BPU11 CONGRESS
SASA, Belgrade 30/08/2022

Transport in strongly correlated systems: the Hubbard model perspective

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Hanna Terletska (FSU at the time)
Marcelo Rozenberg (LPS)
Ana Vranić (IPB)

Resistivity calculations in 2D

J. Vučičević, S. Predin, M. Ferrero, arXiv:2208.04047 (2022)

A. Vranić, J. Vučičević, J. Kokalj, J. Skolimowski, R. Žitko, J. Mravlje, D. Tanasković, Phys. Rev. B **102**, 115142 (2020)

J. Vučičević, J. Kokalj, R. Žitko, N. Wentzell, D. Tanasković, J. Mravlje, Phys. Rev. Lett. **123**, 036601 (2019)

Resistivity in the presence of perpendicular magnetic field

J. Vučičević, R. Žitko, Phys. Rev. Lett. 127, 196601 (2021)

J. Vučičević, R. Žitko, Phys. Rev. B **104**, 205101 (2021)

Method development: real-frequency diagrammatic Monte Carlo

J. Vučičević, P. Stipsić, M. Ferrero, Phys. Rev. Research **3**, 023082 (2021)

J. Vučičević, M. Ferrero, Phys. Rev. B **101**, 075113 (2020)

Quantum critical scaling of resistivity in inifinite dimensions

J. Vučičević, D. Tanasković, M. Rozenberg, V. Dobrosavljević, Phys. Rev. Lett. **114**, 246402 (2015)

J. Vučičević, H. Terletska, D. Tanasković, V. Dobrosavljević, Phys. Rev. B **88**, 075143 (2013)

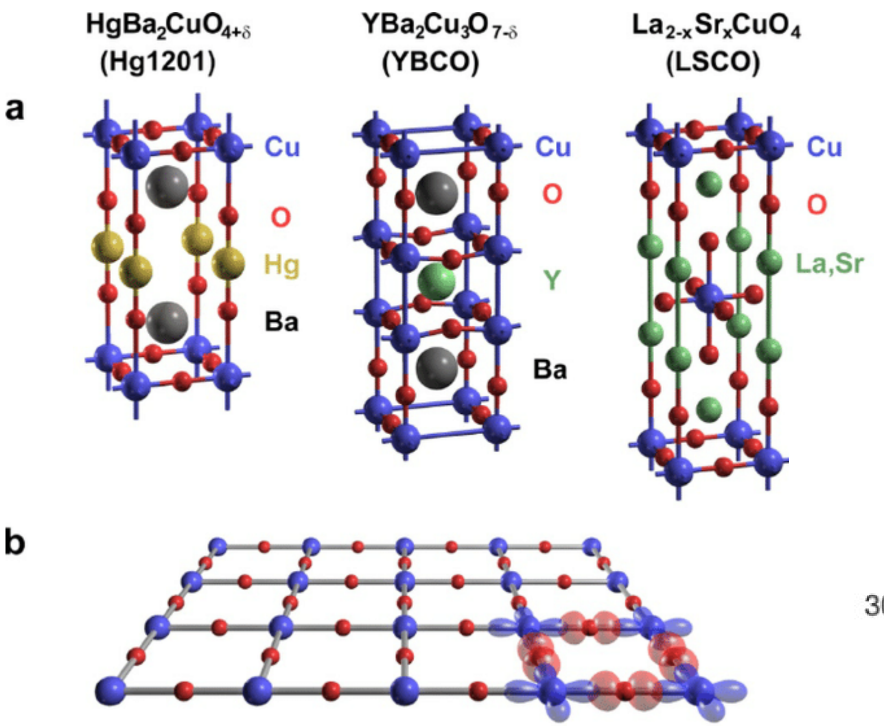
H. Terletska, J. Vučičević, D. Tanasković, V. Dobrosavljević, Phys. Rev. Lett. **107**, 026401 (2011)

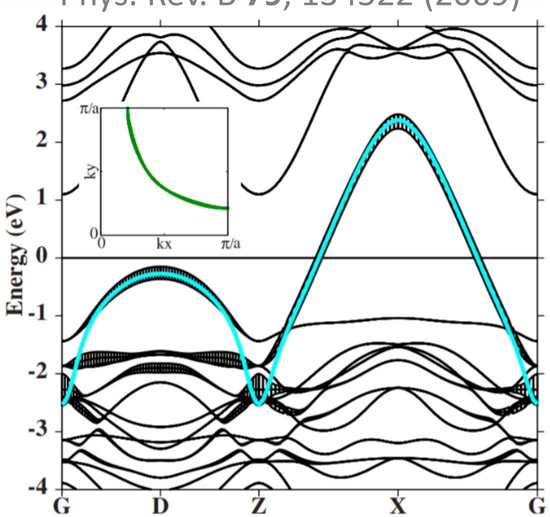
The cuprates

prime example of high-T_c superconductors

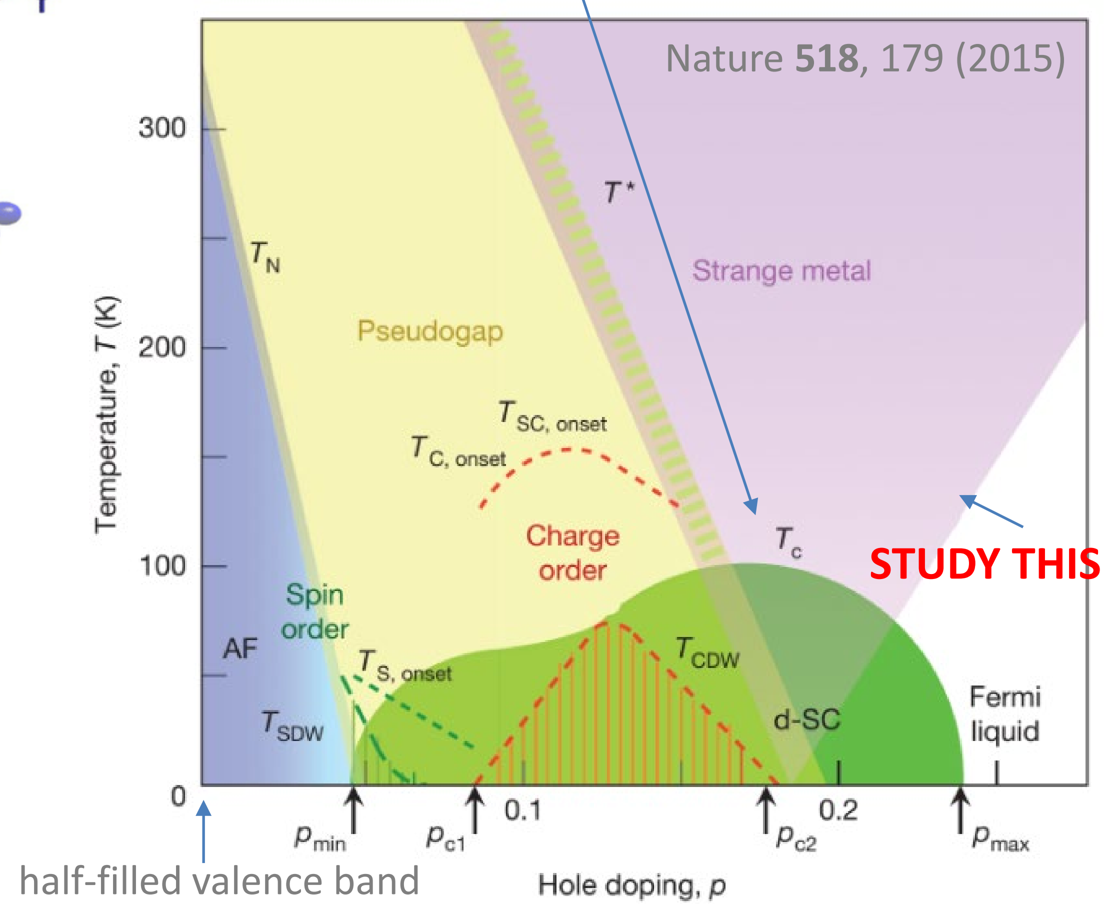
different compounds - same phase diagram

SC T_c as high as 134K, as low as 20K !

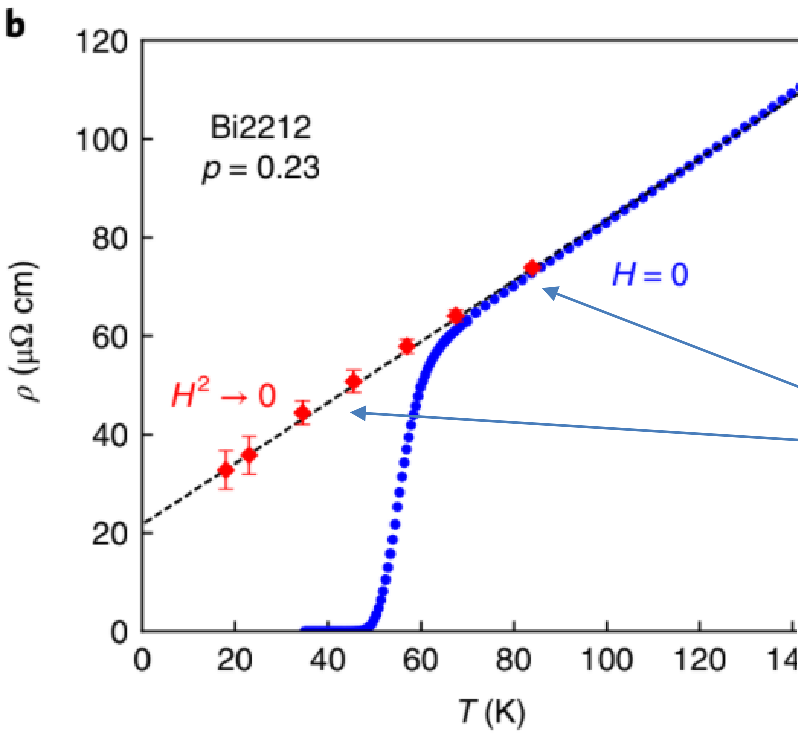




DFT band structure for La_2CuO_4
Phys. Rev. B **79**, 134522 (2009)



The strange metal

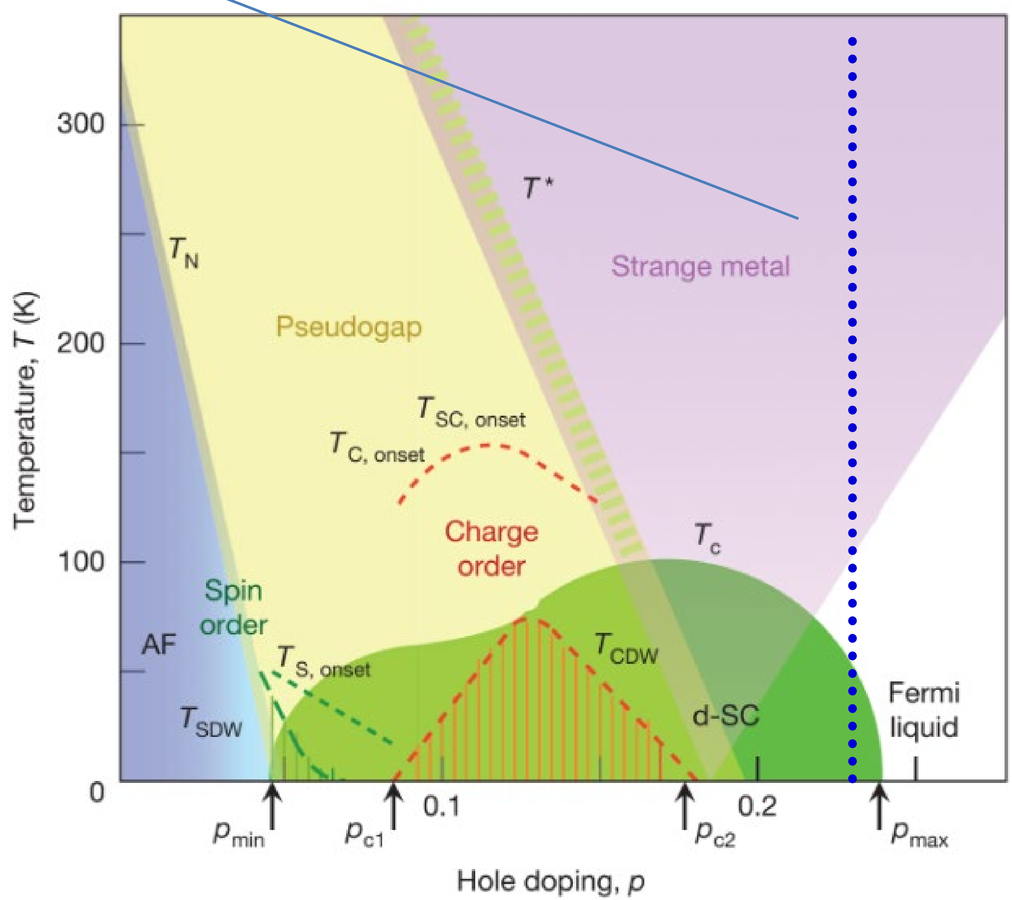


Nature Physics **15**, 142 (2019)

resistivity linear in temperature

magnetic field probes:
trend would continue to T=0 !

