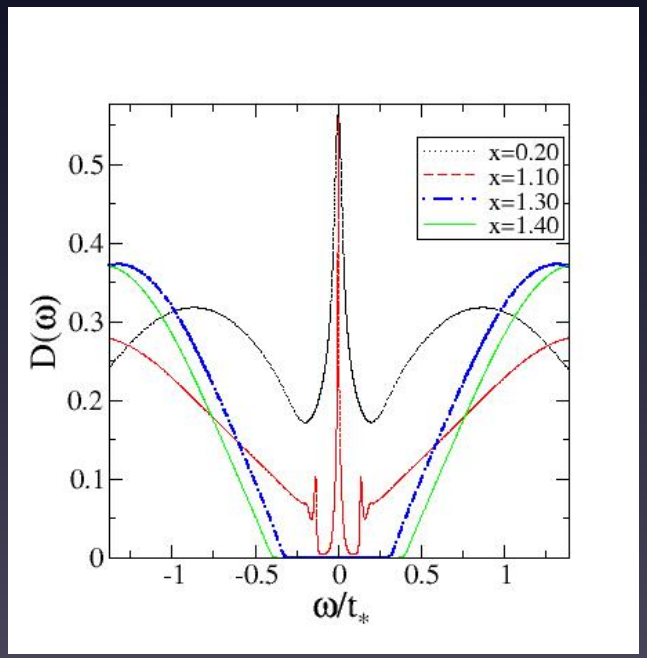




Beyond IPT: Local moment approach (LMA)

- Based on unrestricted Hartree fock (UHF) host Green's function (*Cf.* restricted-HF for IPT).
- Fermi liquid metal obtained by restoring back the broken symmetry.
- Can promise to capture the low-energy scale at strong-coupling (U close to MIT) when the polarization propagators considered in the self-energy.





Summary

- Hubbard model is the minimal model to describe the Mott physics and features can be realized through. DMFT+ impurity problem solver (IPS).
- IPT is such an IPS (approximate), yields MIT with 2 transition pt.s U_{c1} and U_{c2}.
- Universality in the resistivity peak when scaled by low-energy Fermi liquid scale.
- IPT can mimic the thermal hysteresis observed in real materials, e.g. V_2O_3. Can be understood by geometry of the phase diagram.
- However, DMFT misses the avalanches phenomena. Can be realised through RRNM+RFIM based models.
- To capture the strong-coupling behaviour other IPS, e.g. LMA could be a potential candidate.

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