Metal-Insulator Transition with Charge Fractionalization

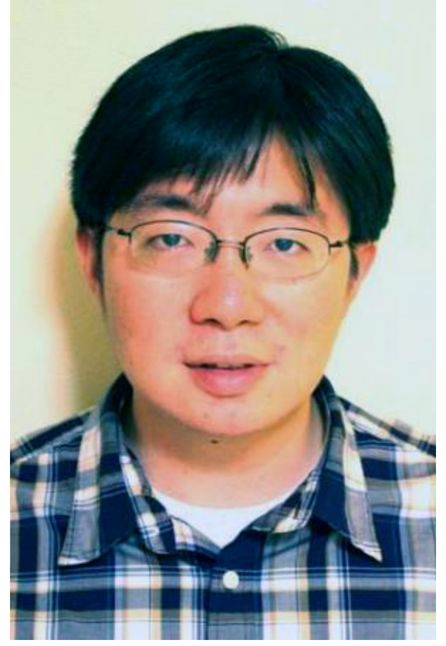
Xiao-Chuan Wu (吴啸川)

UCSB → UChicago

HKU-UCAS young physicist forum (May 10, 2023)

Collaborators

UCSB



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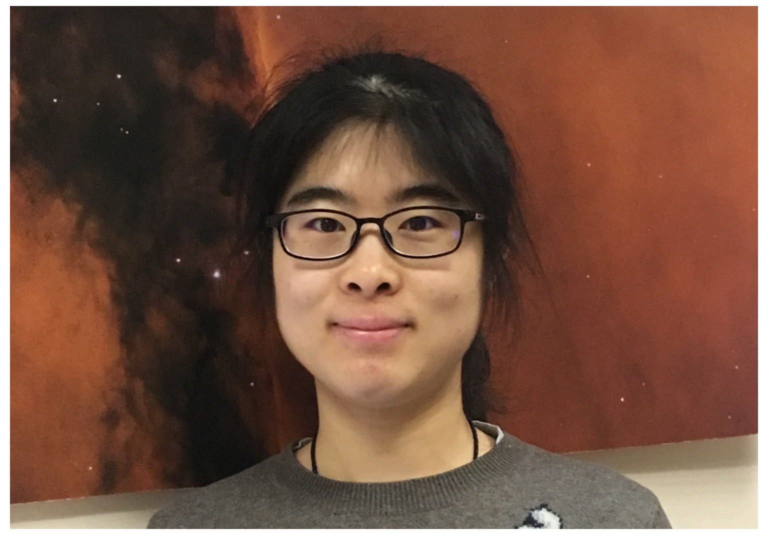

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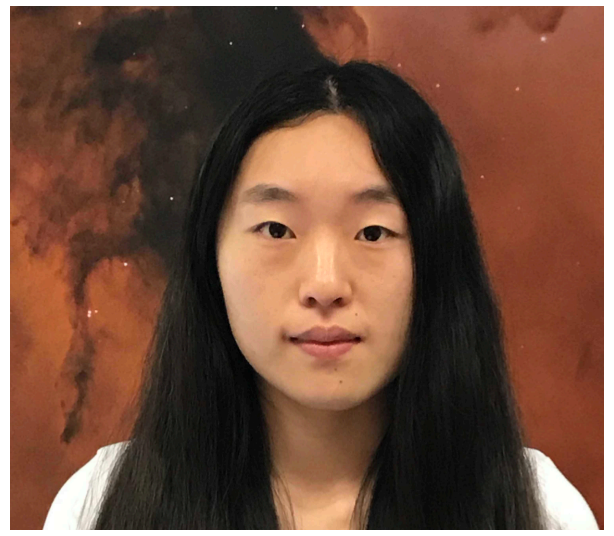


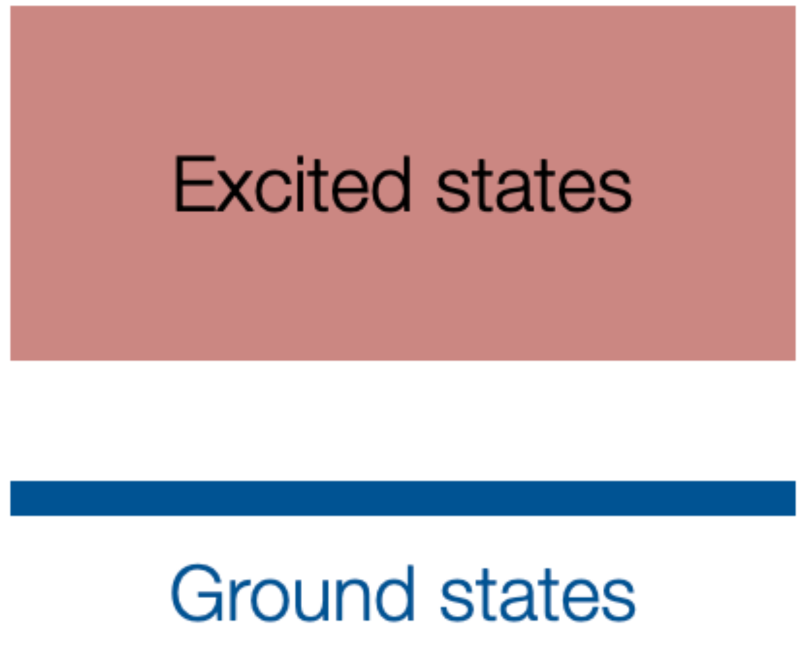
Zhu-Xi Luo

Y. Xu, XW, M. Ye, Z.-X. Luo, C.-M. Jian, and C. Xu,
(arXiv:2106.14910) PRX 12, 021067 (2022)

Content

- **I.** Brief introduction to quantum phases and phase transitions.
- **II.** Experimental motivations and a theoretical proposal for continuous Mott transition with charge fractionalization.

Quantum phases of matter (equilibrium)



Gapped phases

- **Trivial gapped phases**
  i.e., trivial product states
- **Symmetry-protected topological (SPT) phases**
  e.g., topological insulators/superconductors
- **Topologically ordered phases**
  e.g., fractional quantum Hall, gapped spin liquids

  ……

Gapless phases

- **Goldstone modes (Landau ordered phases)**
  e.g., superfluid, Néel order
- **Landau Fermi liquids**
  i.e., all ordinary metals
- **Coulomb phase (emergent gauge theories)**
  e.g., emergent photons in quantum spin ice

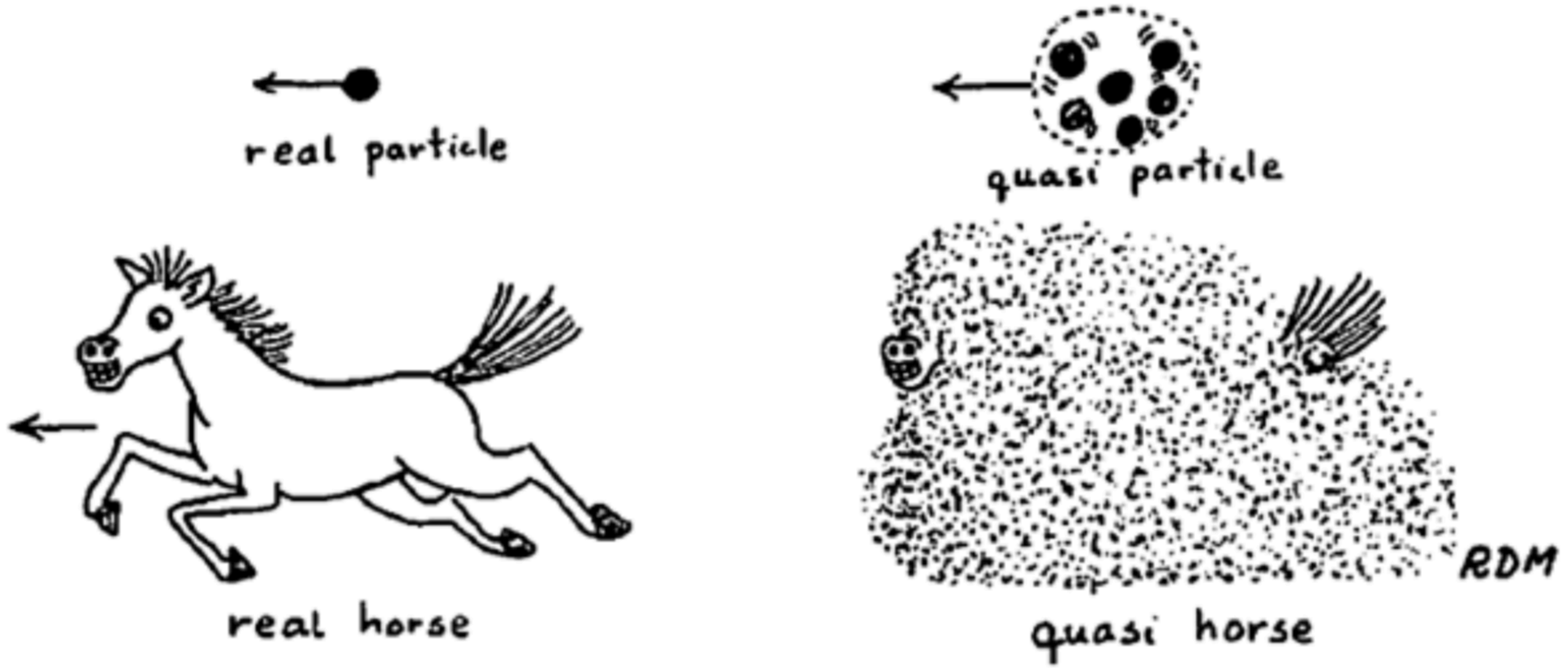
  ……

Quantum phases of matter: **two cornerstones**

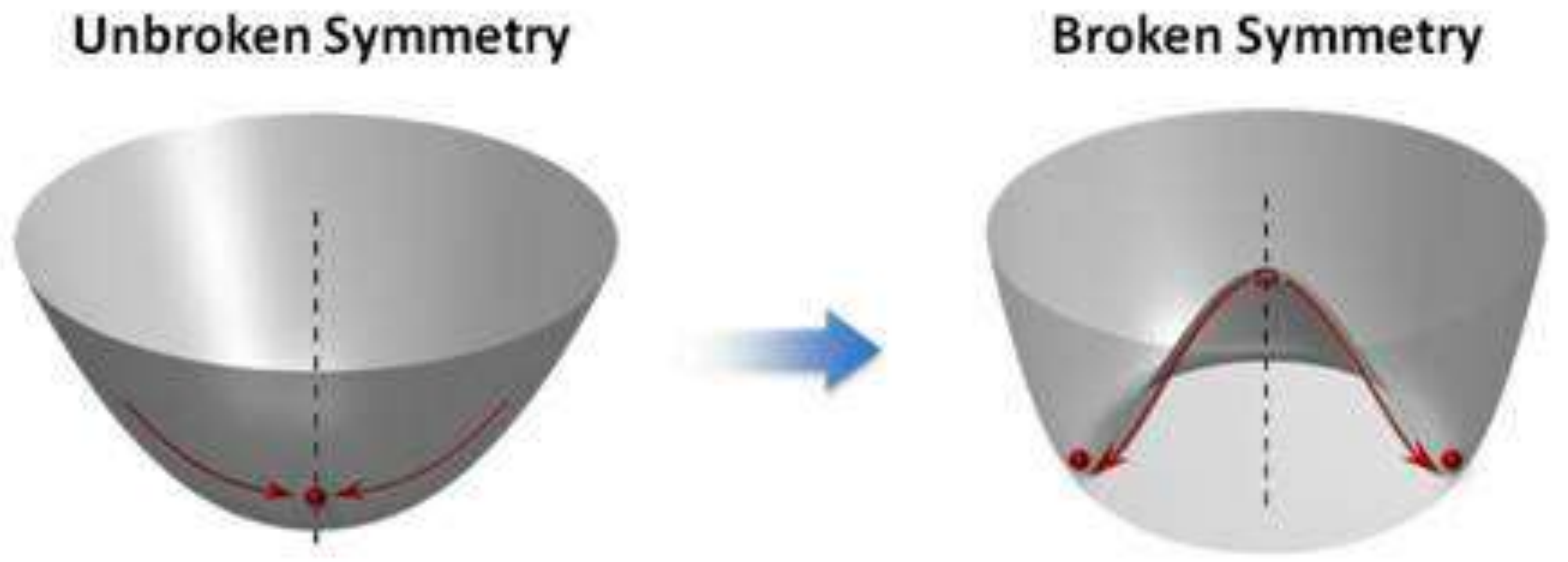
- **Landau Fermi liquid theory:** despite interactions between electrons, collective excitations (quasiparticles) are adiabatically connected to original electrons (with the same quantum numbers and statistics).

- **Landau symmetry paradigm:** phases of matter → by how states represent their symmetries (whether symmetries are spontaneously broken, whether symmetries are anomalous).