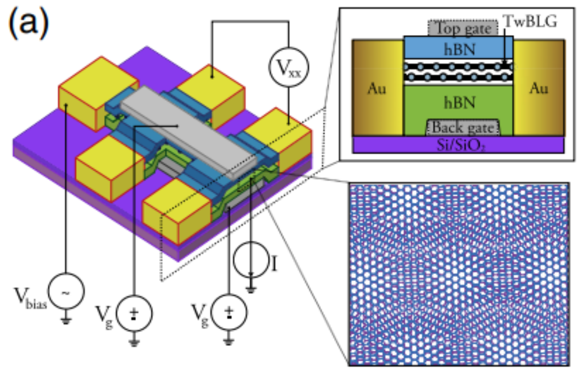
$$\rho_{\rm dc}(T) = \rho_0 + aT$$

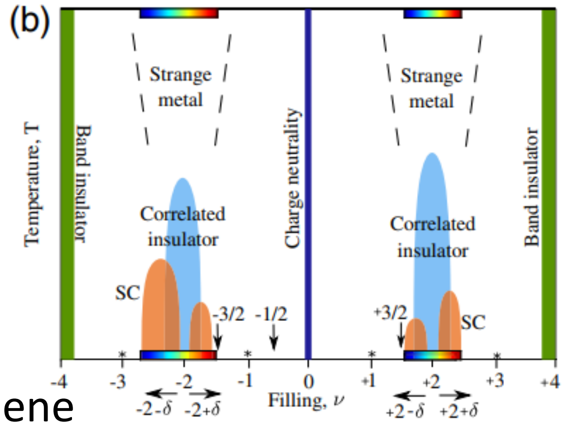


Moiré lattices

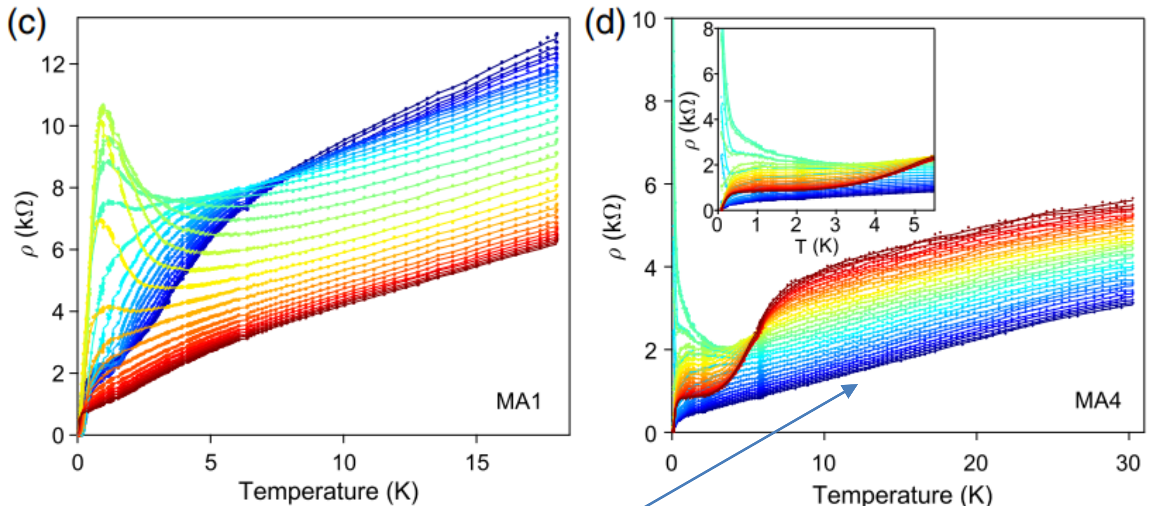
half-way between
- real materials and
- optical lattice simulators

in terms of
- length and time scales
- tunability/control





magic-angle twisted bilayer graphene

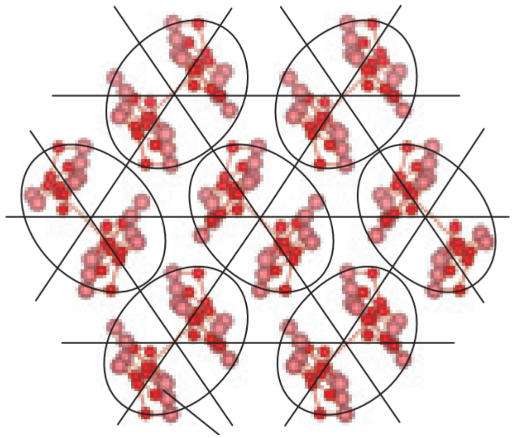


Phys. Rev. Lett **124**, 076801 (2020)

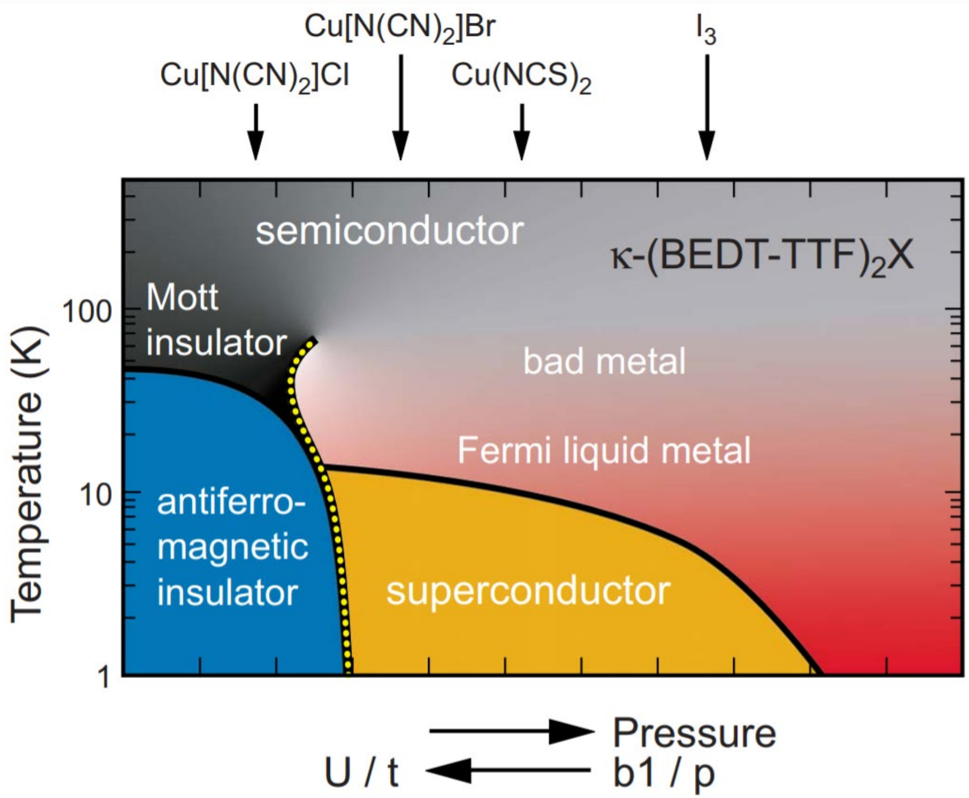
Strange metal down to very low temperature
also in vicinity of a SC phase and an insulating phase

Strange metal - a universal phenomenon

e.g. κ-$(ET)_2Cu_2(CN)_3$



κ-organic materials



Phys. Rev. B **79**, 195106 (2009)

Half-filled valence band throughout the phase diagram
pressure tunes effective interactions

Another generic phase diagram, a manifestation of strong correlations

AFM insulator
unconventional superconductivity
rapid metal-insulator crossover at high-temp

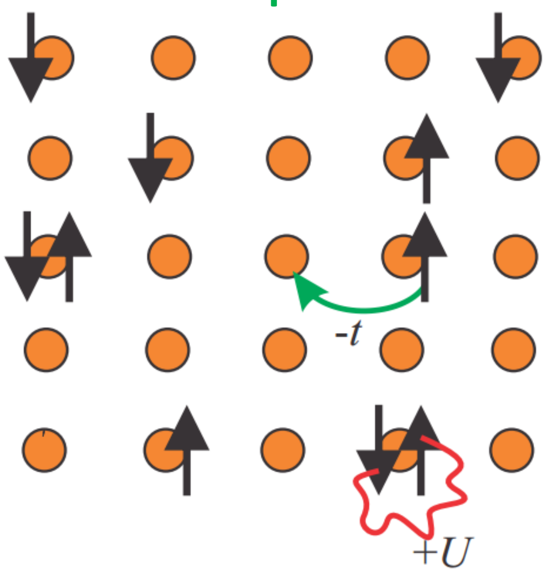
Hubbard model

One of the most studied models in condesed matter theory, more than 50 years old

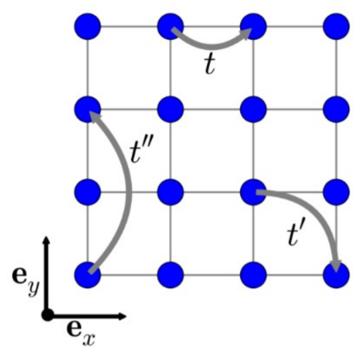
$$H = -t \sum_{\sigma,\langle i,j\rangle} c^\dagger_{\sigma,i} c_{\sigma,j} + U \sum_i n_{\uparrow,i} n_{\downarrow,i} - \mu \sum_{\sigma,i} n_{\sigma,i}$$

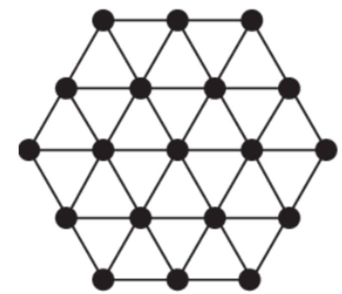
kinetic interaction chemical potential

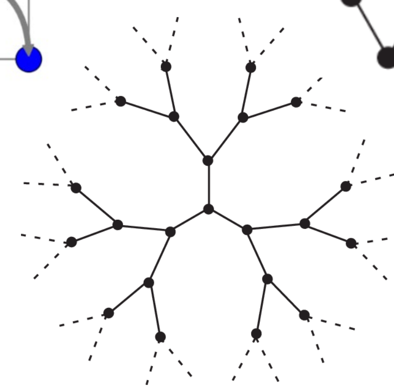
electrons hop between lattice sites



interact when they meet







$d = \infty$

Bethe lattice
solvable with DMFT

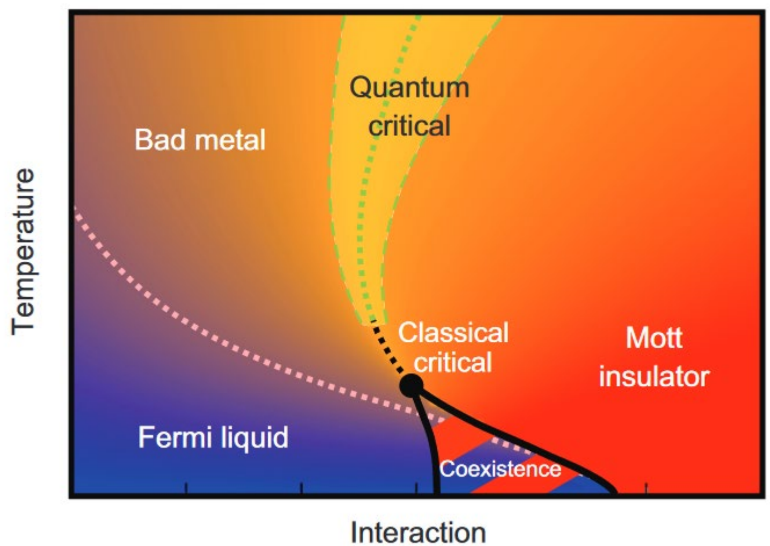
can be formulated for any kind of lattice

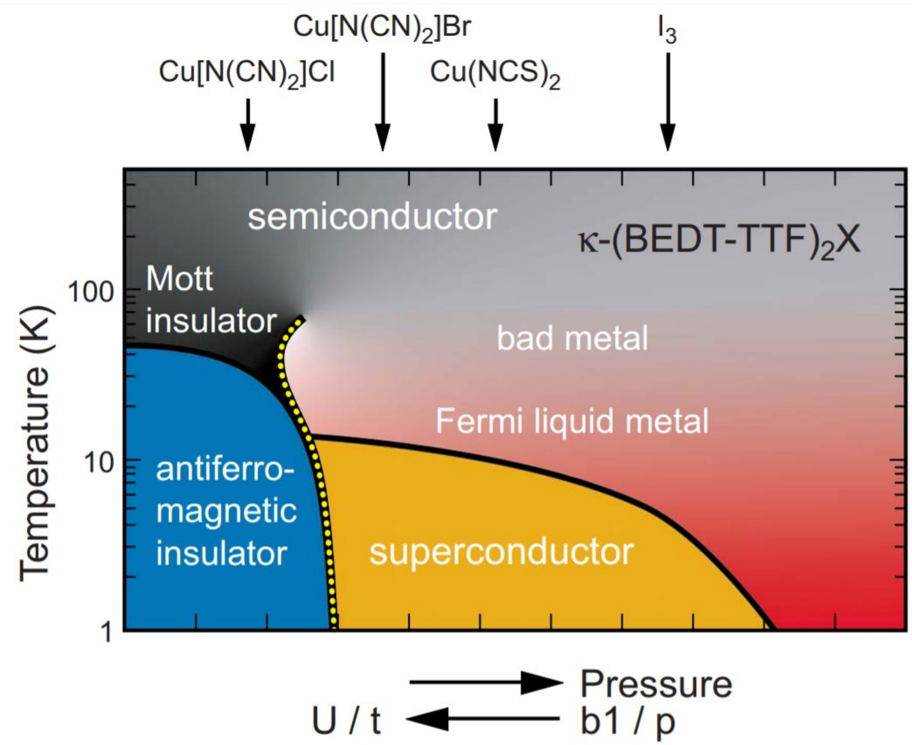
Based on the Hubbard model, progress is made in understanding the phenomenology related to resistivity in strongly correlated systems

1) dependence of **resistivity** on **temperature and doping/pressure** can be understood in terms of the **Mott transition and its quantum criticality**

κ-organics vs. Hubbard model

Phys. Rev. B **88**, 075143 (2013)



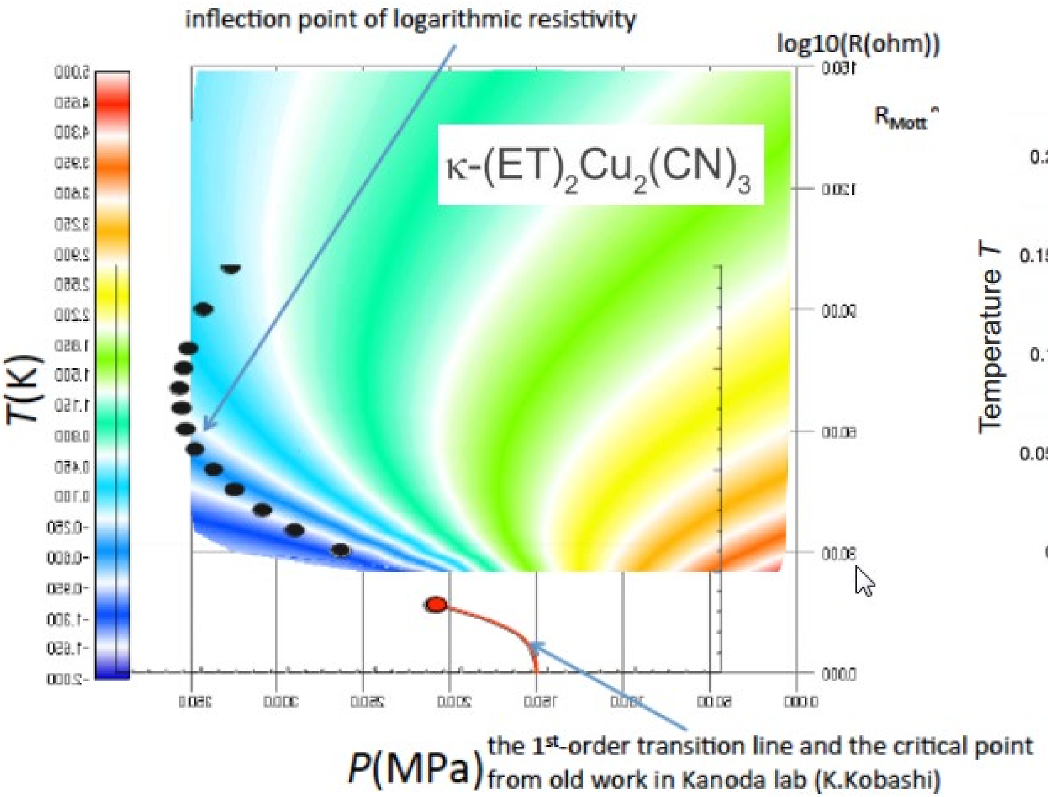


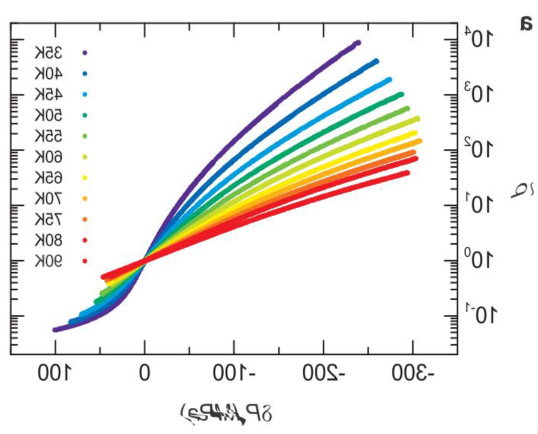
Phys. Rev. B **79**, 195106 (2009)

Central notion: **first-order Mott metal-insulator transition**

Experiment

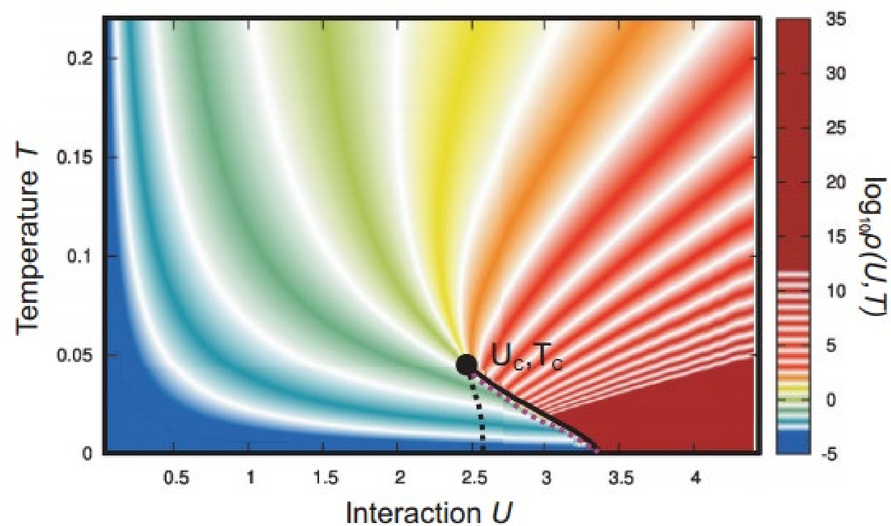
Nat. Phys. **11**, 221 (2015)

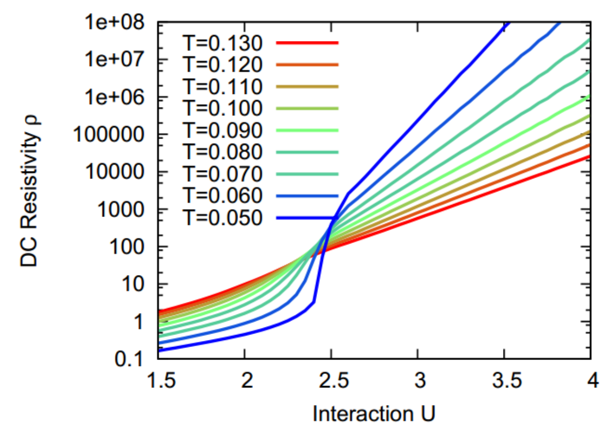




Hubbard model, DMFT(IPT) solution

JV et al. Phys. Rev B **88**, 075143 (2013)





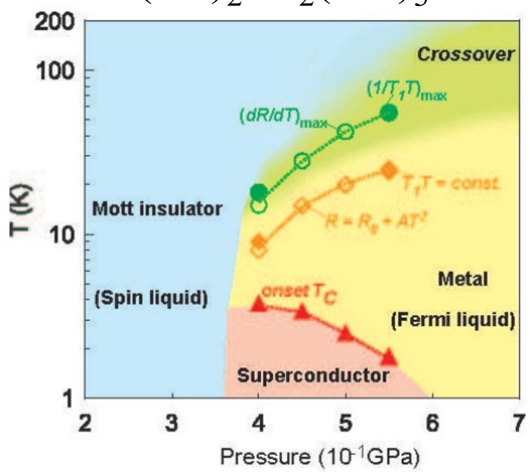
See also Phys. Rev. Lett **91**, 016401 (2003)

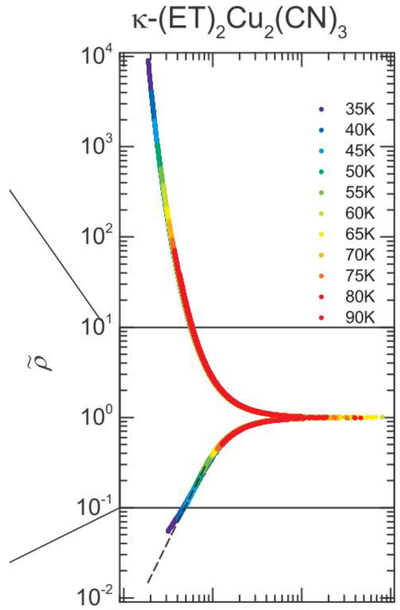
Quantum ctitical scaling

Nat. Phys. **11**, 221 (2015)

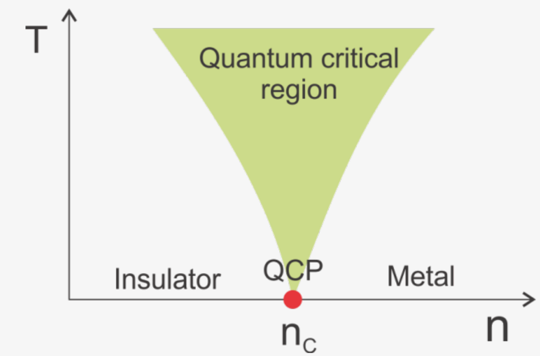
Experiment

κ-$(ET)_2Cu_2(CN)_3$





Similar to 2D electron gas in MOSFETs

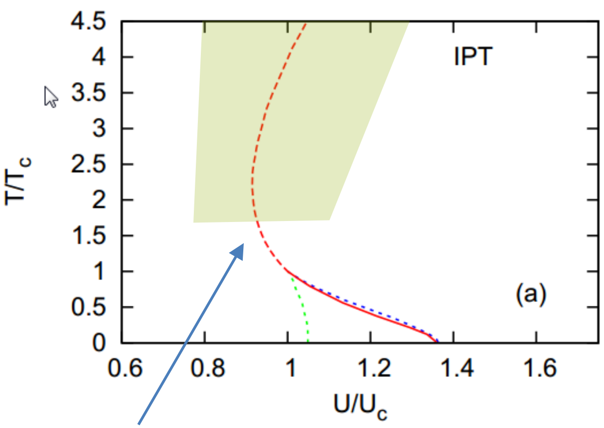


relevant variable $\frac{T}{\delta U^{z\nu}}$

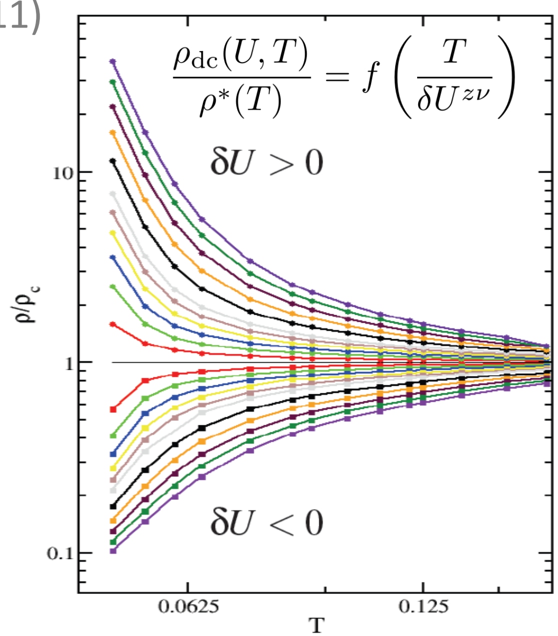
Phys. Rev. Lett. **107**, 026401 (2011)

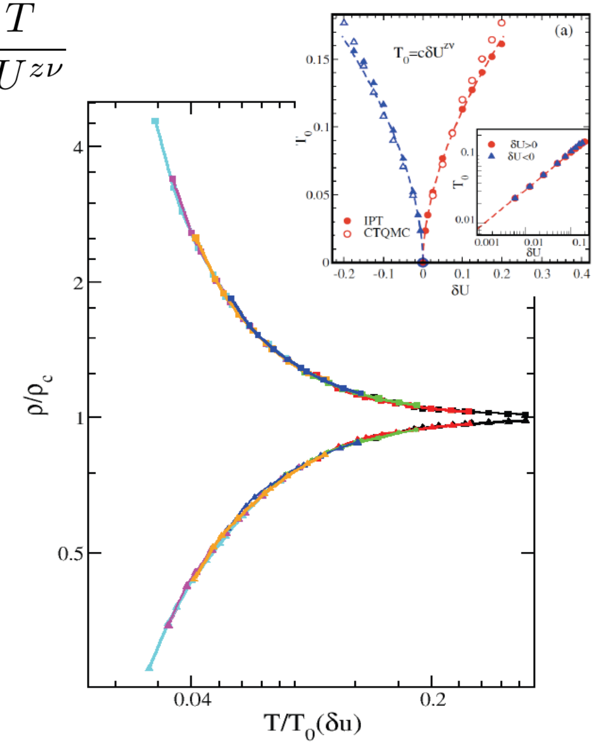
Hubbard model

DMFT(IPT) solution



quantum Widom line





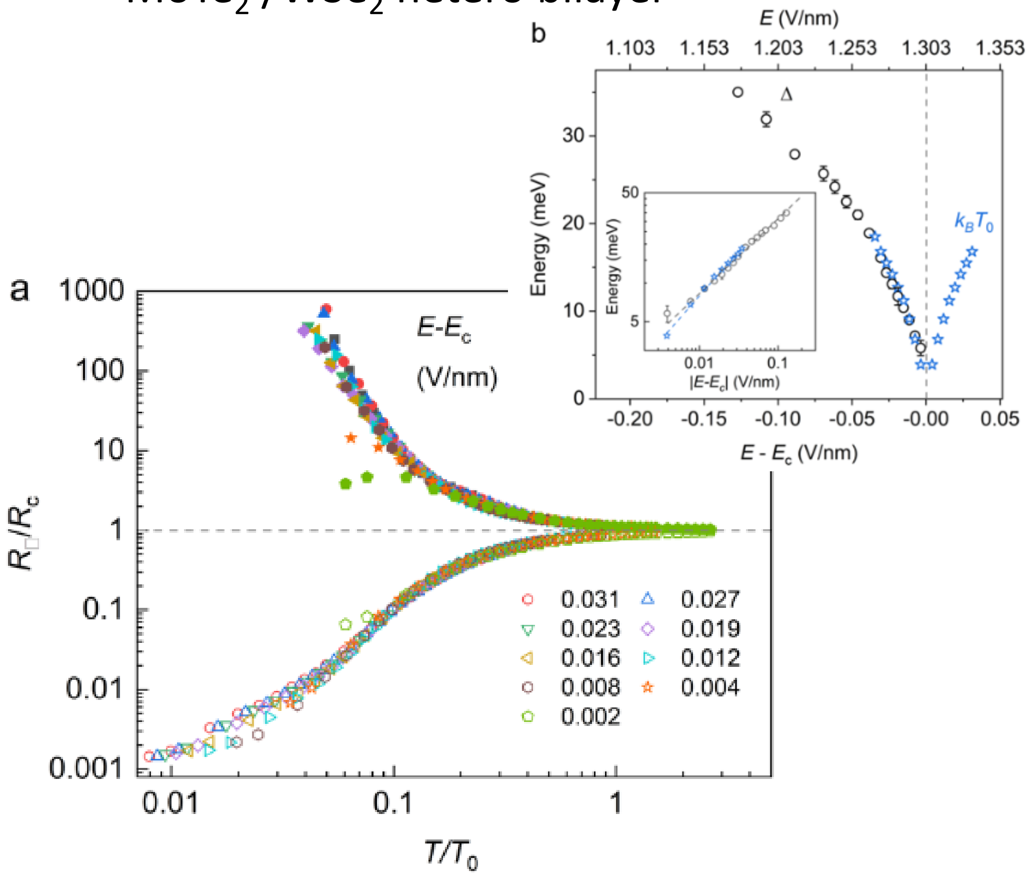
Moiré lattices vs. Hubbard model

Mott QCP

1st order MIT

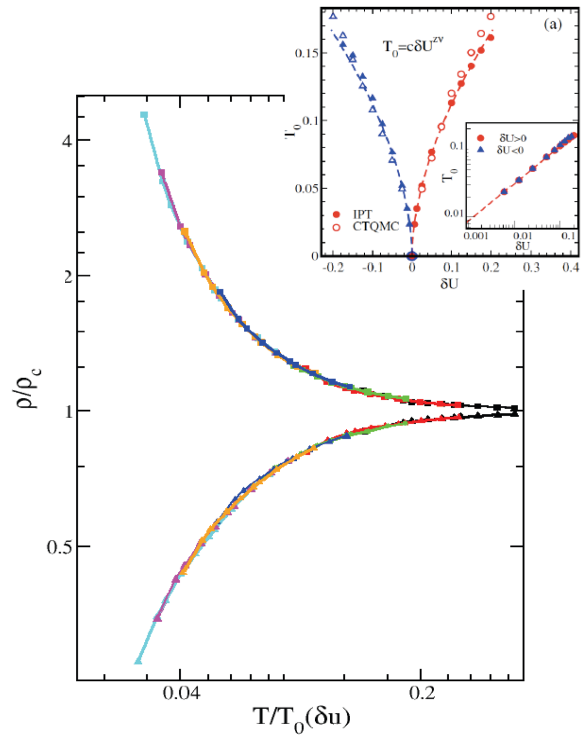
Experiment

$MoTe_2$ /WSe_2 hetero bilayer



Nature **597**, 350 (2021)