- The modern extension of the Landau paradigm by generalized symmetries (e.g., higher-form symmetries) and 't Hooft anomalies.



(figure credit: R. Mattuck)



(figure credit: Peking University)

Quantum phases of matter

- **Landau symmetry paradigm**
- **Landau Fermi liquid theory**

- **Trivial gapped phases**
  i.e., trivial product states
- **Symmetry-protected topological (SPT) phases**
  e.g., topological insulators/superconductors
- **Topologically ordered phases**
  e.g., fractional quantum Hall, gapped spin liquids
  ……

Symmetry is anomalous (boundary)

Spontaneous symmetry breaking

Landau quasiparticles

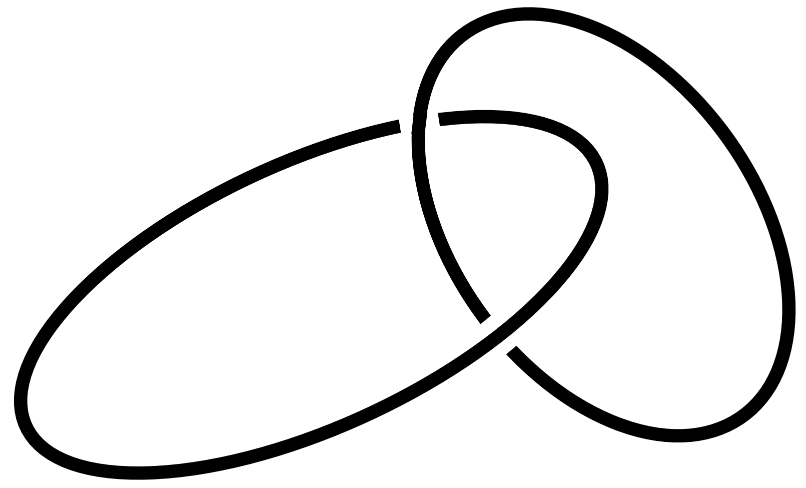
- **Goldstone modes (Landau ordered phases)**
  e.g., superfluid, Néel order
- **Landau Fermi liquids**
  i.e., all ordinary metals
- **Coulomb phase (emergent gauge theories)**
  e.g., emergent photons in quantum spin ice
  …… (photons = Goldstone modes of 1-form symmetry)

Aside: topological order as SSB of 1-form symmetry

- Ordinary symmetries (0-form symmetries) are acting on 0-dimensional objects (quantum numbers are carried by quasiparticles); p-form symmetries are acting on p-dimensional objects.

Aside: topological order as SSB of 1-form symmetry

- Ordinary symmetries (0-form symmetries) are acting on 0-dimensional objects (quantum numbers are carried by quasiparticles); p-form symmetries are acting on p-dimensional objects.
- $\nu = 1/k$ Laughlin quantum Hall state has $\mathbb{Z}_k$ 1-form symmetry acting on Wilson loops
- $\mathbb{Z}_k$ 1-form symmetry transformations are given by braiding of anyons



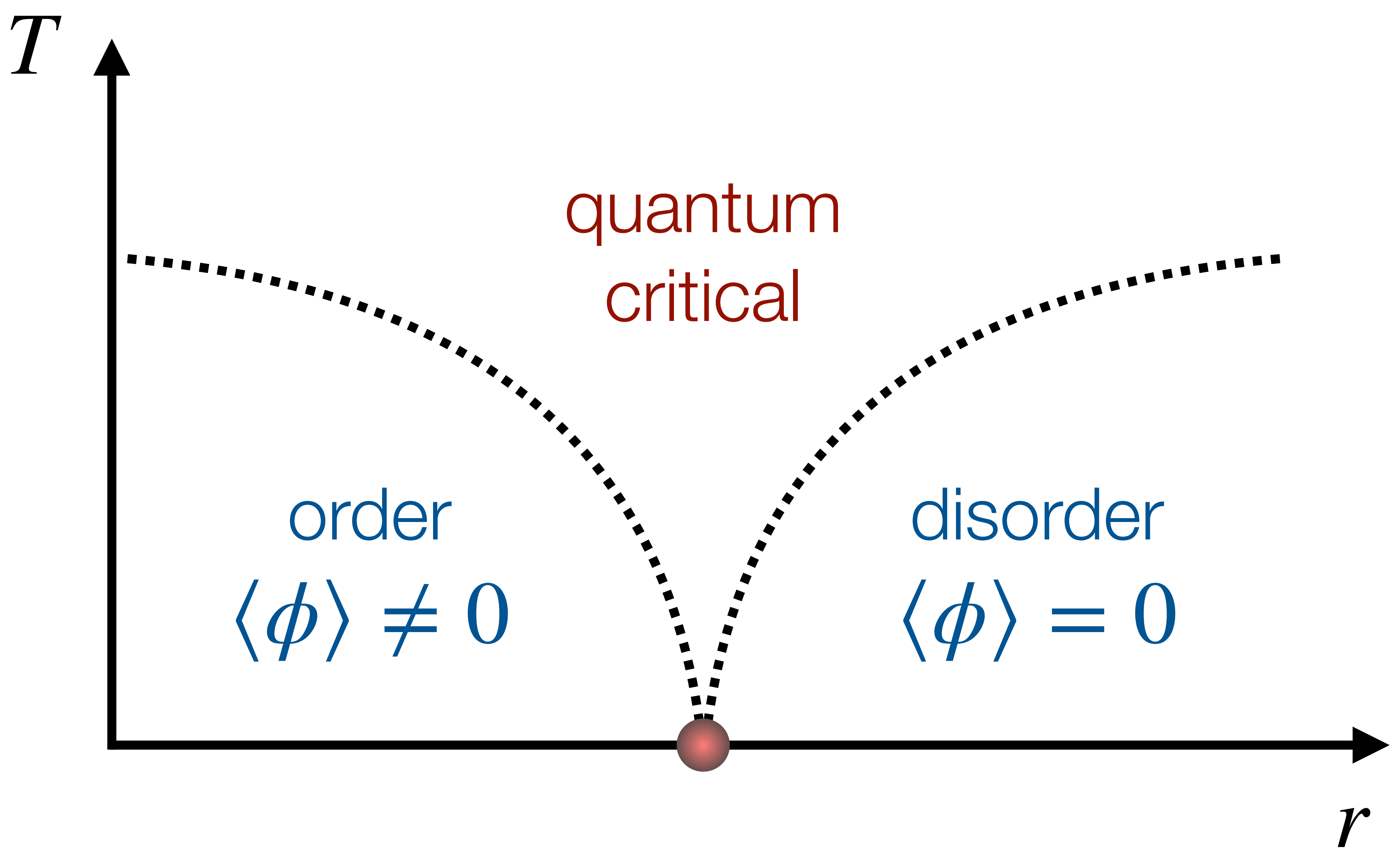
- $U(1)$ Chern-Simons at level k invariant under $a \to a + \gamma/k$ with flat connection γ
- Deconfined phase of gauge theory $\leftrightarrow$ Spontaneous symmetry breaking of 1-form symmetry

Modern generalizations of symmetries:
higher-form symmetries, subsystem symmetries,
categorical symmetries (non-invertible symmetries),
higher-group symmetries, loop-group symmetries, etc.

See reviews
McGreevy, arXiv:2204.03045
Cordova et al, arXiv:2205.09545

Quantum phase transitions in insulators

Landau ordinary symmetry-breaking transitions (order parameter ϕ)



Quantum phase transitions in insulators

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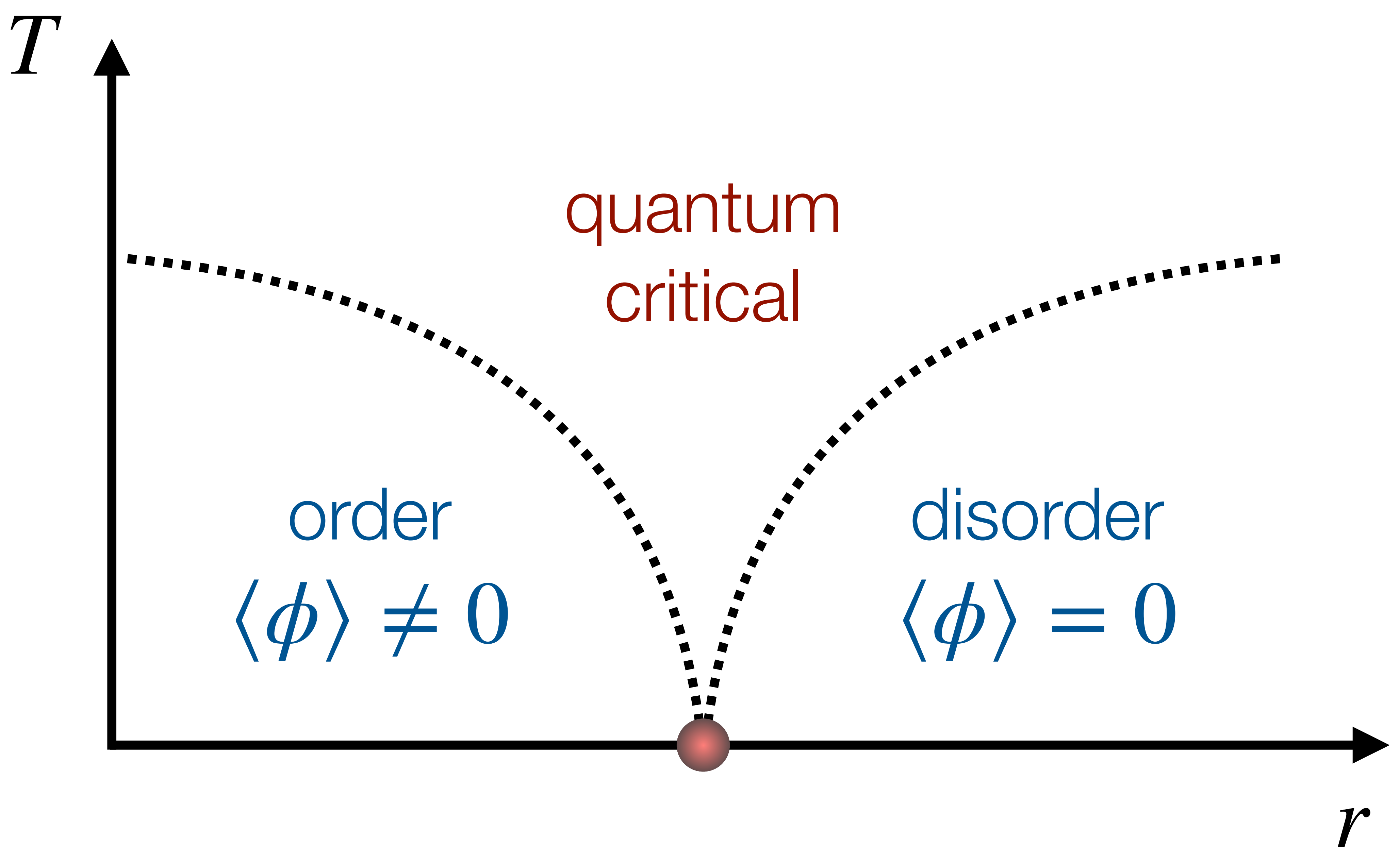
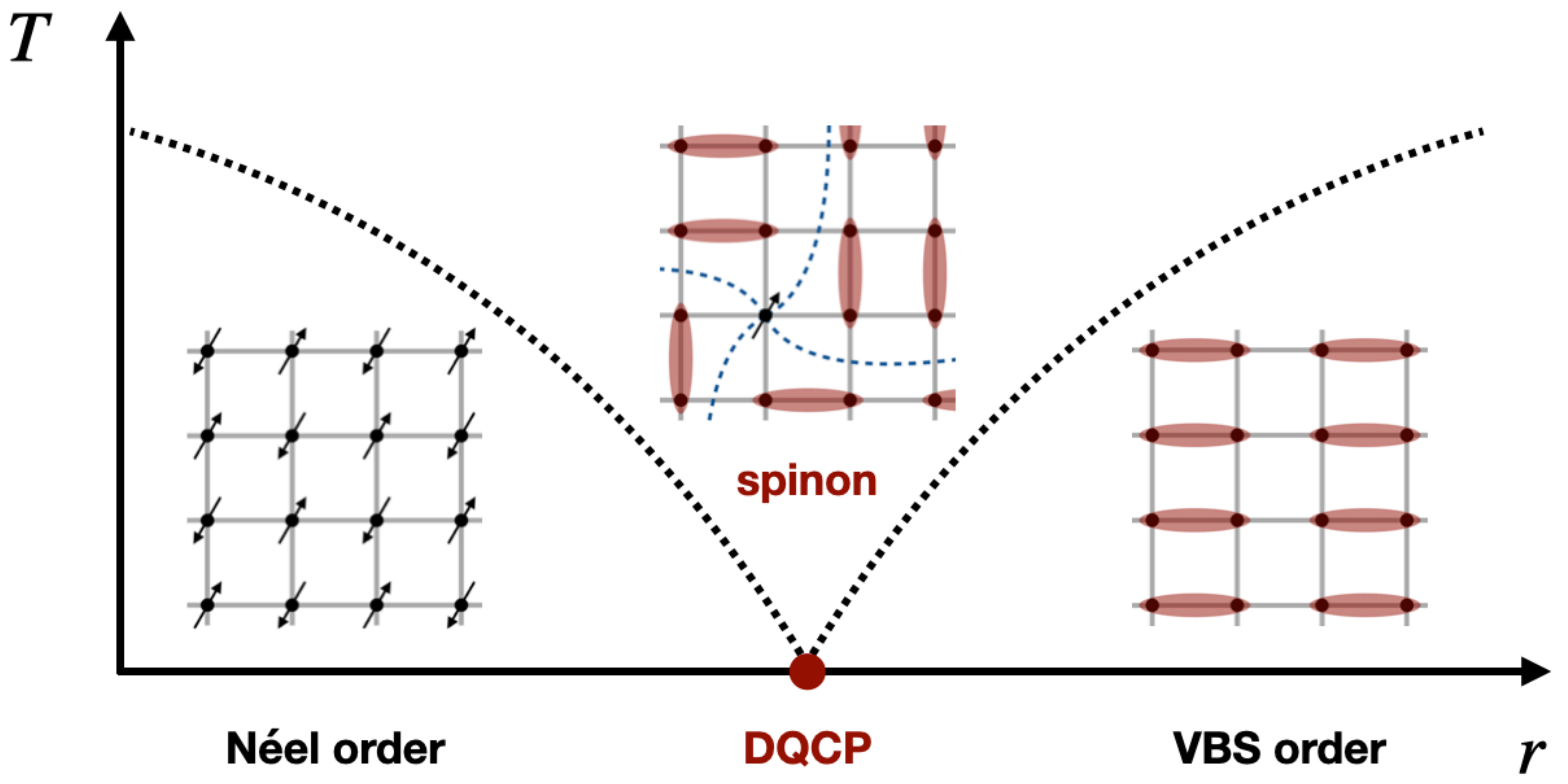