Hubbard model
DMFT(IPT) solution



Phys. Rev. Lett. **107**, 026401 (2011)

Moiré lattices vs. Hubbard model

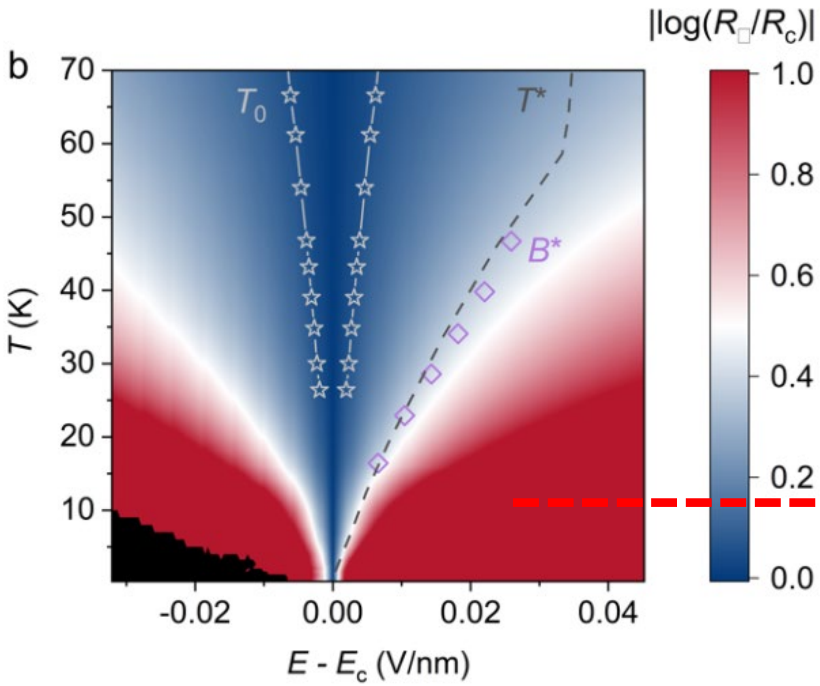
Mott QCP

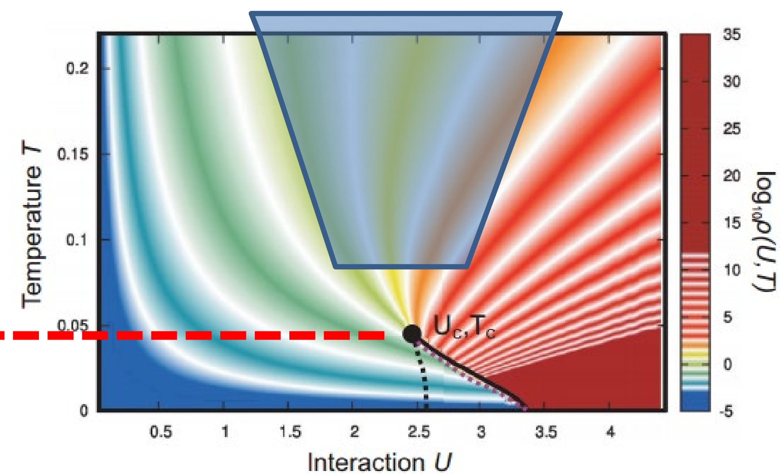
1st order MIT

Experiment
$MoTe_2$ /WSe_2 hetero bilayer

Hubbard model
DMFT(IPT) solution

W = 0,07eV ~ 700K, T_c should be around 10 K



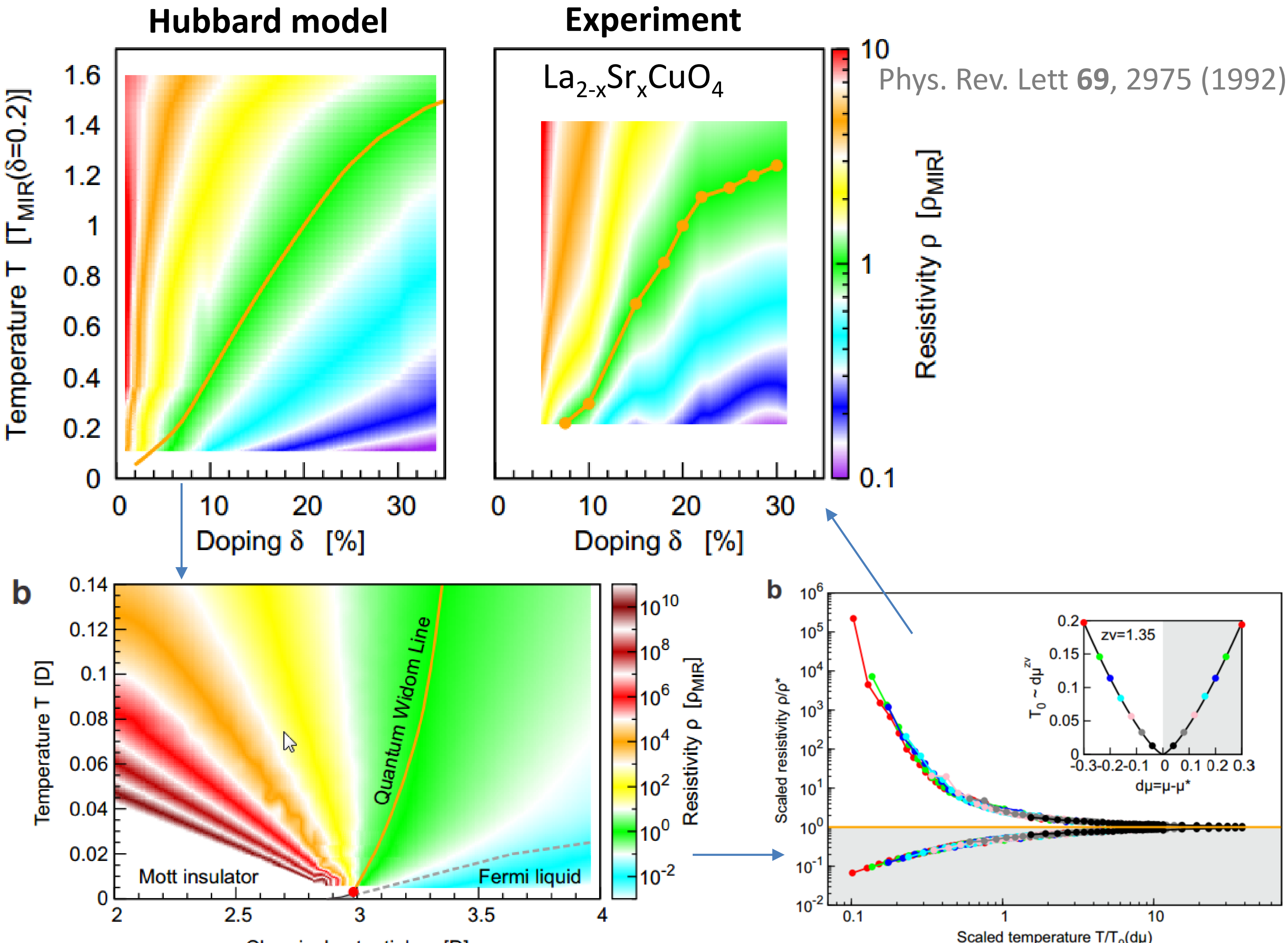


Nature **597**, 350 (2021)

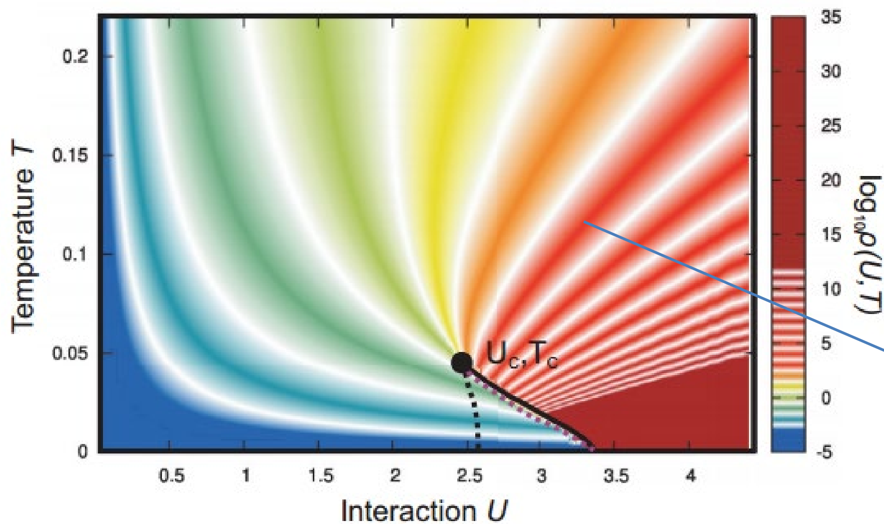
Phys. Rev. Lett. **107**, 026401 (2011)

Cuprates vs. Hubbard model

JV et al., Phys. Rev. Lett. **114**, 246402 (2015)

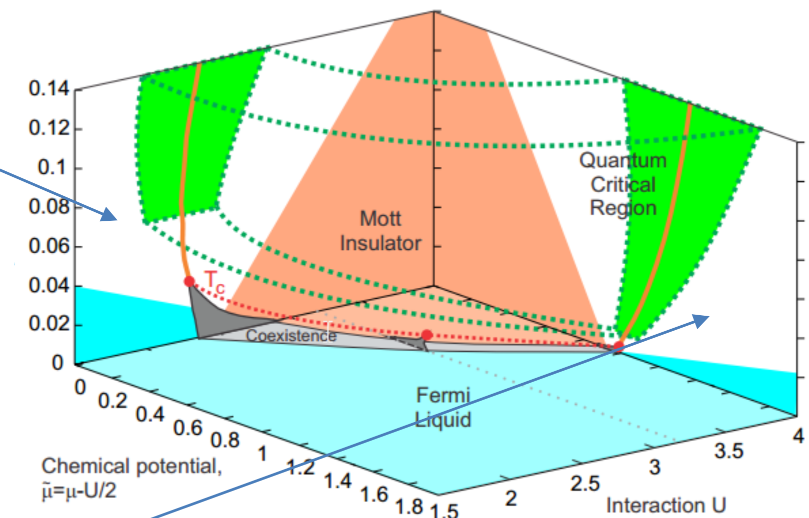


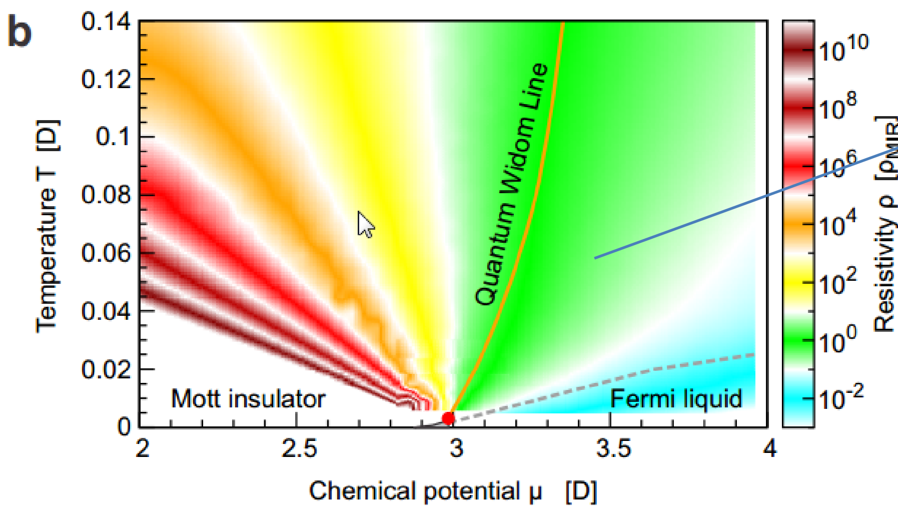
Cuprates vs. κ-organics
= doping driven Mott MIT vs. interaction driven Mott MIT



Phys. Rev. Lett. **114**, 246402 (2015)

half-filled Hubbard model
=κ-organics

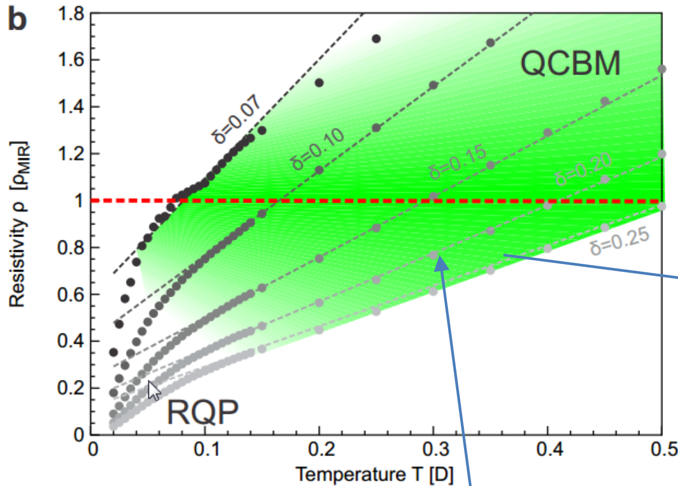




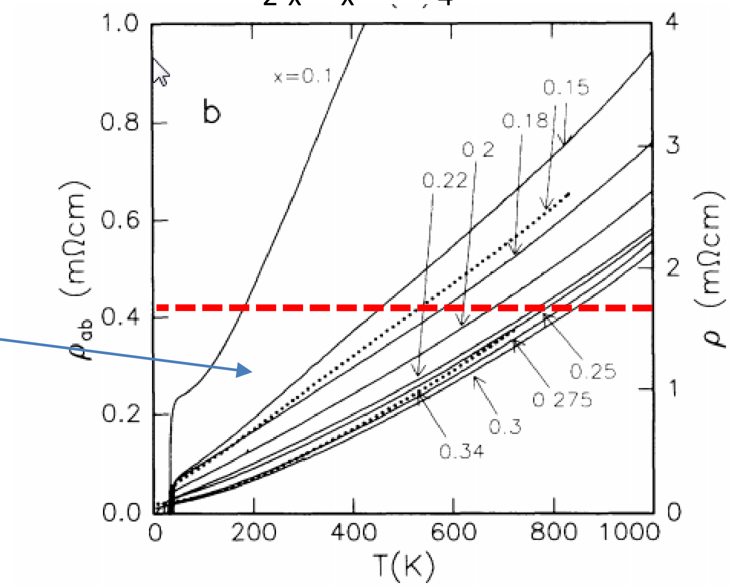
doped Hubbard model
=cuprates

T-linear resistivity vs. QC scaling region

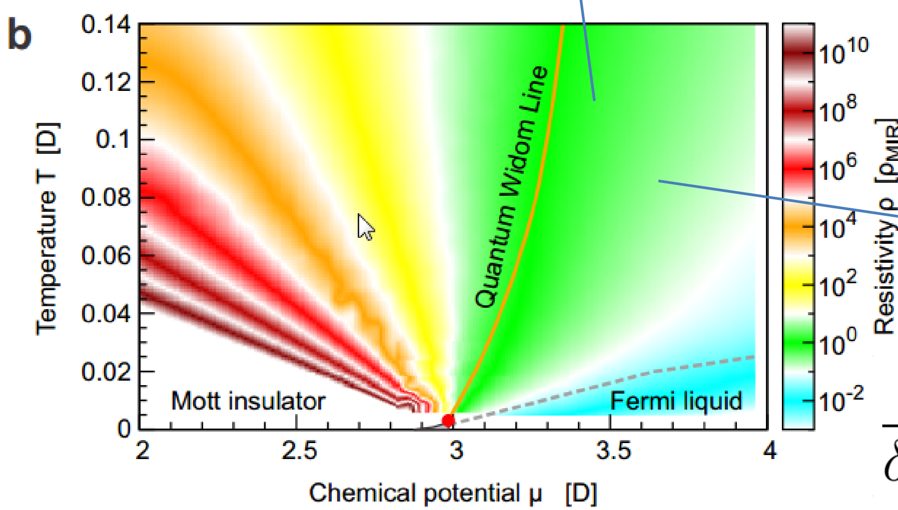
Phys. Rev. Lett. **114**, 246402 (2015)



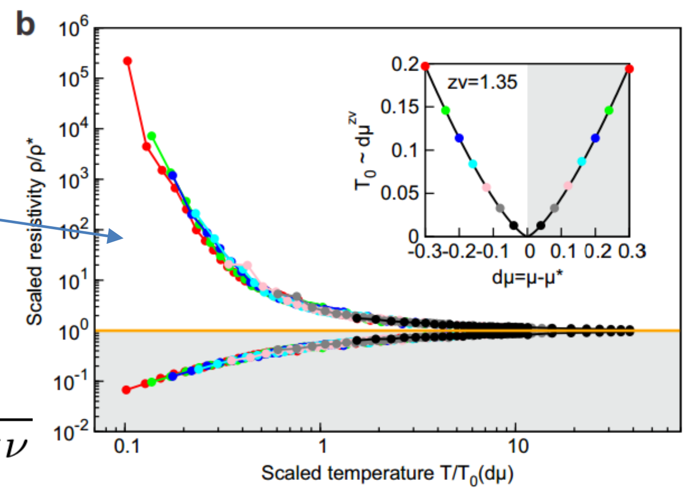
$La_{2-x}Sr_xCuO_4$



Phys. Rev. Lett **69**, 2975 (1992)



$$\frac{T}{\delta\mu^{z\nu}}$$

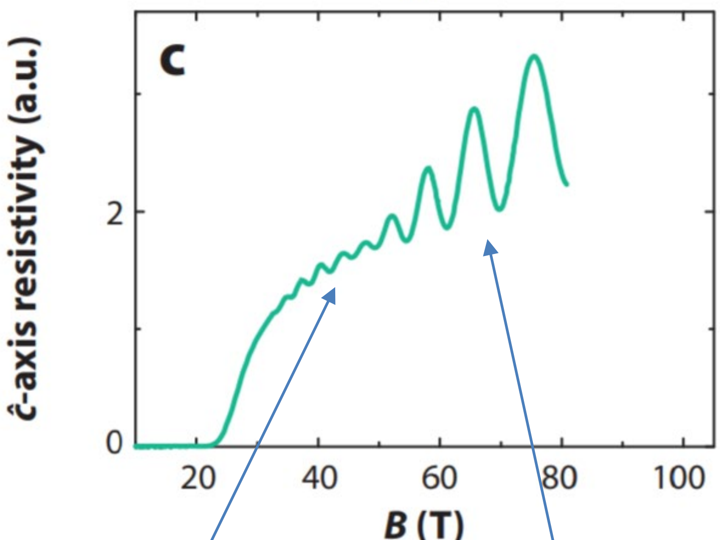


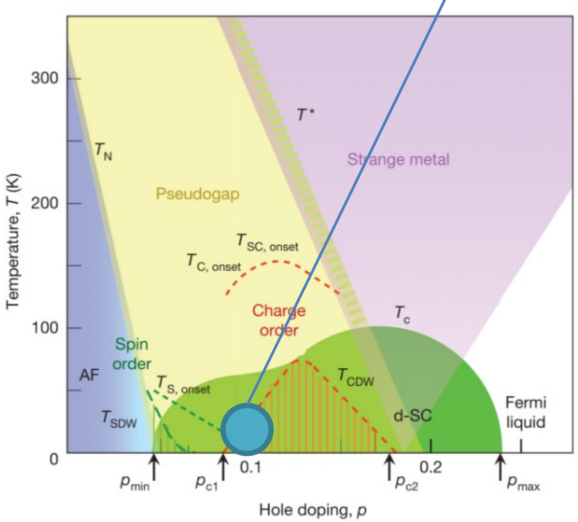
2) to understand magnetoresistance, one must consider **interactions**

Quantum oscillations of resistivity

Annu. Rev. Condens. Matter Phys. 6, 411 (2015)

$T = 4.2$ K, $p = 0.108$ YBCO

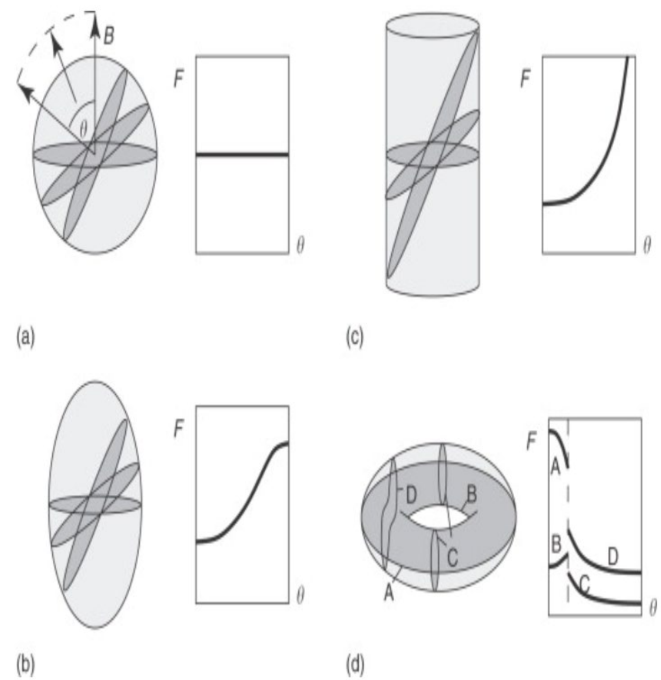




constant period
when plotted vs. B^{-1}

Shubnikov-de Haas effect
known since 1930

very low temperature needed,
very strong fields



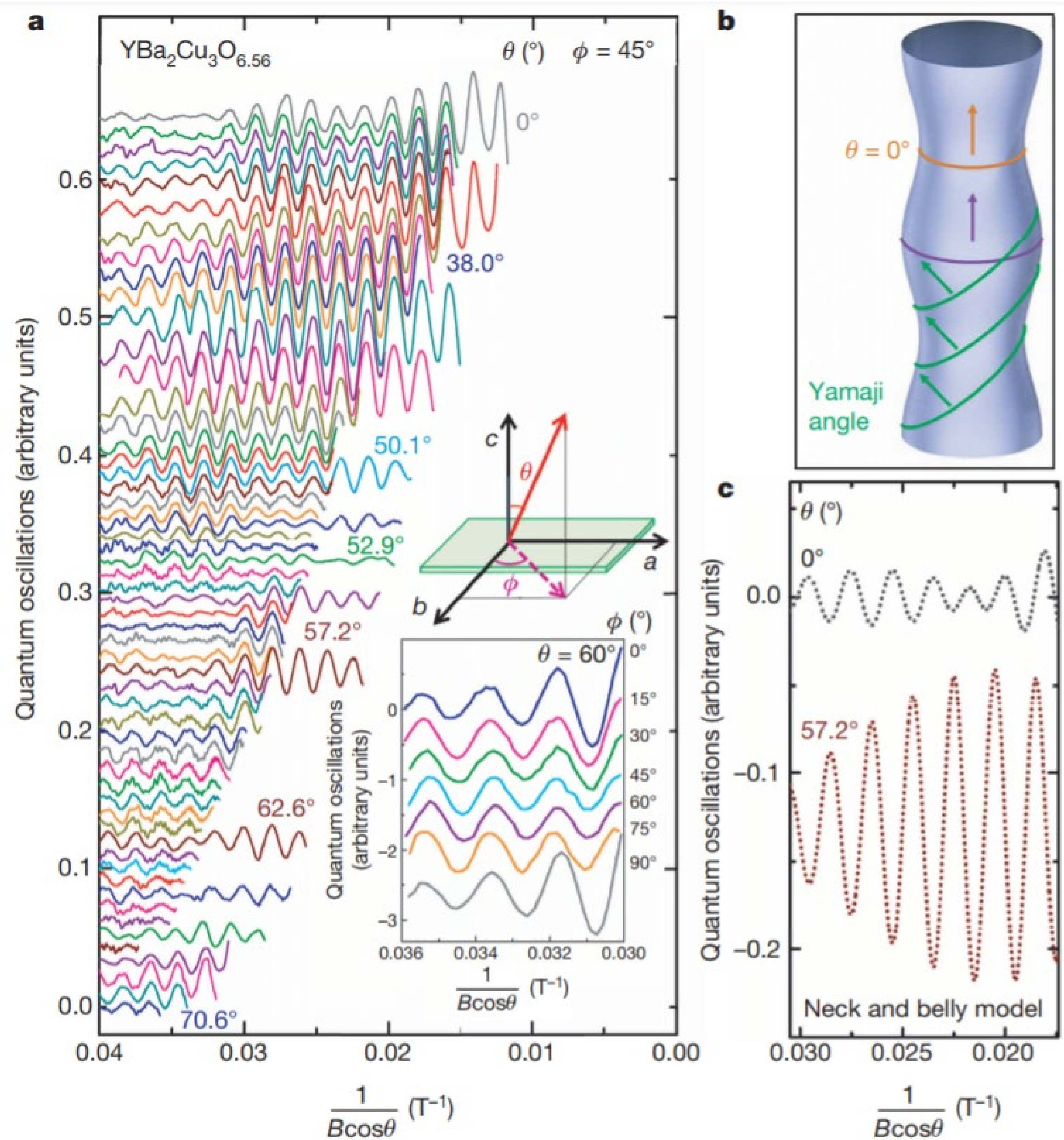
Encyclopedia of Condensed Matter Physics, Elsevier, 185 (2005)

Quantum oscillations of resistivity

Nature **511**, 61 (2014)

very useful!