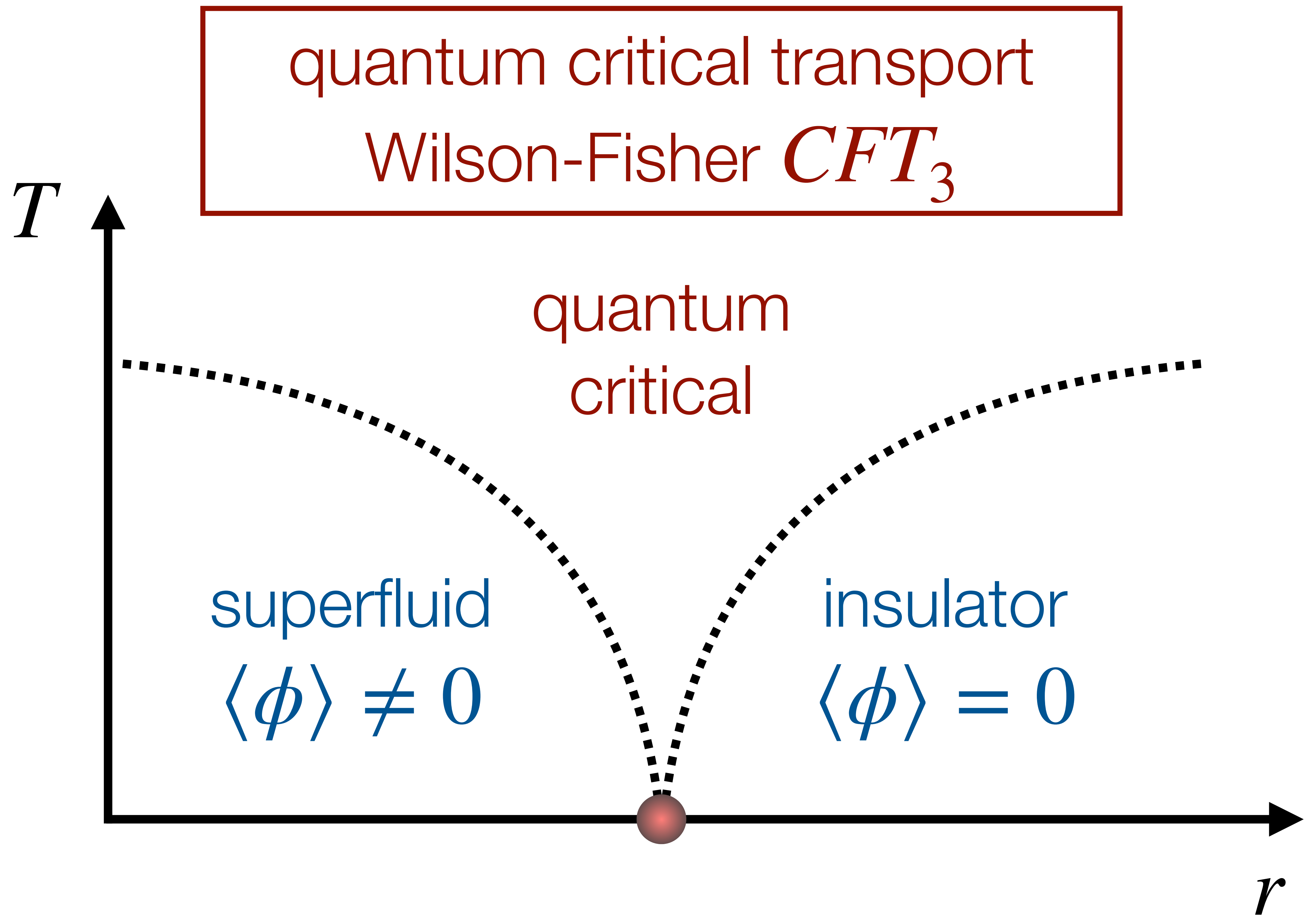
Deconfined quantum criticality (Néel-VBS transition)
Senthil-Vishwanath-Balents-Sachdev-Fisher 2004



Critical transport in 3D XY universality class

Landau symmetry-breaking transition in 2+1D

$$S = \int d\tau d^2\boldsymbol{x}\, |\partial_\tau \phi|^2 + |\nabla \phi|^2 + r|\phi|^2 + u|\phi|^4 + \ldots$$



Haviland et al. PRL 62, 2180 (1989)
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Cha et al. PRB 44, 6883 (1991)
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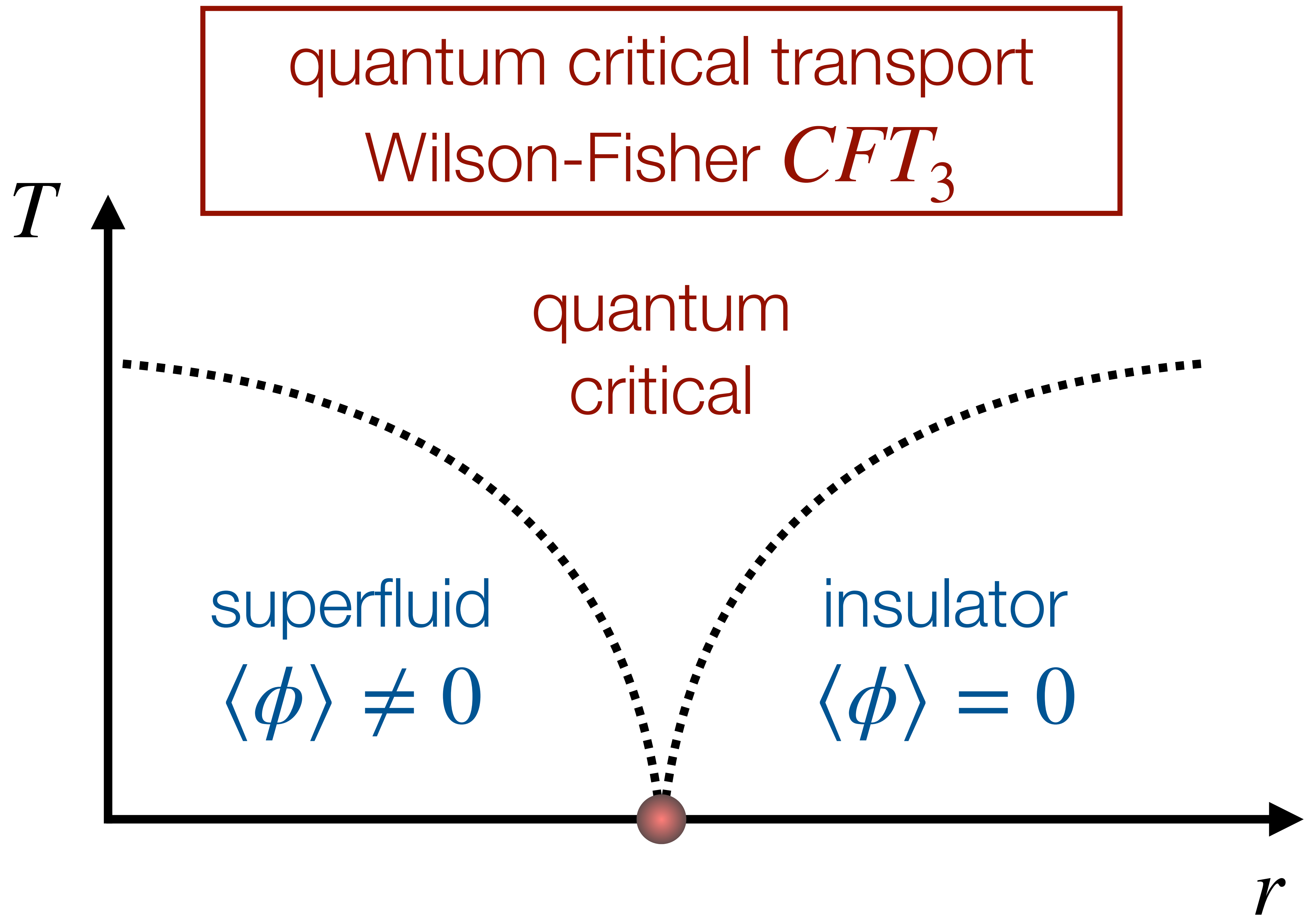
Fazio-Zappalà PRB(R) 8883 (1996)
Damle-Sachdev PRB 56, 8714 (1997)
Šmakov-Sørensen PRL 95, 180603 (2005)
Witczak-Krempa et al. PRB 86, 245102 (2012)
Chen et al. PRL 112, 030402 (2014)
Chester et al. JHEP 2020, 142 (2020)

Critical transport in 3D XY universality class

Universal conductivity: $\Sigma(\tilde{\omega})$ is a dimensionless universal scaling function in 2+1D

$$\sigma(\omega/T) = \frac{e^2}{h}\Sigma\left(\frac{\hbar\omega}{k_B T}\right)$$



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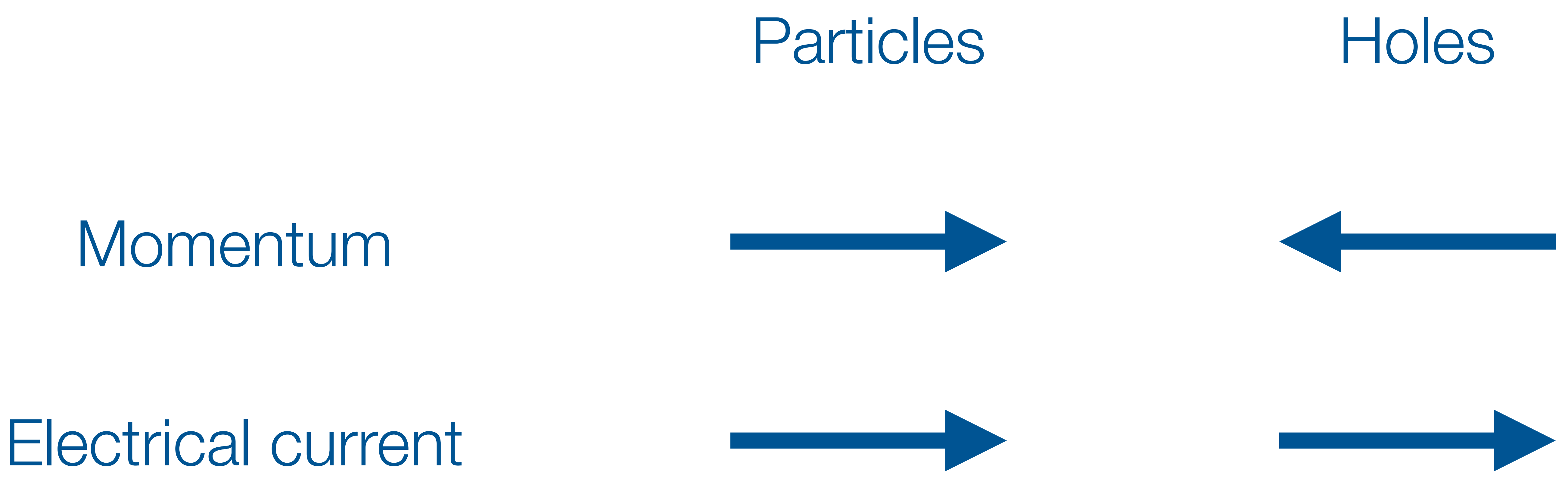
Ordinary transport:
finite conductivity always needs impurity or Umklapp scattering (for momentum relaxation)

Quantum critical transport (with particle-hole symmetry):
conductivity is finite **without disorder and Umklapp**



Critical transport in 3D XY universality class

Universal conductivity: $\Sigma(\tilde{\omega})$ is a dimensionless universal scaling function in 2+1D

$$\sigma(\omega/T) = \frac{e^2}{h}\Sigma\left(\frac{\hbar\omega}{k_B T}\right)$$

- Fully determining the shape of the scaling function $\Sigma(\tilde{\omega})$ is challenging using conventional field-theory methods.
- Under the limits $\hbar\omega \gg k_B T$ and $\hbar\omega \ll k_B T$, people have calculated $\sigma(0)$ and $\sigma(\infty)$ using analytical methods like small-ϵ expansion and large-N expansion, or numerical methods like Monte Carlo simulation and conformal bootstrap.
- The DC conductivity $\sigma(0)$ is easier to measure in experiments.