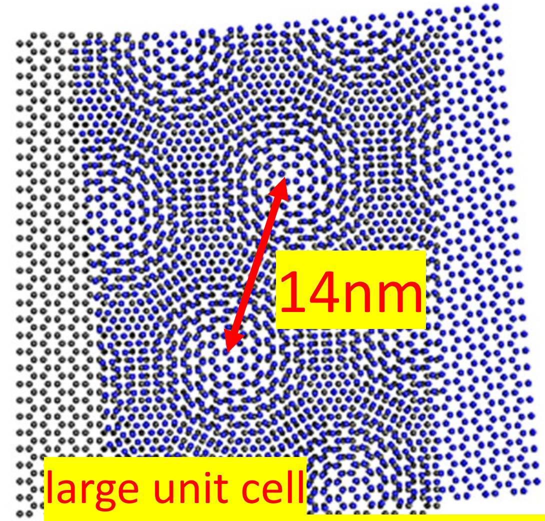
vary the angle of magnetic field
monitor the oscillation freq.
reconstruct the Fermi surface



Simple theory
not considered in the context
of strong correlations
until recently

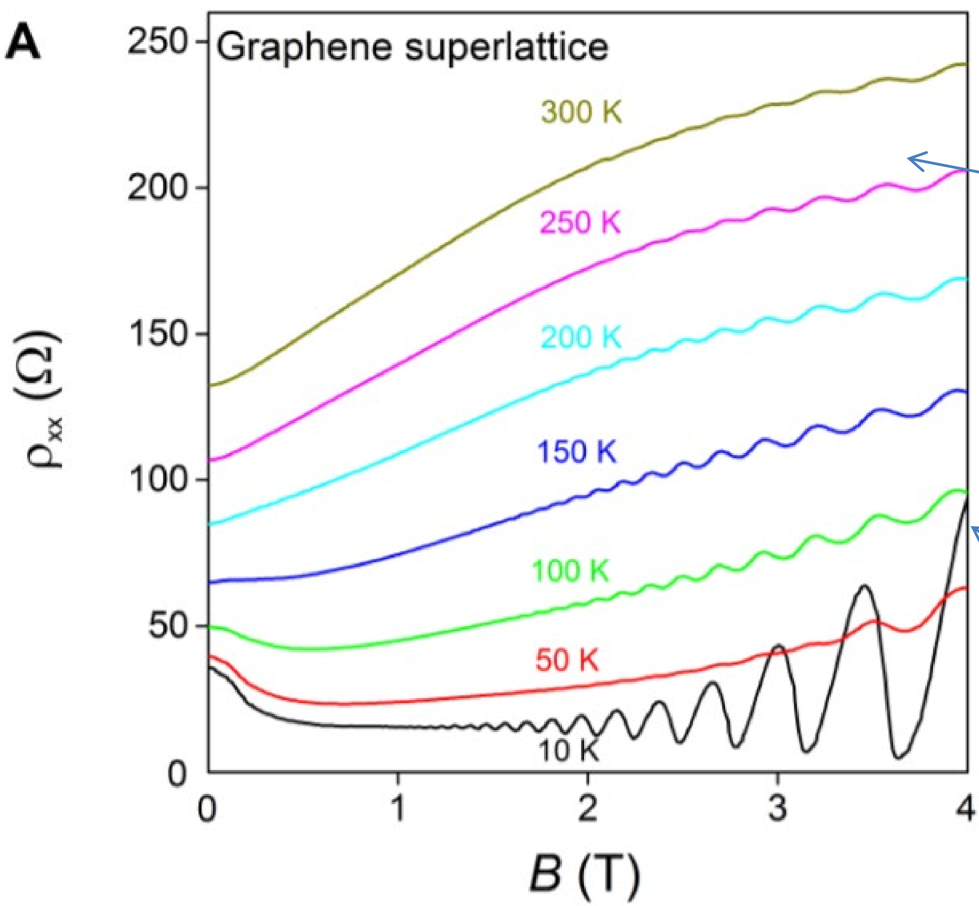
Quantum oscillations of resistivity ...at room temperature

Science **357**, 181 (2017)



large unit cell
=orbital effects of magnetic field
much more pronounced

hBN+graphene Moiré lattice



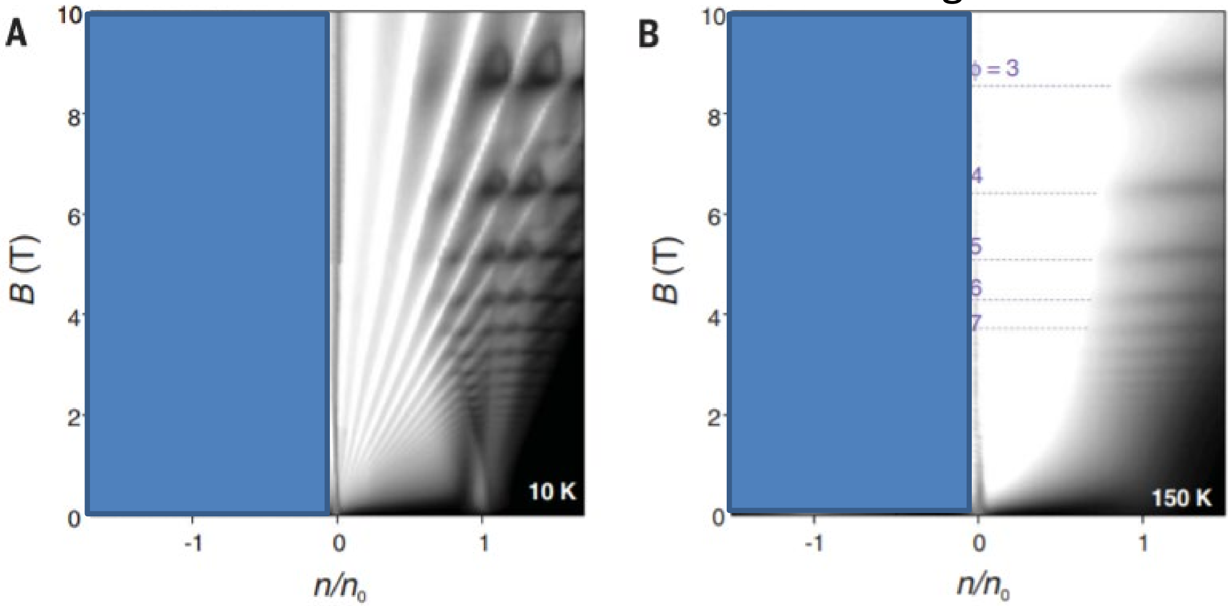
something completely different
Brown-Zak oscillations

Shubnikov-de Haas oscillations

Moiré lattice vs. Hubbard model

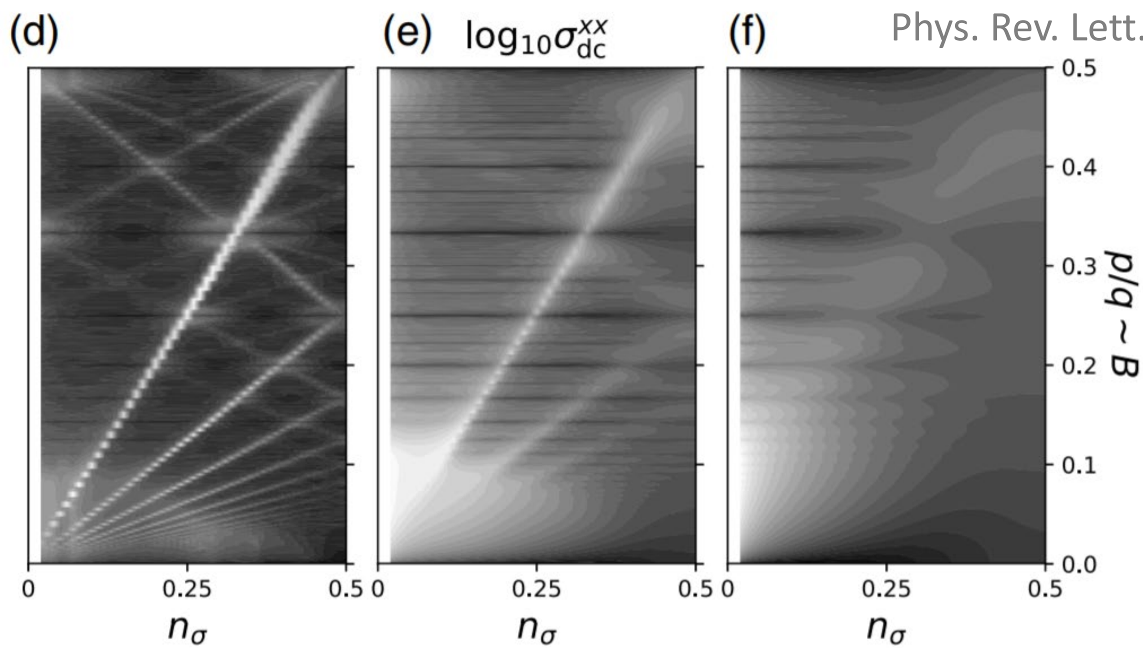
low T high T Science **357**, 181 (2017)

Experiment



Phys. Rev. Lett. **127**, 196601 (2021)

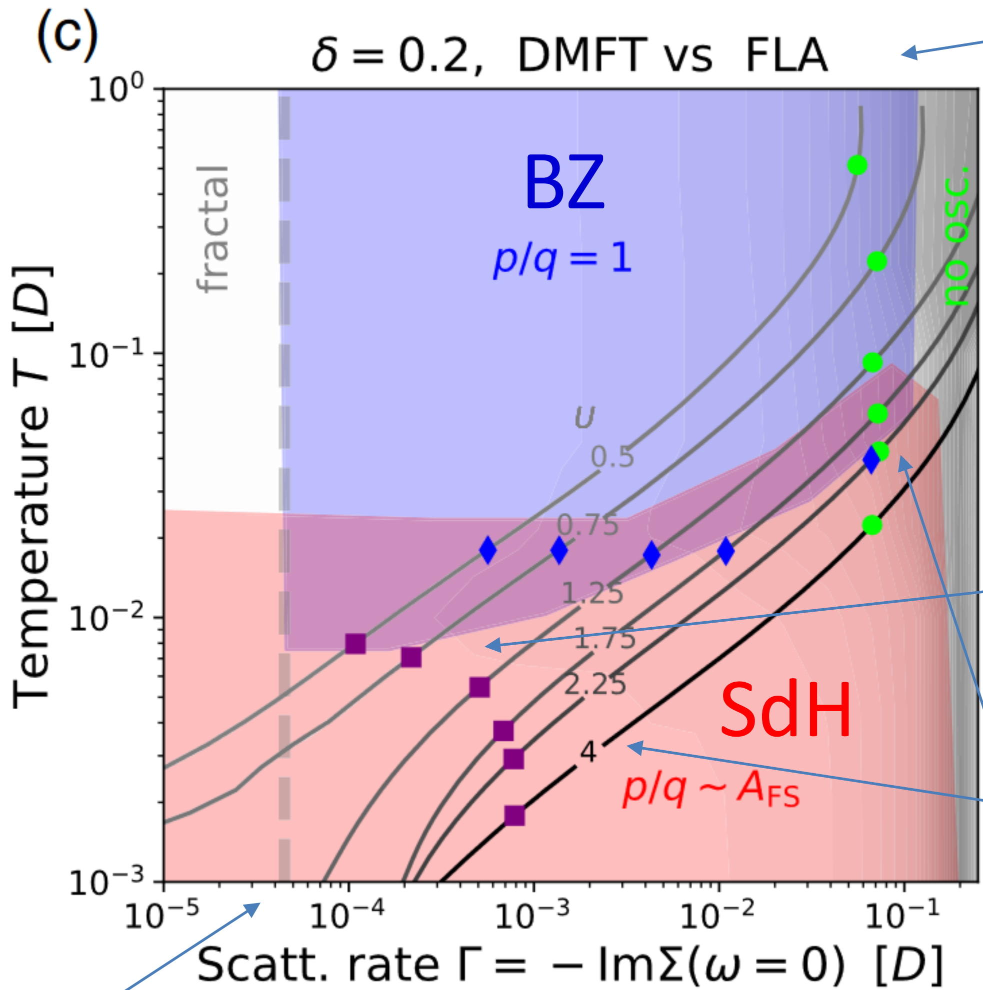
Hubbard model (2D, DMFT(NRG))



Hubbard model vs. fixed lifetime model

Phys. Rev. Lett. **127**, 196601 (2021)

up to inf. temp. !



minimal temp.
only at weak coupling

in highly corr. regimes
should be observed at
lower temp

minimal scattering rate

maximal scattering rate

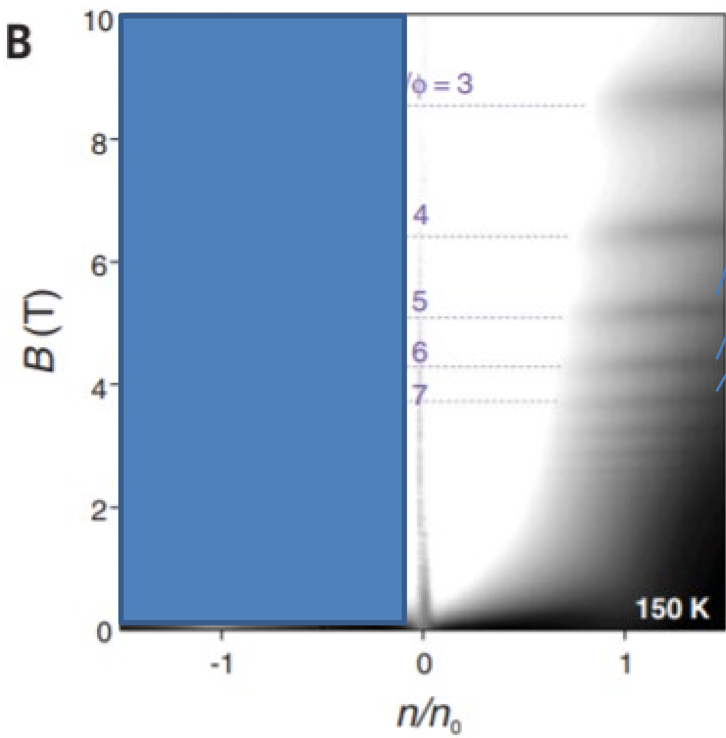
Moiré lattice vs. fixed lifetime model

Phys. Rev. B **104**, 205101 (2021)

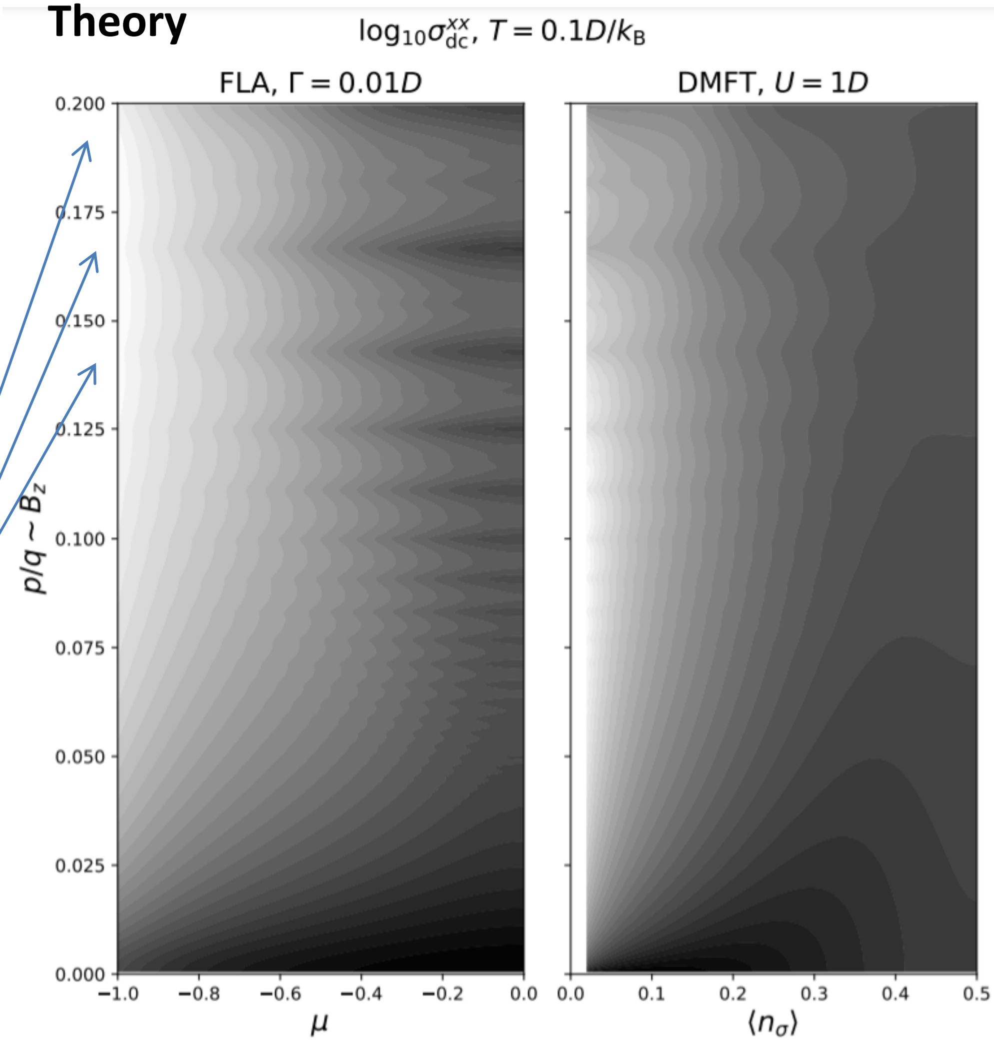
Experiment

Science **357**, 181 (2017)

high T



Theory



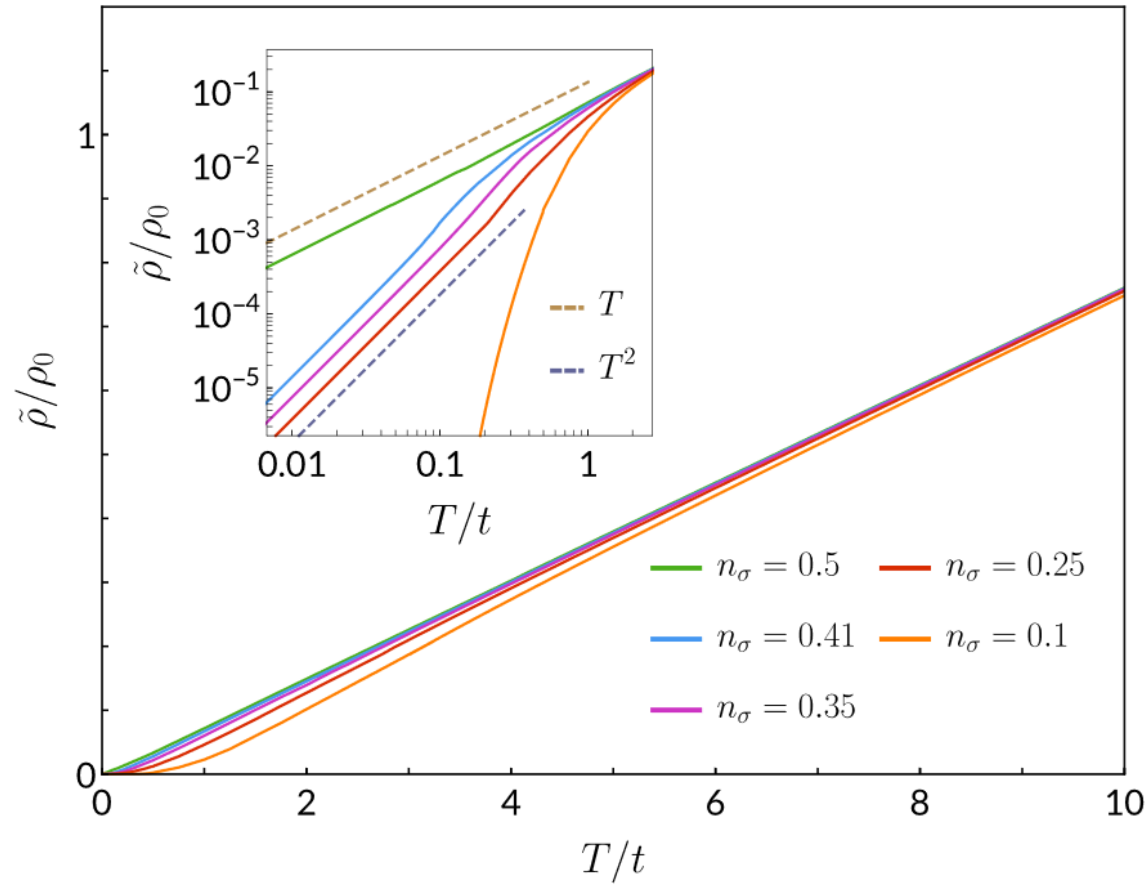
Doping dependence in better agreement with FLA: **the scattering is not of Coulomb origin**

BZ oscillations can perhaps be useful in determining the effective lattice model

3) linear resistivity is not necessarily a strong coupling phenomenon

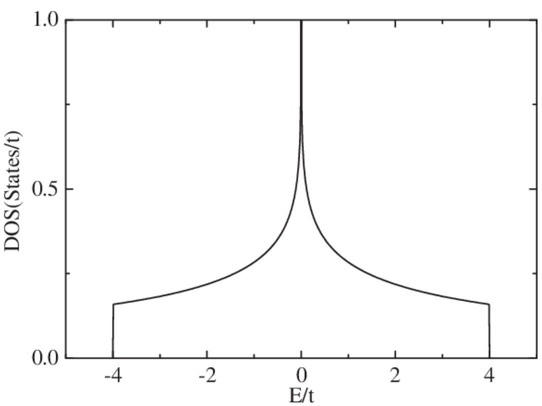
Semi-classical Boltzmann approach to **Hubbard model at weak coupling**
at half-filling, linear resistivity down to zero temperature!

Phys. Rev B **104**, 165143 (2021)



Phys. Rev B **99**, 184107 (2019)

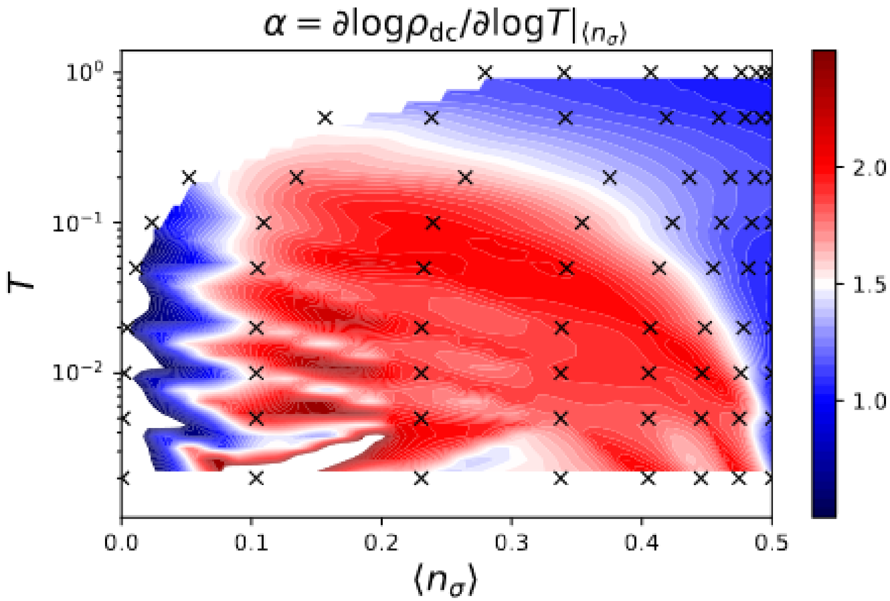
important role of van Hove singularities in DOS

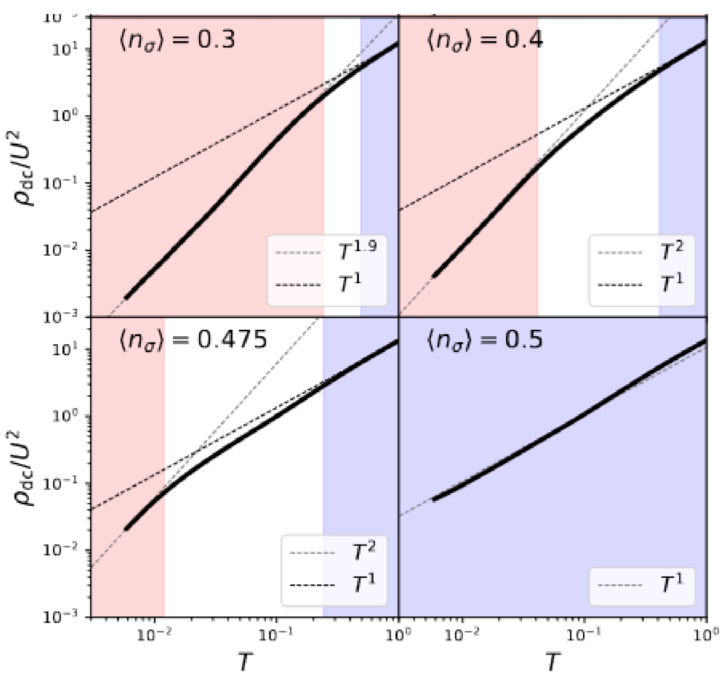


High-T linear regime
at any doping easy to understand
also in the infinite coupling limit

Phys. Rev. B **94**, 235115 (2016)

Phys. Rev. B **73**, 035113 (2006)





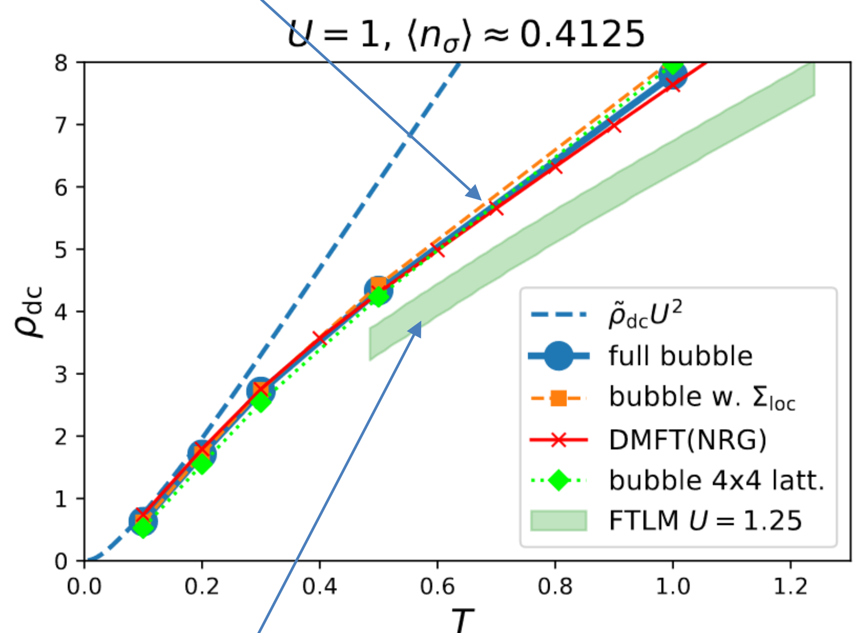
Kubo bubble calculation at weak coupling

arXiv:2208.04047 (2022)

same conclusion!

...but Boltzmann approach yields ~30x smaller resistivity

Kubo bubble results in better agreement with reference method at moderate coupling



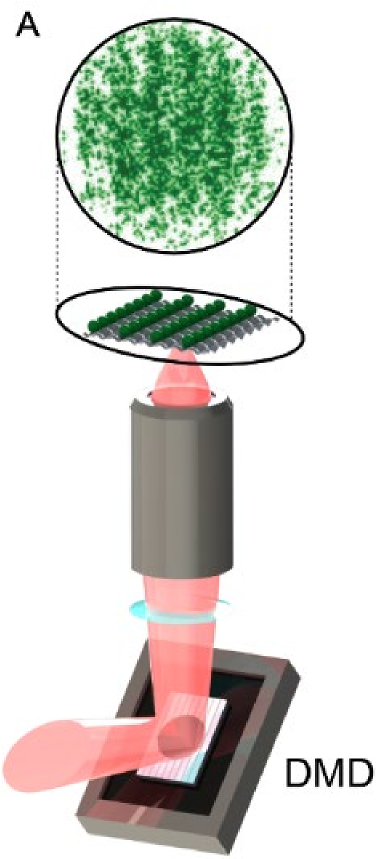
FTLM: numerically exact results at high temperature at strong, but also moderate coupling

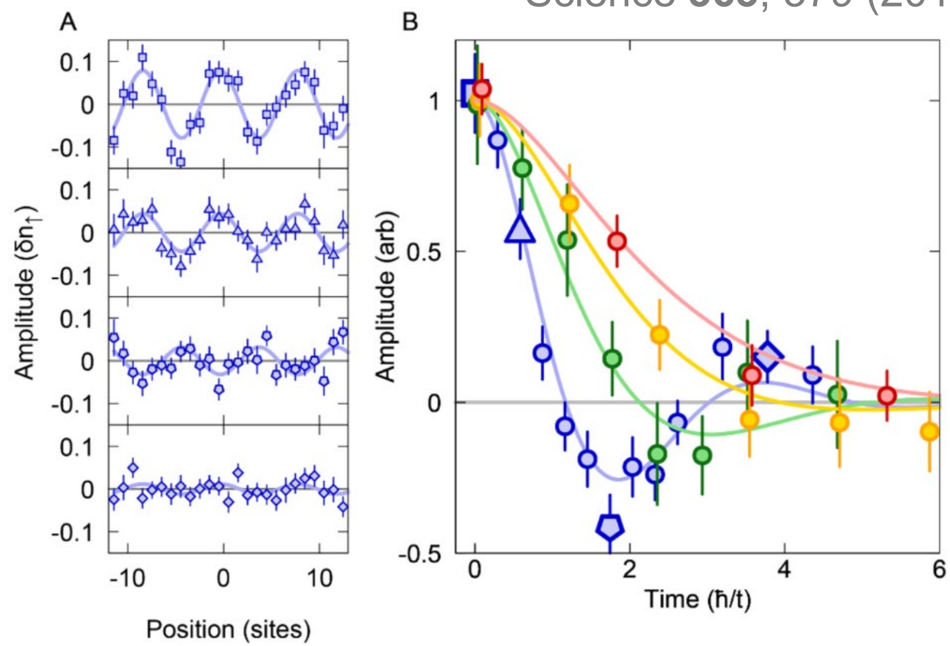
Phys. Rev. Lett. **123**, 036601 (2019)

4) the resistivity is determined by effective hydrodynamics at long wavelengths/low freqs.