Critical transport in 3D XY universality class

Universal conductivity: $\Sigma(\tilde{\omega})$ is a dimensionless universal scaling function in 2+1D

$$\sigma(\omega/T) = \frac{e^2}{h}\Sigma\left(\frac{\hbar\omega}{k_B T}\right)$$

$\Sigma(0)$	$\Sigma(\infty)$	
≈ 1		experiment in PRL 62, 2180 (1989)
≈ 1		experiment in PRL 67, 2068 (1991)
	0.315	ϵ-expansion in PRB 8883 (1996)
1.037	0.3927	ϵ-expansion in PRB 56, 8714 (1997)
1.068		large-N in PRB 86, 245102 (2012)
	0.359(4)	Monte Carlo in PRL 112, 030402 (2014)
	0.355155(11)	conformal bootstrap in JHEP 2020, 142 (2020)

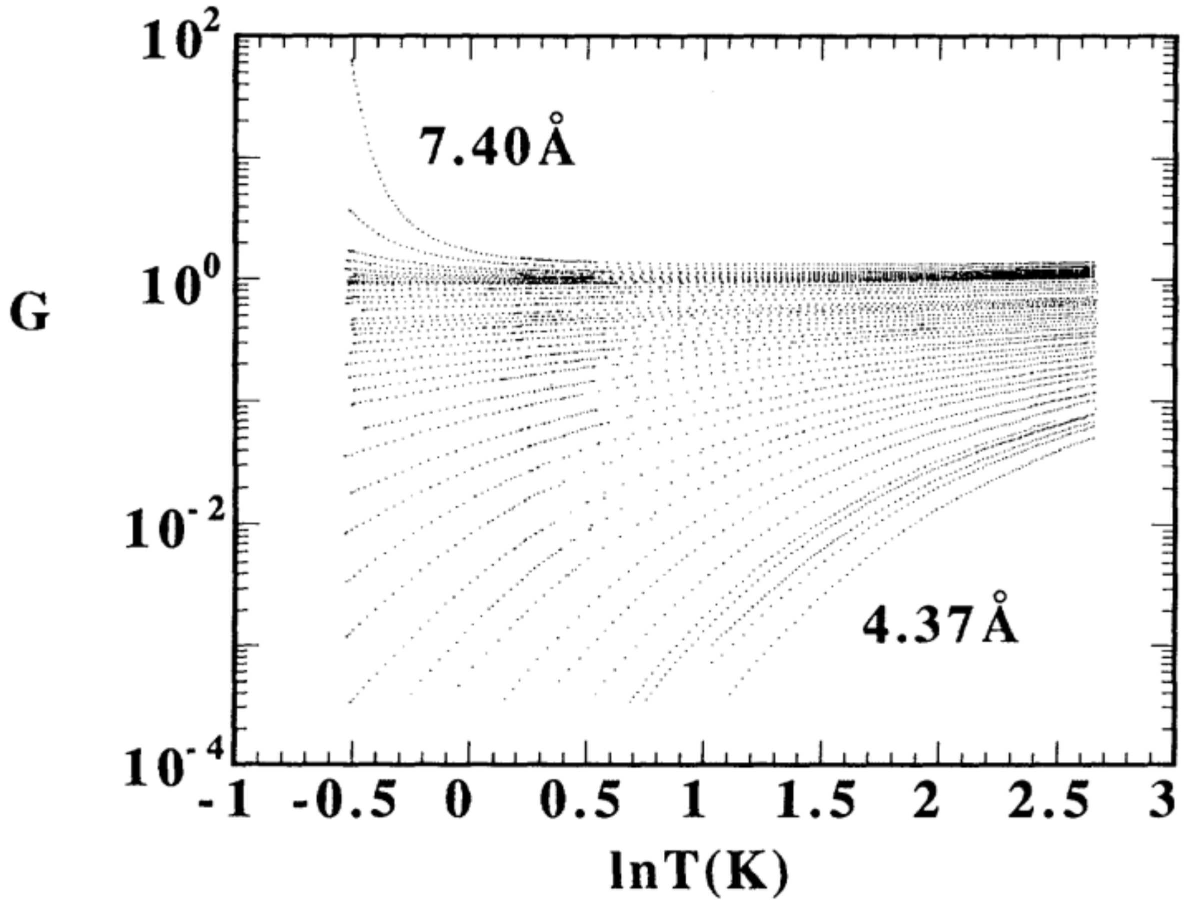


FIG. 1. Logarithm of the conductance G, in units of $4e^2/h$, vs $\ln(T)$ for a number of different Bi films. The thickness of the first (thinnest) and last (thickest) films are indicated.

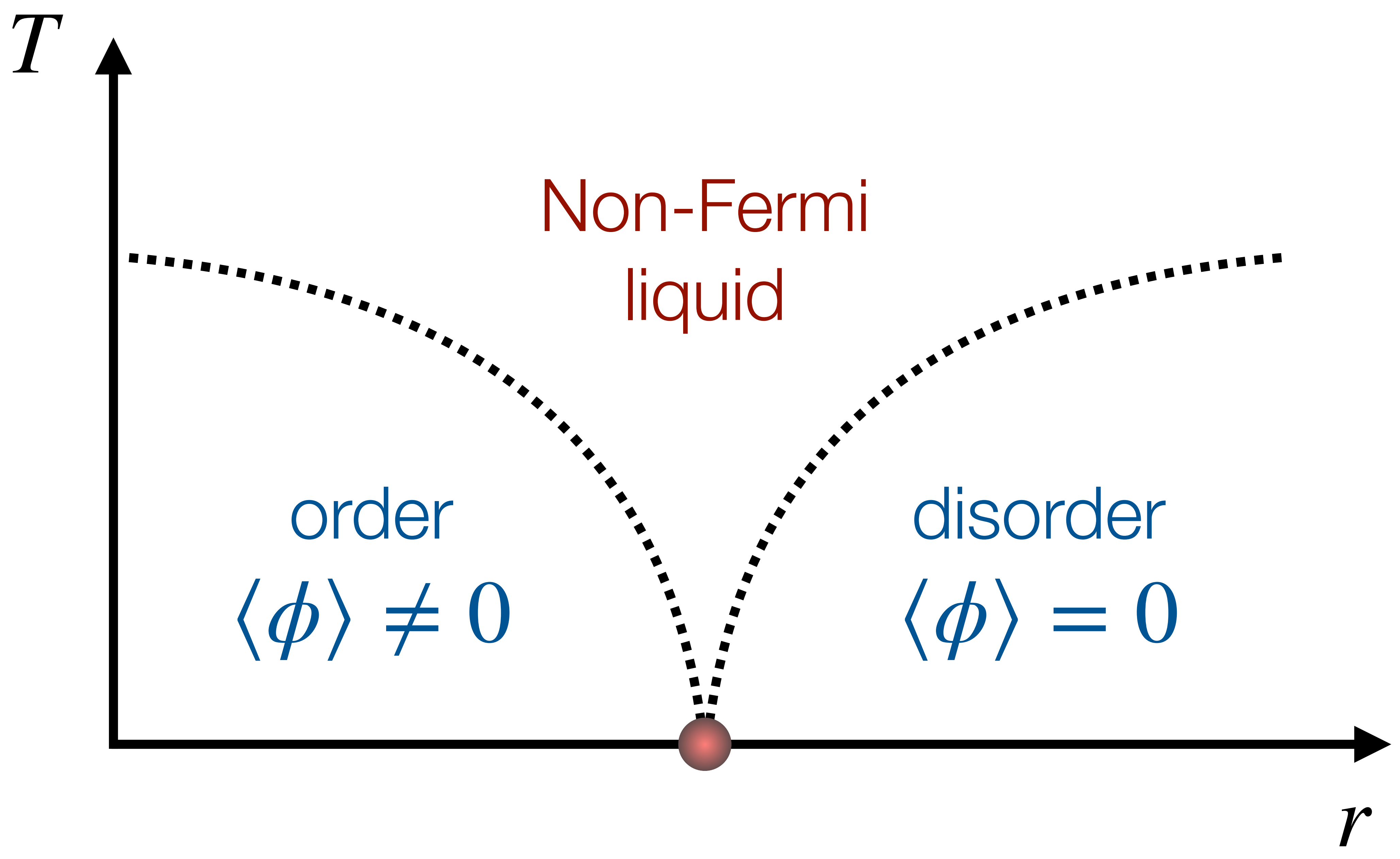
- Maybe we can trust $\Sigma(\infty) \approx 0.36$ (conformal bootstrap) and $\Sigma(0) \approx 1$ (experiment).

- Universal resistivity $\rho = \sigma^{-1}$ (two values the same order): $\rho(\infty) \approx 3\rho(0) \approx 3\dfrac{h}{e^2}$.

Quantum phase transitions in metals

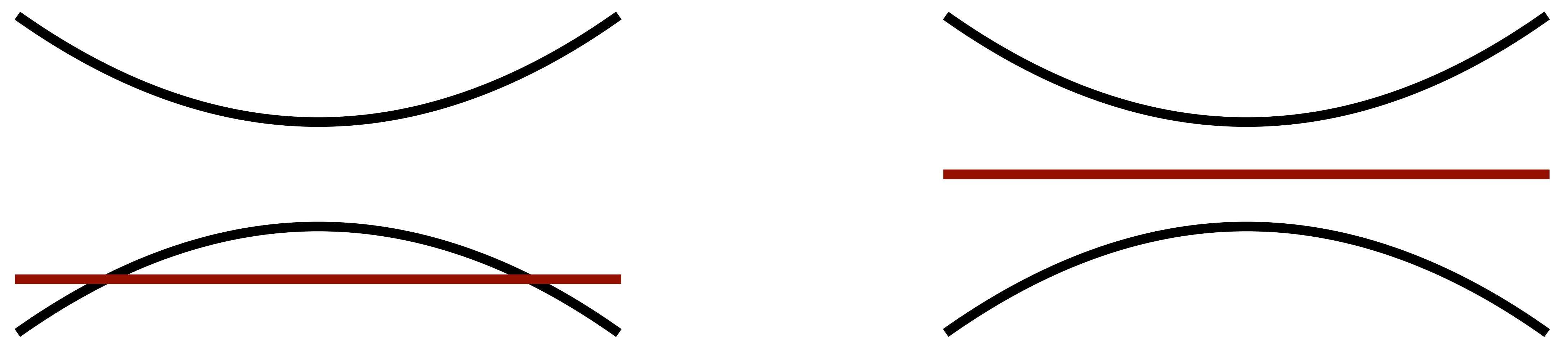
- Quantum phase transitions involving **fermi-surface** states remain poorly understood (technically and conceptually).

- For conventional symmetry-breaking transitions in 2+1D metals, the fermi-surface states strongly renormalized $\rightarrow$ breakdown of Landau Fermi liquid theory (no controlled theory, even today).



Quantum phase transitions in metals

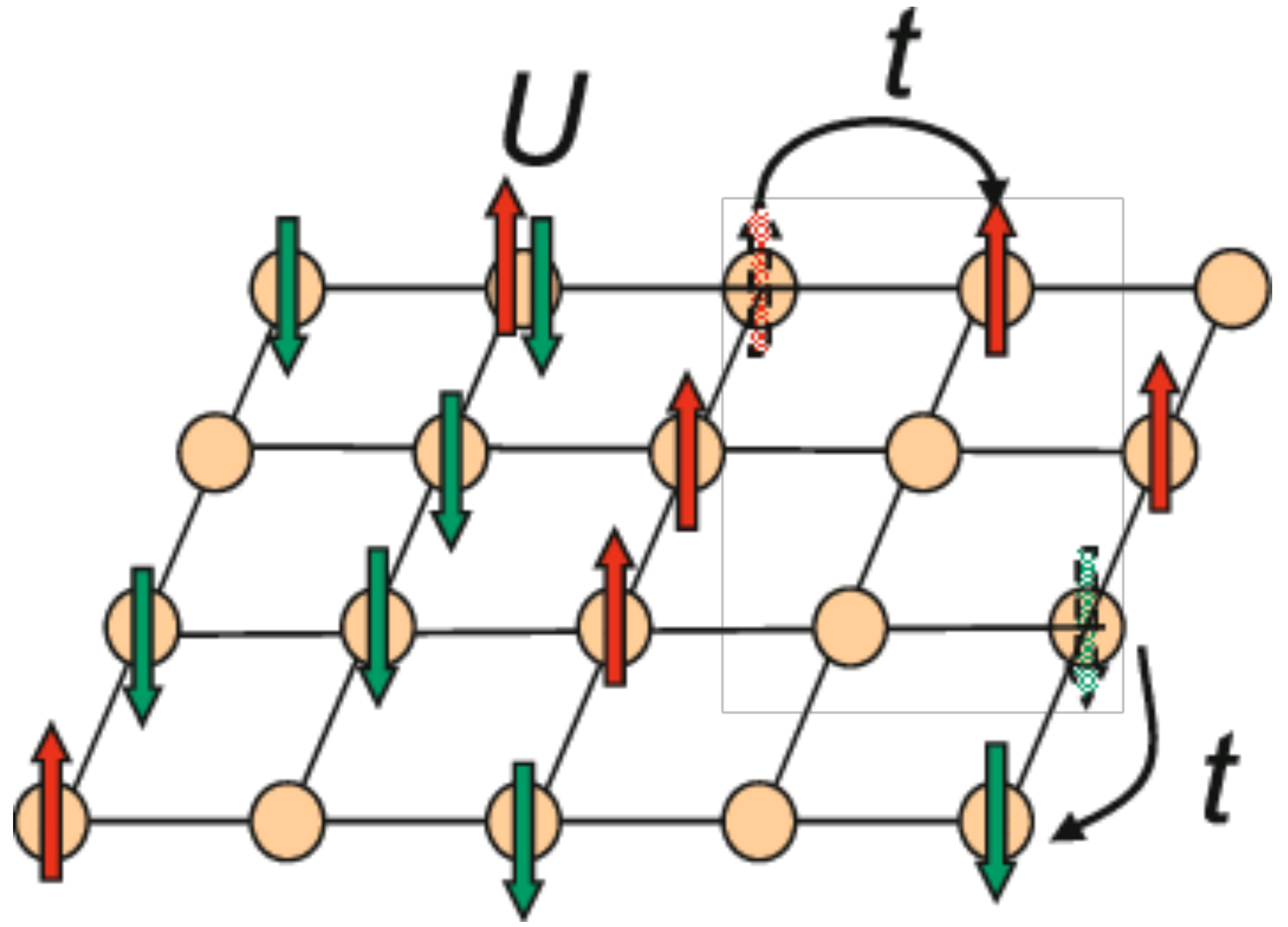
- Quantum phase transitions involving **fermi-surface** states remain poorly understood (technically and conceptually).
- For conventional symmetry-breaking transitions in 2+1D metals, the fermi-surface states strongly renormalized $\rightarrow$ breakdown of Landau Fermi liquid theory (no controlled theory, even today).
- This talk will be about **metal-insulator transition (MIT)** without symmetry breaking.
- The simple scenarios within band theory:



- Beyond band theory: (1) disorder-driven MIT; (2) **interaction-driven MIT** (our focus today)

Interaction-driven metal-insulator transition

- The one-band Hubbard model at half-filling
- $$H = -\sum_{\langle i,j \rangle} \sum_{\alpha=\uparrow,\downarrow} t_{ij}(c^{\dagger}_{i,\alpha} c_{j,\alpha} + c^{\dagger}_{j,\alpha} c_{i,\alpha}) + U \sum_{j} n_{j,\uparrow} n_{j,\downarrow}$$
- There is a competition between the hopping energy t and the on-site Coulomb repulsion U.
- (1) metal when $t/U \gg 1$; (2) insulator when $t/U \ll 1$
- The value of t/U (i.e., the bandwidth) is tunable in experiments by changing external parameters.



(figure credit: Yamada et al. 2018)

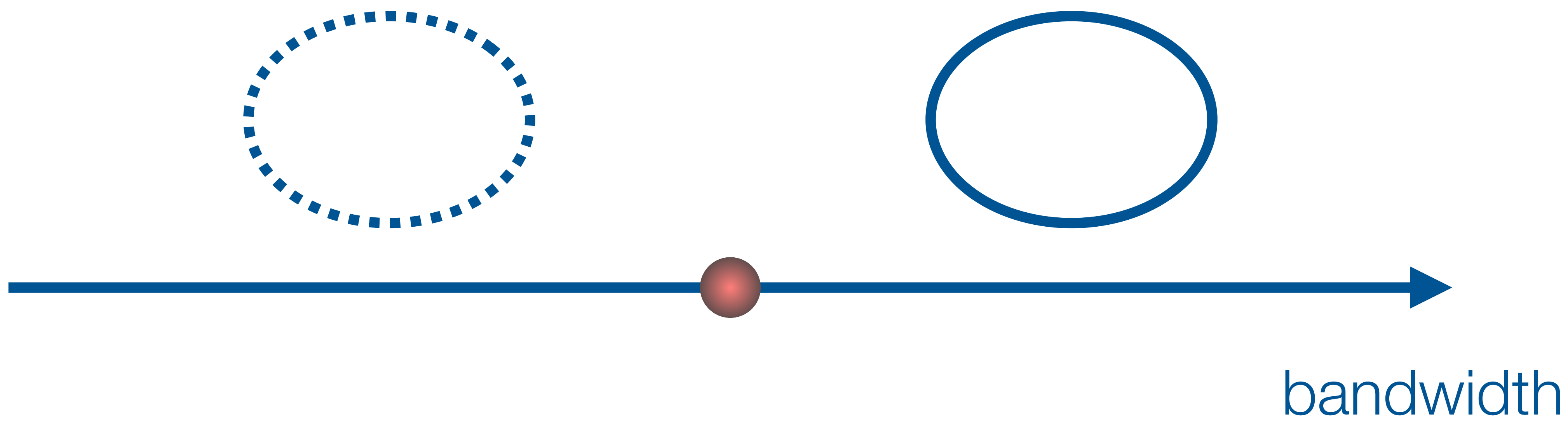
Interaction-driven metal-insulator transition

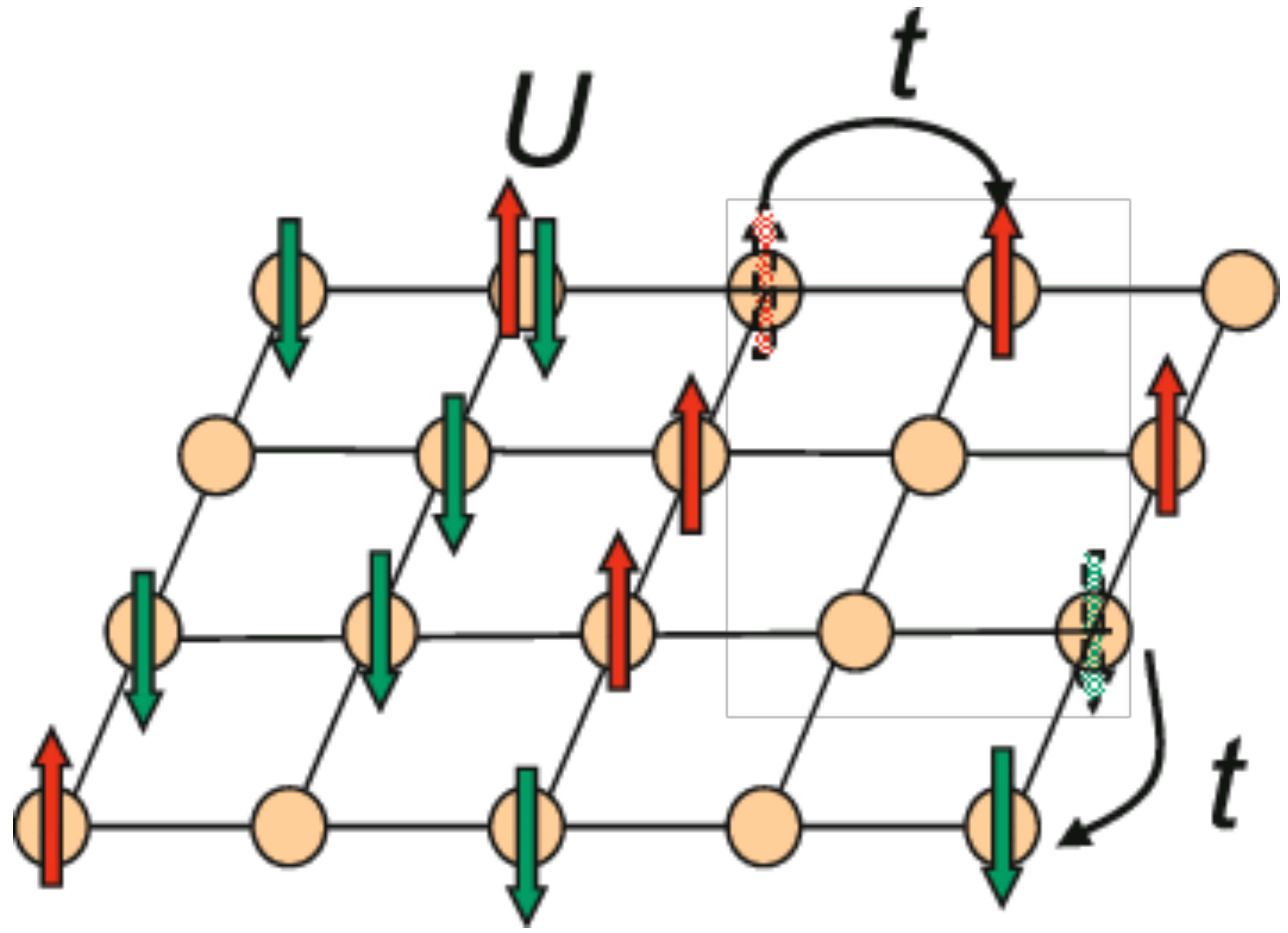
- The one-band Hubbard model at half-filling

- $$H = -\sum_{\langle i,j \rangle} \sum_{\alpha=\uparrow,\downarrow} t_{ij}(c^\dagger_{i,\alpha} c_{j,\alpha} + c^\dagger_{j,\alpha} c_{i,\alpha}) + U \sum_j n_{j,\uparrow} n_{j,\downarrow}$$

- Continuous metal-insulator transition?

- An idea (Senthil 2008): to make the electron Fermi surface disappear abruptly in a continuous fashion, a neutral Fermi surface remains on the insulator side.