Info comes not from theory but from cold atoms in optical lattice
quantum simulation of the Hubbard model

Science **363**, 379 (2019)





relaxation of CDW
well described by a simple
hydrodynamic theory

$$\partial_t n = -\nabla \cdot \mathbf{j}$$

$$\partial_t \mathbf{j} = -\Gamma(D\nabla n + \mathbf{j})$$

not at all obvious

Hydrodynamic model vs. Hubbard model

arXiv:2208.04047 (2022)

Hydrodynamic model:

$$\partial_t \mathbf{j} = -\Gamma(D\nabla n + \mathbf{j})$$

Hubbard model:

$$\partial_t j^{\eta}_{\mathbf{r}} = -t^2 \sum_{\sigma} \left\{ 2n_{\sigma,\mathbf{r}+\mathbf{e}_\eta} - 2n_{\sigma,\mathbf{r}} + \sum_{\mathbf{u}\in\{-\mathbf{e}_\eta,\mathbf{e}_{\bar\eta},-\mathbf{e}_{\bar\eta}\}} \left(c^\dagger_{\sigma,\mathbf{r}+\mathbf{u}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta} - c^\dagger_{\sigma,\mathbf{r}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta-\mathbf{u}} + \mathrm{H.c.} \right) \right\}$$
$$-tU \sum_{\sigma} (n_{\bar\sigma,\mathbf{r}+\mathbf{e}_\eta} - n_{\bar\sigma,\mathbf{r}}) (c^\dagger_{\sigma,\mathbf{r}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta} + c^\dagger_{\sigma,\mathbf{r}+\mathbf{e}_\eta} c_{\sigma,\mathbf{r}}).$$

Hydrodynamic model vs. Hubbard model

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???

diffusion constant

$$D\Gamma \approx 2t^2$$

mom. relax. rate

Hydrodynamic model:

$$\partial_t \mathbf{j} = -\boxed{\Gamma(D\nabla n} + \mathbf{j})$$

Hubbard model:

$$\partial_t j^\eta_{\mathbf{r}} = -\boxed{t^2 \sum_\sigma \Big\{ 2n_{\sigma,\mathbf{r}+\mathbf{e}_\eta} - 2n_{\sigma,\mathbf{r}}} + \sum_{\mathbf{u}\in\{-\mathbf{e}_\eta,\mathbf{e}_{\bar\eta},-\mathbf{e}_{\bar\eta}\}} \Big(c^\dagger_{\sigma,\mathbf{r}+\mathbf{u}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta} - c^\dagger_{\sigma,\mathbf{r}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta-\mathbf{u}} + \mathrm{H.c.}\Big)\Big\}$$

$$-tU\sum_\sigma (n_{\bar\sigma,\mathbf{r}+\mathbf{e}_\eta} - n_{\bar\sigma,\mathbf{r}})(c^\dagger_{\sigma,\mathbf{r}} c_{\sigma,\mathbf{r}+\mathbf{e}_\eta} + c^\dagger_{\sigma,\mathbf{r}+\mathbf{e}_\eta} c_{\sigma,\mathbf{r}}).$$

charge-charge corr. func. $\chi_{ij}(\tau) = \langle n_i(\tau) n_j(0)\rangle - \langle n\rangle^2$

Hydrodynamic model:

$$\chi_{\mathbf{q}}(\nu) = \frac{\chi_c}{1 - \frac{i\nu}{q^2 D} - \frac{\nu^2}{q^2 D\Gamma}}$$

Hubbard model:

$$\mathrm{Re}\chi_{\mathbf{q}\to 0}(i\nu \to i\infty) = -\frac{2t}{\nu^2} \sum_{\eta=\{x,y\}} \sum_{\mathbf{k}} q_\eta \sin k_\eta \mathbf{q}\cdot\nabla\langle n_{\mathbf{k}}\rangle$$

If the hyd. theory holds in the Hubbard model it must be

$$\lim_{\substack{U\to 0\\ T\to\infty}} D\Gamma = 2t^2$$

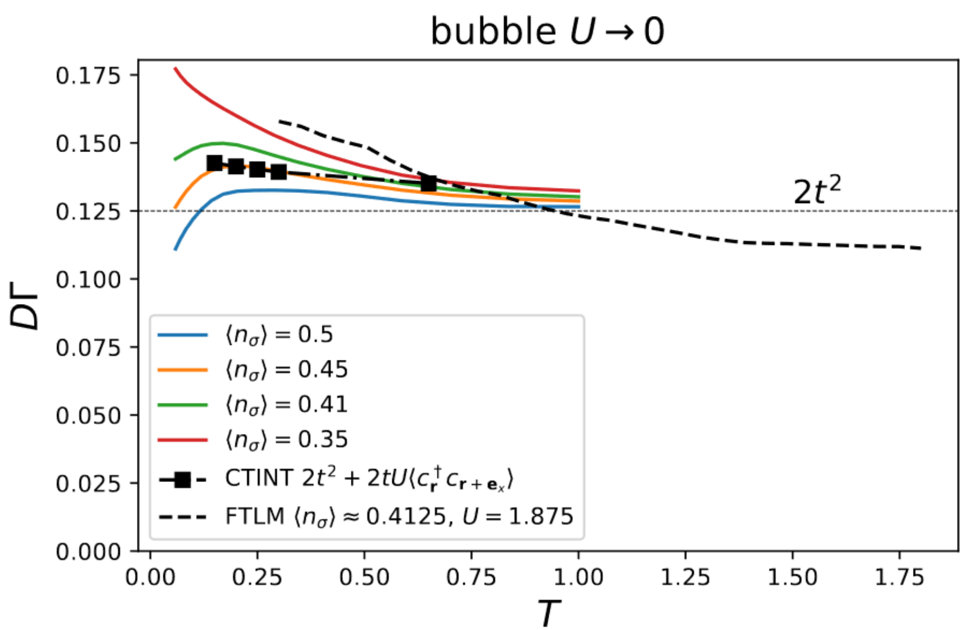
$$\sigma^{xx}_{\mathbf{q}=0}(\nu) = \frac{\chi_c D}{1 + \left(\frac{\nu}{\Gamma}\right)^2}$$

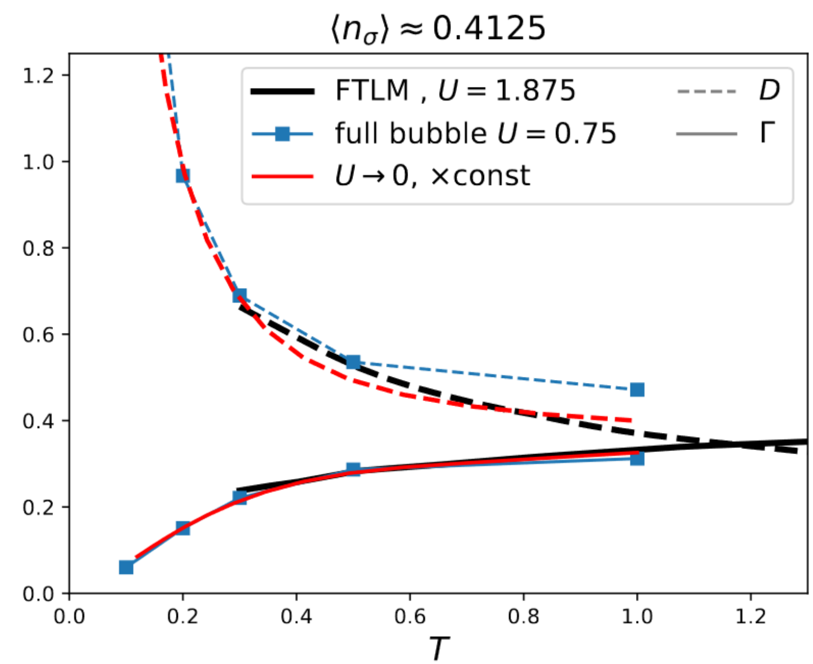
We take the Hydrodynamic model for granted
and combine it with what we know for theHubbard model analytically

Hydrodynamic model vs. Hubbard model

arXiv:2208.04047 (2022)

$$D\Gamma \;\approx\; 2t^2$$ satisfied in a broad range of parameters, including strong coupling





Microscopic support for the hydrodynamic theory but still inconclusive

no qualitative difference between weak and strong coupling

Linear resistivity at high temperature is the inverse of charge compressibility because diffusion constant D saturates

$$\sigma_{\mathrm{dc}} = \chi_c D \qquad \chi_c \sim 1/T \qquad \rho_{\mathrm{dc}} \sim T$$

Phys. Rev. B **94**, 235115 (2016)
Phys. Rev. B **95**, 041110(R) (2017)

1) dependence of **resistivity** on **temperature and doping/pressure**
can be understood in terms of the **Mott transition and its quantum criticality**

Strongly correlated systems at high T exhibit rapid metal-insulator crossovers governed by simple quantum critical scaling laws related to underlying Mott transition

2) to understand magnetoresistance, one must consider **interactions**

Brown-Zak quantum oscillations at high-temperature are brought about by a combination of scattering and temperature in a way that reveals dominant scattering mechanisms

3) linear resistivity is not necessarily a strong coupling phenomenon

Linear resistivity is always expected at high temperature, but at weak coupling it extends to zero temperature when the Fermi level is at a van Hove singularity.

4) the resistivity is determined by effective hydrodynamics at long wavelengths/low freqs.

The precise form of the hydrodynamic theory is unclear, but quantum simulation results are starting to receive support from microscopic calculations.

Task for the future work, necessary to resolve the puzzle of linear resistivity

Numerically exact solutions formulated in real-frequency
in 2D, thermodynamic limit
at low temperature, strong coupling
in the presence of the magnetic fields

avoid analytical continuation from Matsubara formalism at all costs!

Bonus points awarded if
model includes weak disorder
model includes weak e-ph coupling
model treats details of the lattice structure (includes multiple bands)

Real-frequency diagrammatic Monte Carlo new kid in town

$$Q(z) = \sum_l (-U)^l Q_l(z)$$

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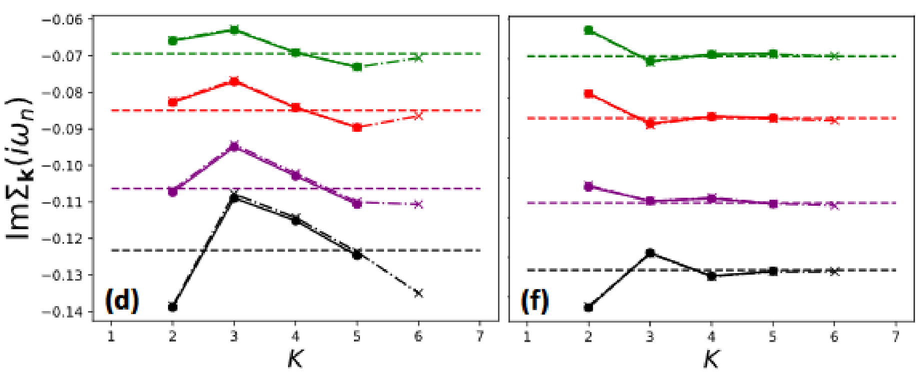

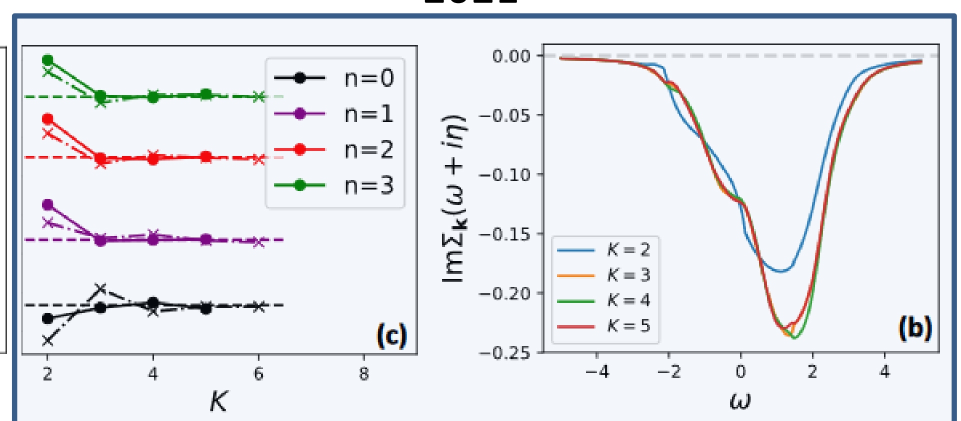

Phys. Rev. B **96**, 041105(R) (2017)

Thank you for your attention!