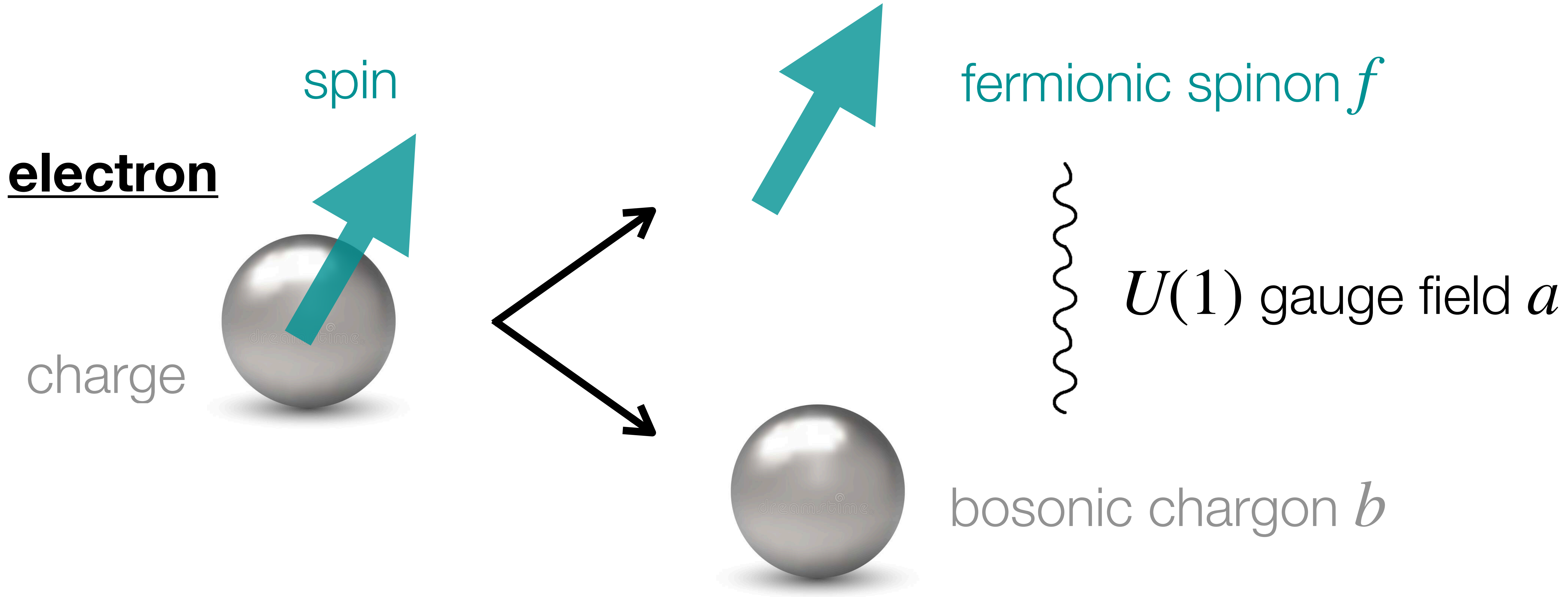


(figure credit: Yamada et al. 2018)

Lee-Lee, PRL (2005), Senthil, PRB (2008), etc

Continuous metal-insulator transition

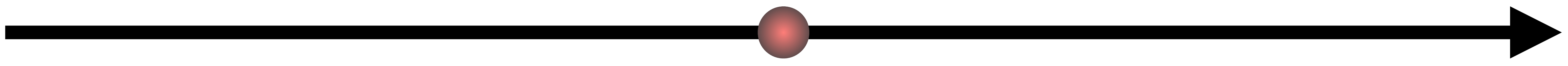
Interaction-driven transition at half-filling



b (dynamically decoupled from f, a): 3D XY transition

Mott insulator (spinon FS)

a is Higgsed, $c \sim \langle b \rangle f$ (electron FS)



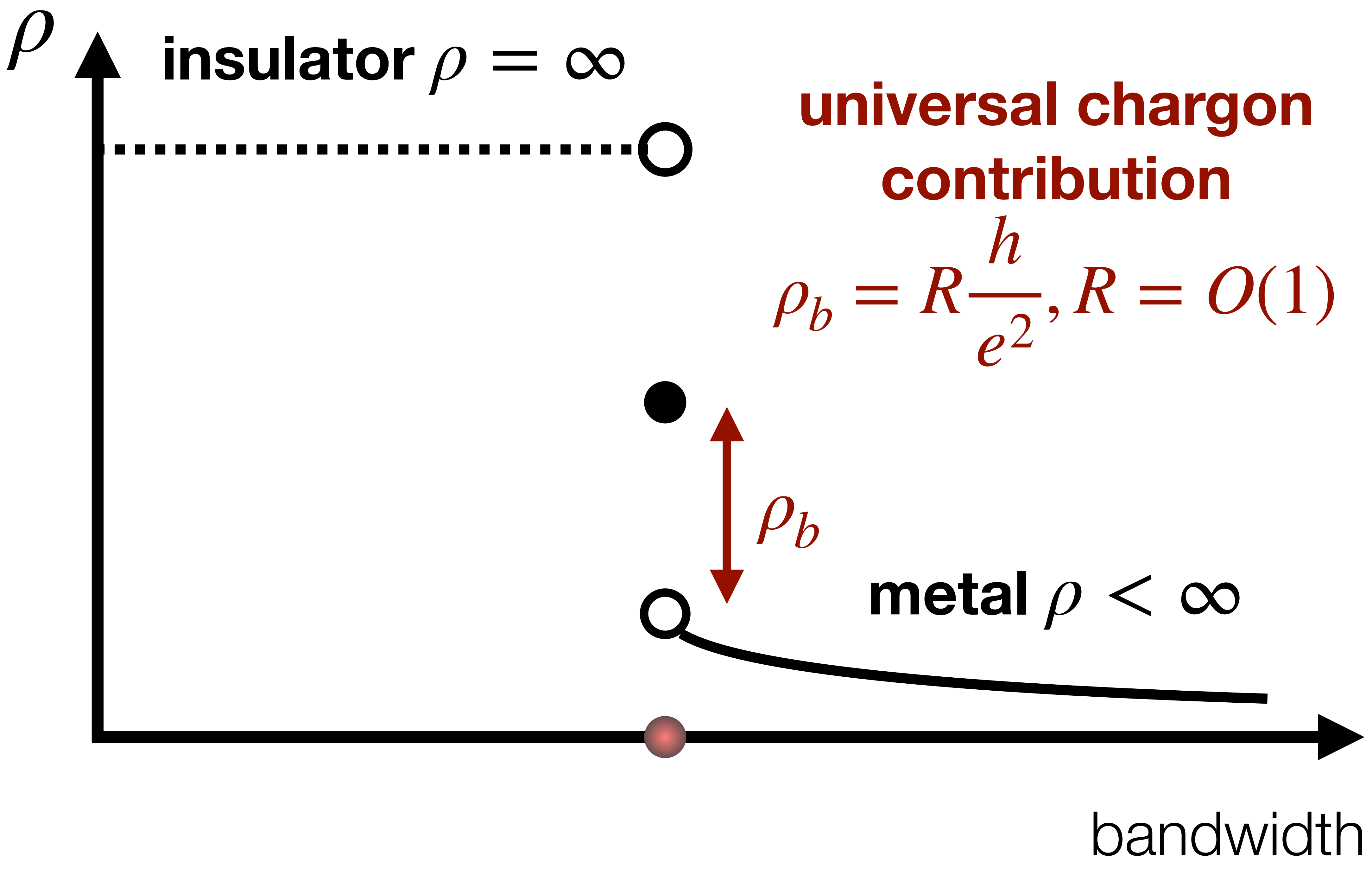
$\langle b \rangle = 0$

$\langle b \rangle \neq 0$

bandwidth

Electrical resistivity at continuous metal-insulator transition

- Ioffe-Larkin rule $\rho = \rho_f + \rho_b$; Insulator $\rho_b = \infty \Rightarrow \rho = \infty$; Metal $\rho_b = 0 \Rightarrow \rho = \rho_f$.
- Critical point: $\rho_b = R\frac{h}{e^2} \Rightarrow \rho = \rho_f + R\frac{h}{e^2}$, where R is of the order $1 < R < 10$.



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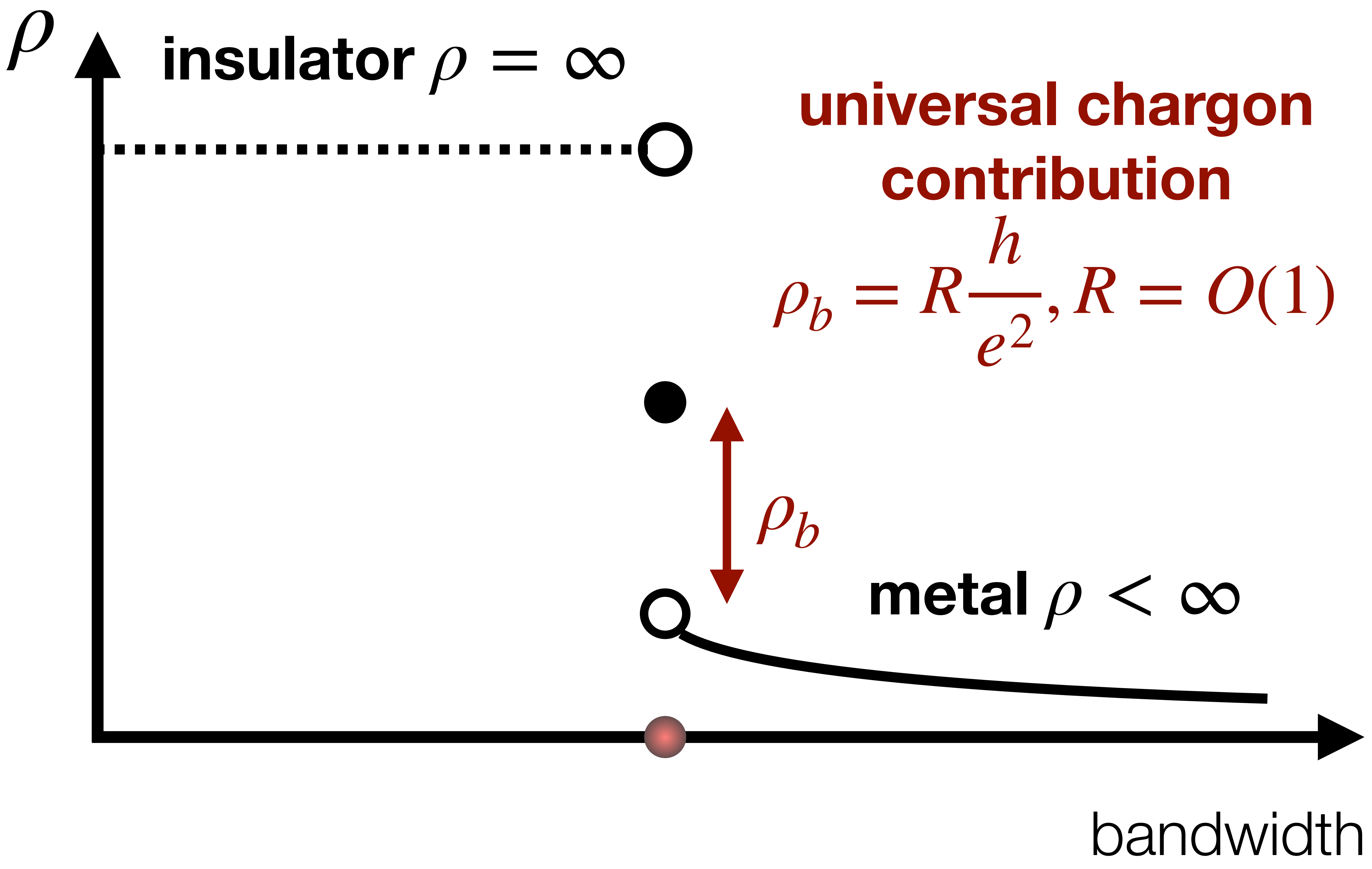

Universal chargon contribution $\rho_b(\omega/T)$ (large-N, MC results in Witczak-Krempa et al. PRB (2012)):

$$\rho_b(\infty) = 3.51\frac{h}{e^2} \text{ (Wilson-Fisher CFT)}$$

$$\rho_b(0) = 7.93\frac{h}{e^2} \text{ (WF CFT + damped gauge)}$$

ρ_b is NOT significantly larger than $\frac{h}{e^2}$

Electrical resistivity at continuous metal-insulator transition

- Ioffe-Larkin rule $\rho = \rho_f + \rho_b$; Insulator $\rho_b = \infty \Rightarrow \rho = \infty$; Metal $\rho_b = 0 \Rightarrow \rho = \rho_f$.
- Critical point: $\rho_b = R\frac{h}{e^2} \Rightarrow \rho = \rho_f + R\frac{h}{e^2}$, where R is of the order $1 < R < 10$.
- ρ_f is from weak disorder scattering, and below the Mott-Ioffe-Regel limit $\sim \frac{h}{e^2}$.
- In total, the critical resistivity $\rho = \rho_f + \rho_b$ is NOT significantly larger than $\frac{h}{e^2}$.

Content

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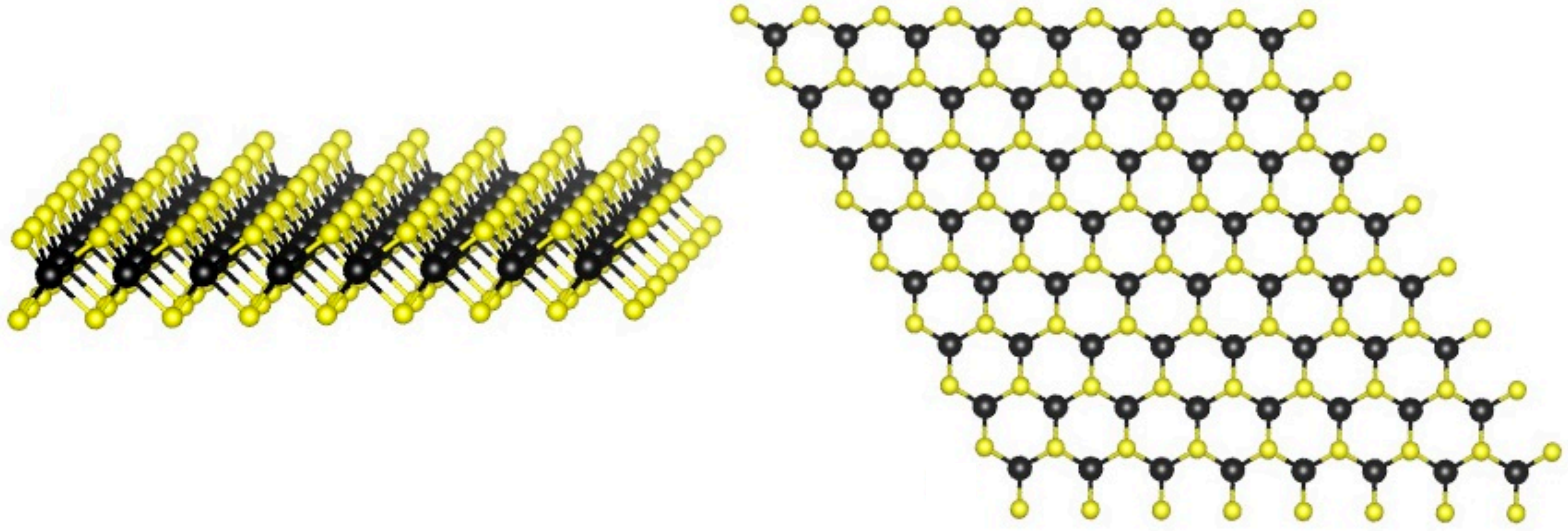
- **II.** Experimental motivations: a potentially interaction-driven continuous metal-insulator transition in transition-metal dichalcogenide (TMD) Moiré heterobilayer $MoTe_2/WSe_2$, which has anomalously large critical resistivity.

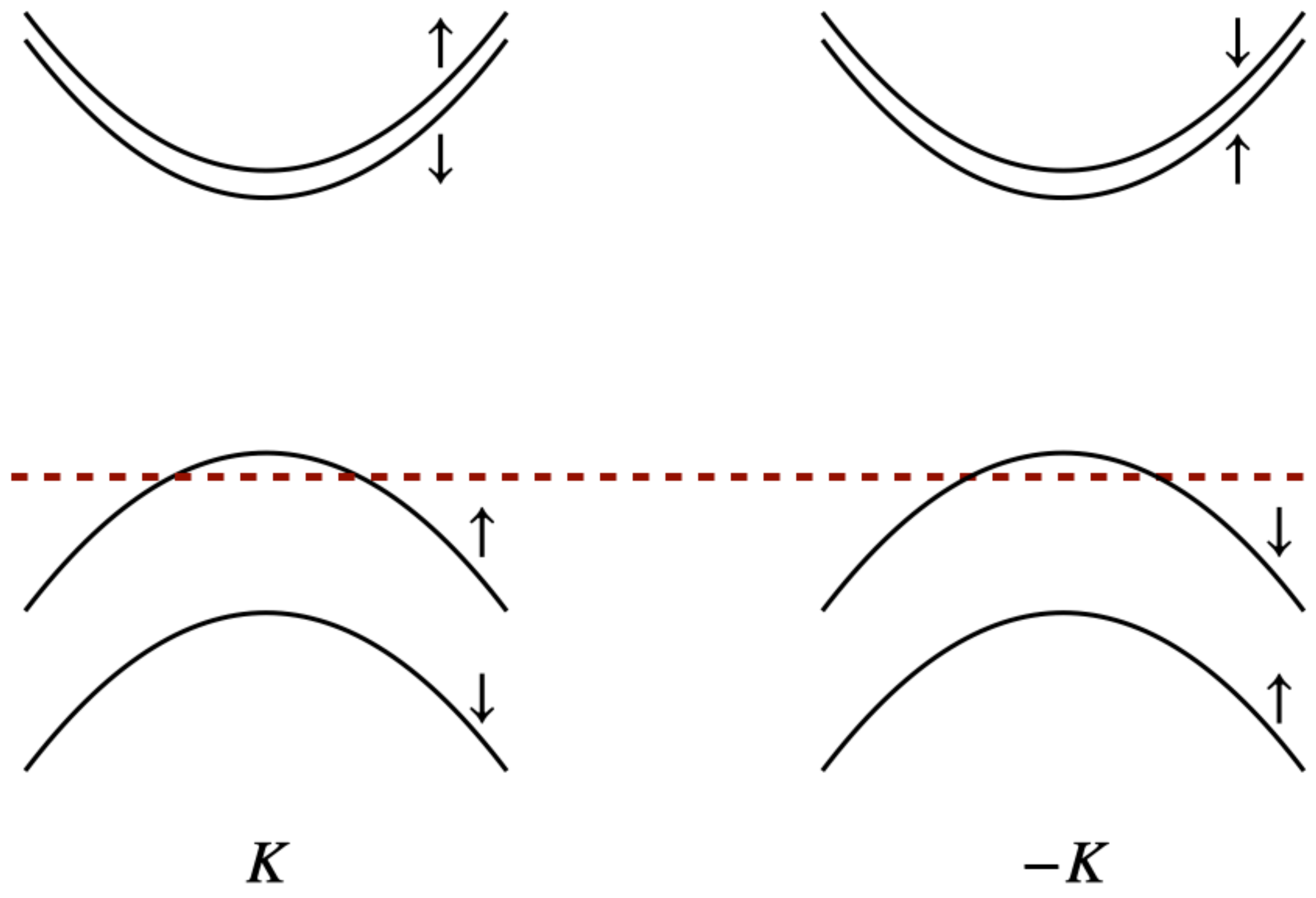
- **III.** Theoretical proposal for the interaction-driven continuous metal-insulator transition with charge fractionalization.

Transition metal dichalcogenides (TMDs)

- The hexagonal TMD monolayers (MoS_2, WS_2, $MoSe_2$, WSe_2, $MoTe_2$) are two-dimensional semiconductors with a direct band gap

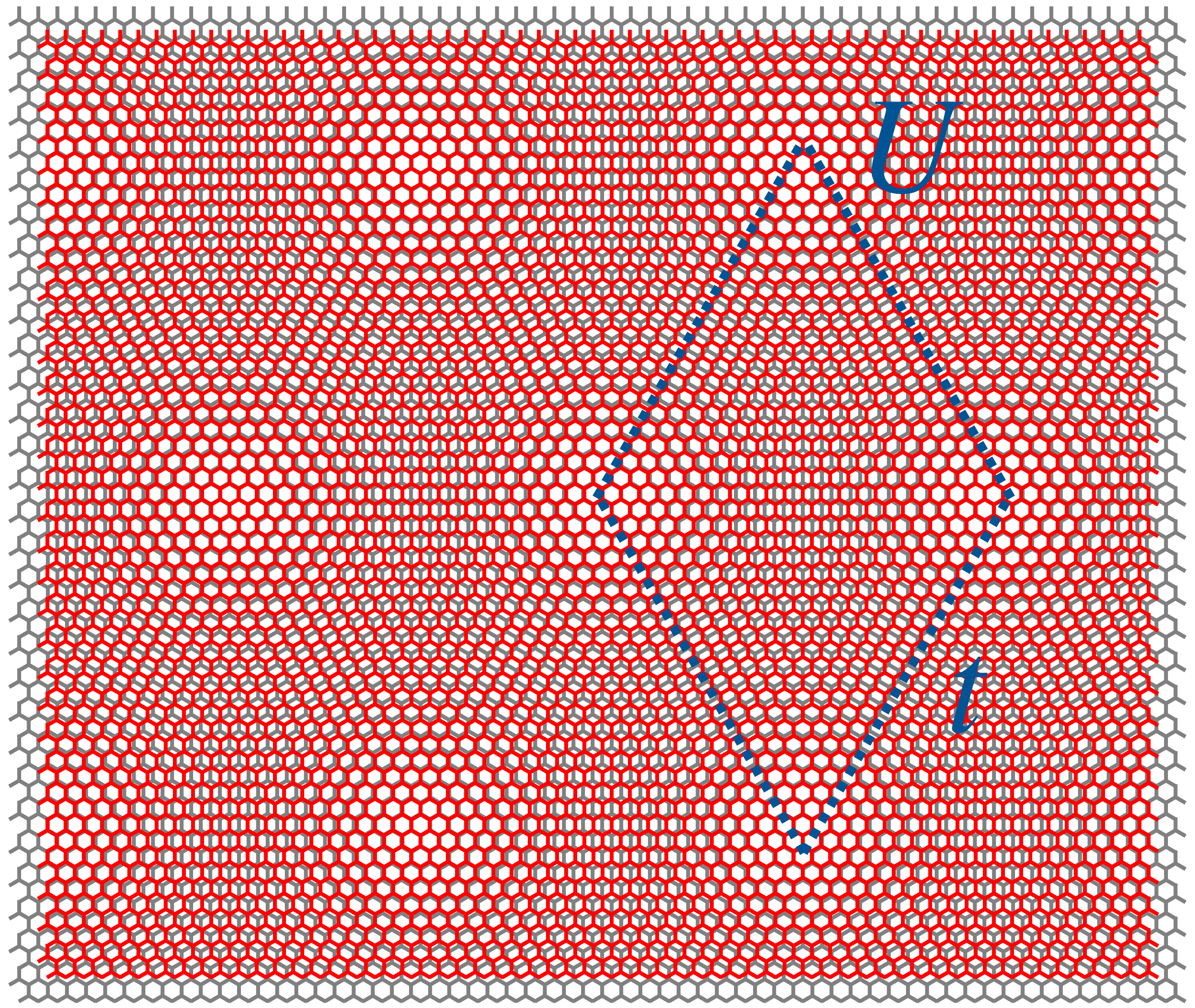
- The strong spin-orbit coupling in TMD monolayers leads to a spin-orbit splitting of hundreds of meV in the valence band and a few meV in the conduction band (**spin-valley locking**)





Hubbard physics in TMD heterobilayer $MoTe_2/WSe_2$

$MoTe_2/WSe_2$ bilayers (0-degree)



7% lattice mismatch

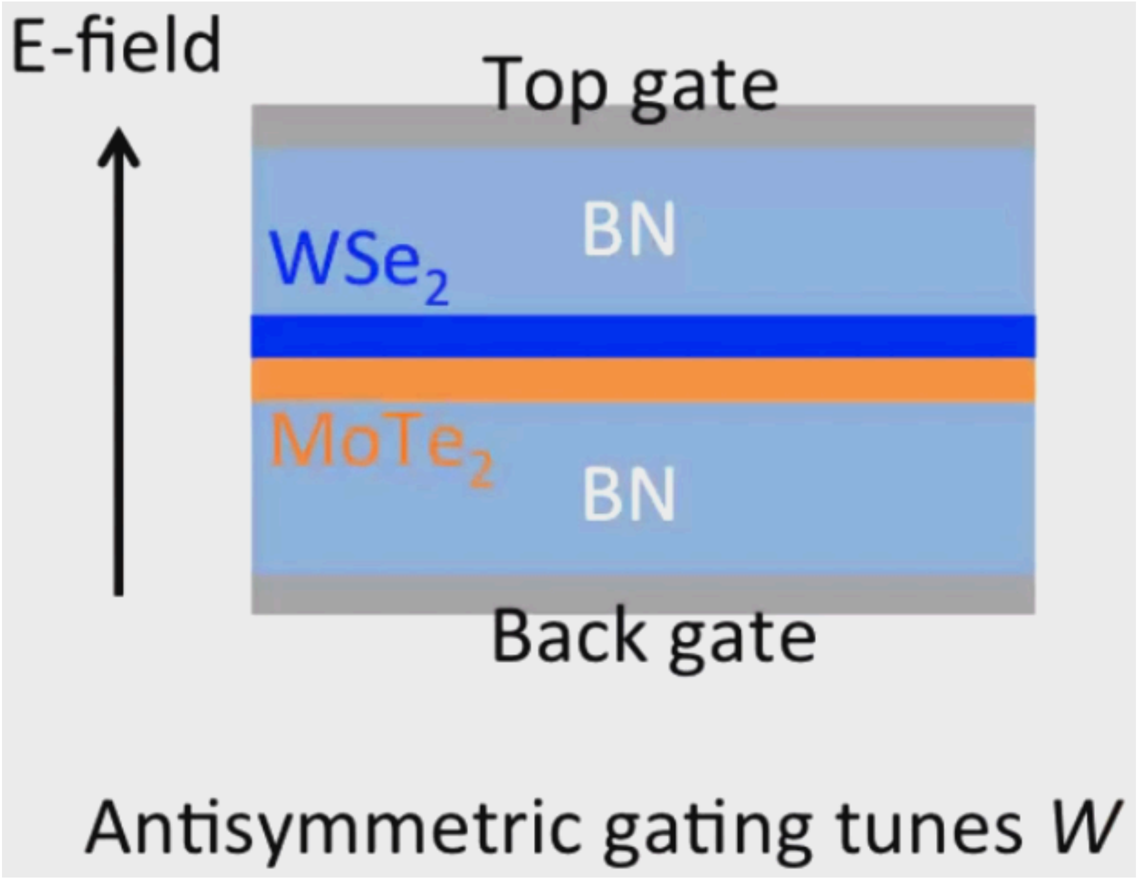
⇓

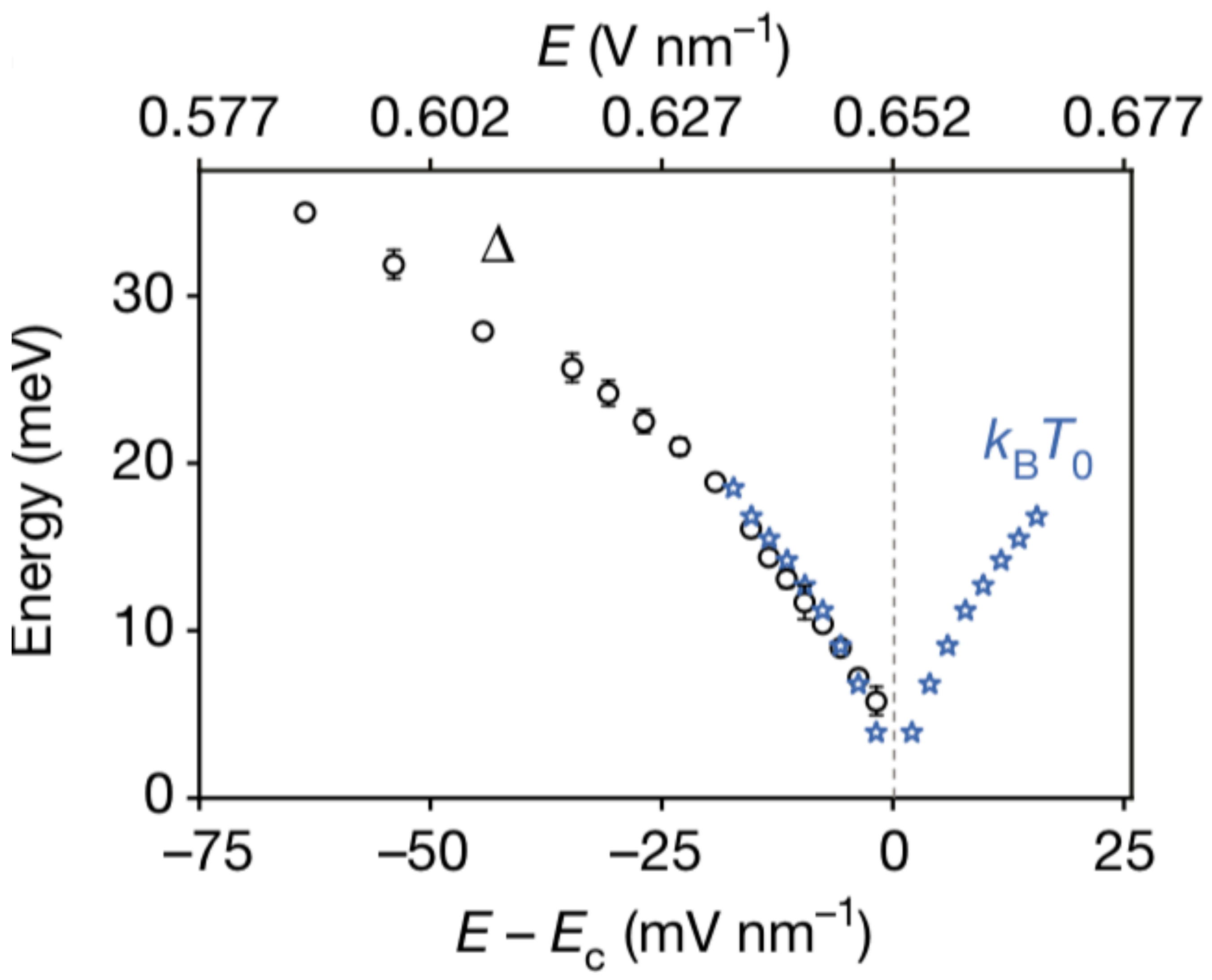
Moiré superlattice

$a_M \sim$ 5 nm

- TMD Moiré systems: t ~ 1-10 meV $\ll$ U ~ 50-100 meV.
- Topologically trivial bands ⇒ No Wannier obstruction
- Spin-valley locking ⇒ two degrees per site
- $$H = -\sum_{\langle i,j \rangle} \sum_{\alpha=\uparrow,\downarrow} t_{ij}(c^\dagger_{i,\alpha} c_{j,\alpha} + c^\dagger_{j,\alpha} c_{i,\alpha}) + U \sum_j n_{j,\uparrow} n_{j,\downarrow}$$
- The pseudo-spin degeneracy by time-reversal symmetry.
- But pseudo-spin $SU(2)$ is not guaranteed by microscopic symmetries (unlike the standard Hubbard model).

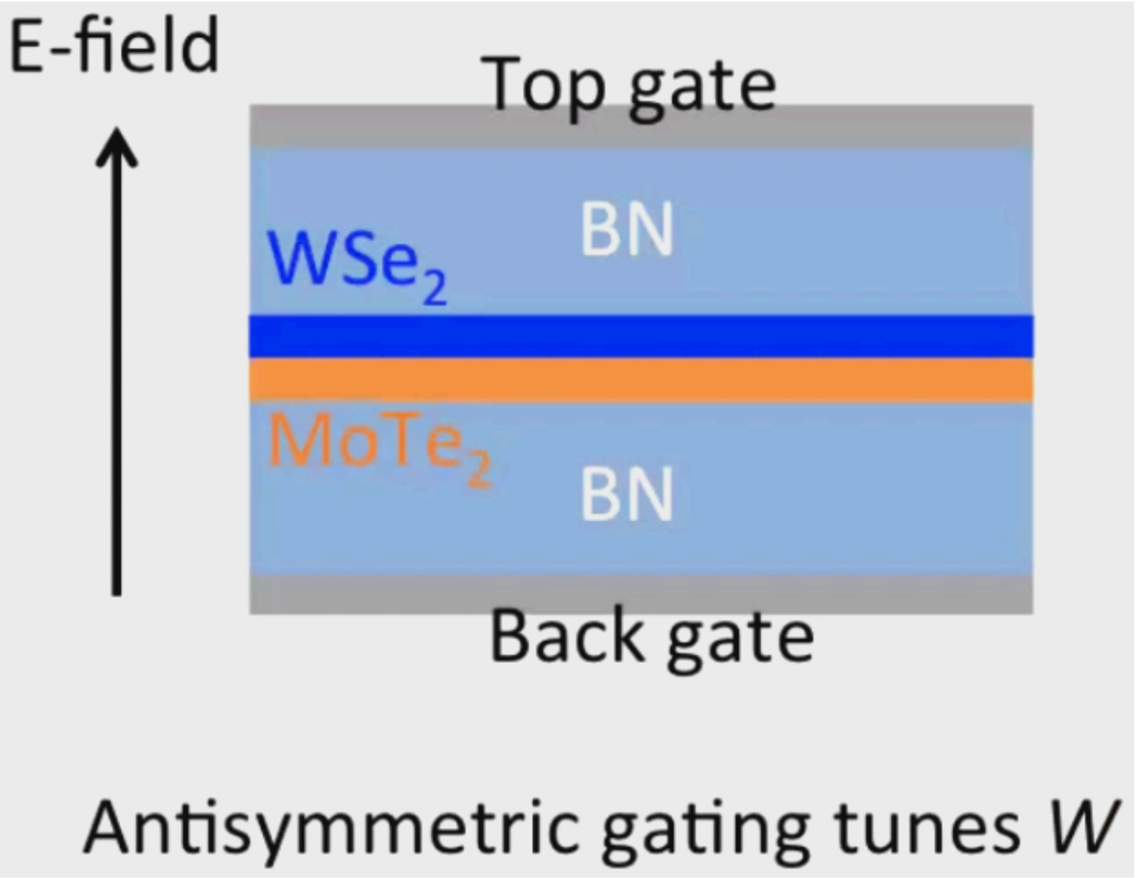
Continues metal-insulator transition in heterobilayer $MoTe_2/WSe_2$

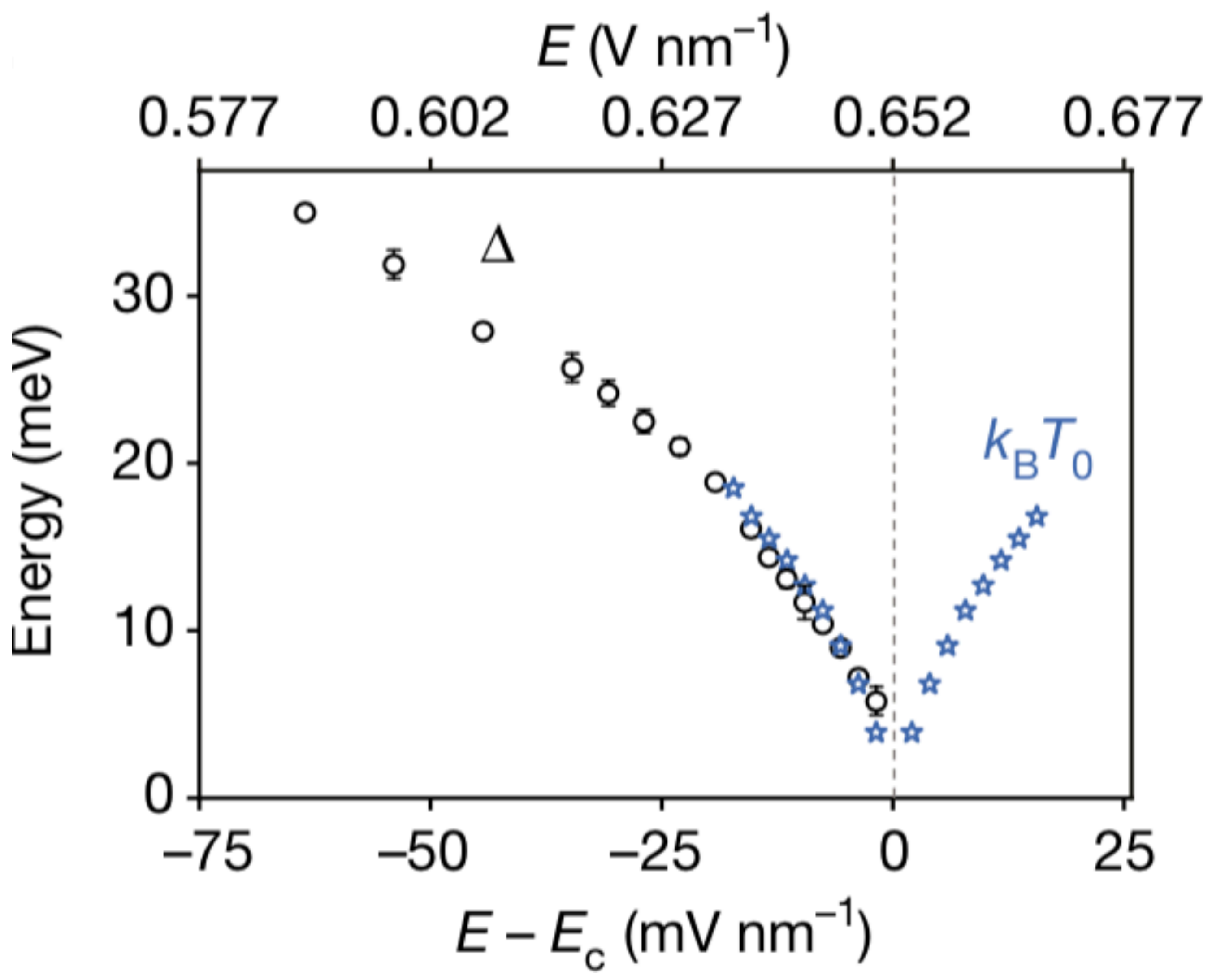




- bandwidth tuned by the interlayer displacement field ⇒ continuous metal-insulator transition
- From the insulator side, the charge gap vanishes continuously.
- From the metal side, the electron effective mass (from Kadowaki–Woods scaling in resistivity measurements) diverges near the critical point.
- No sign of long-range magnetic ordering (down to 5% of Curie-Weiss temperature), and magnetic susceptibility shows a smooth dependence on the displacement field across the transition.

Continues metal-insulator transition in heterobilayer $MoTe_2/WSe_2$

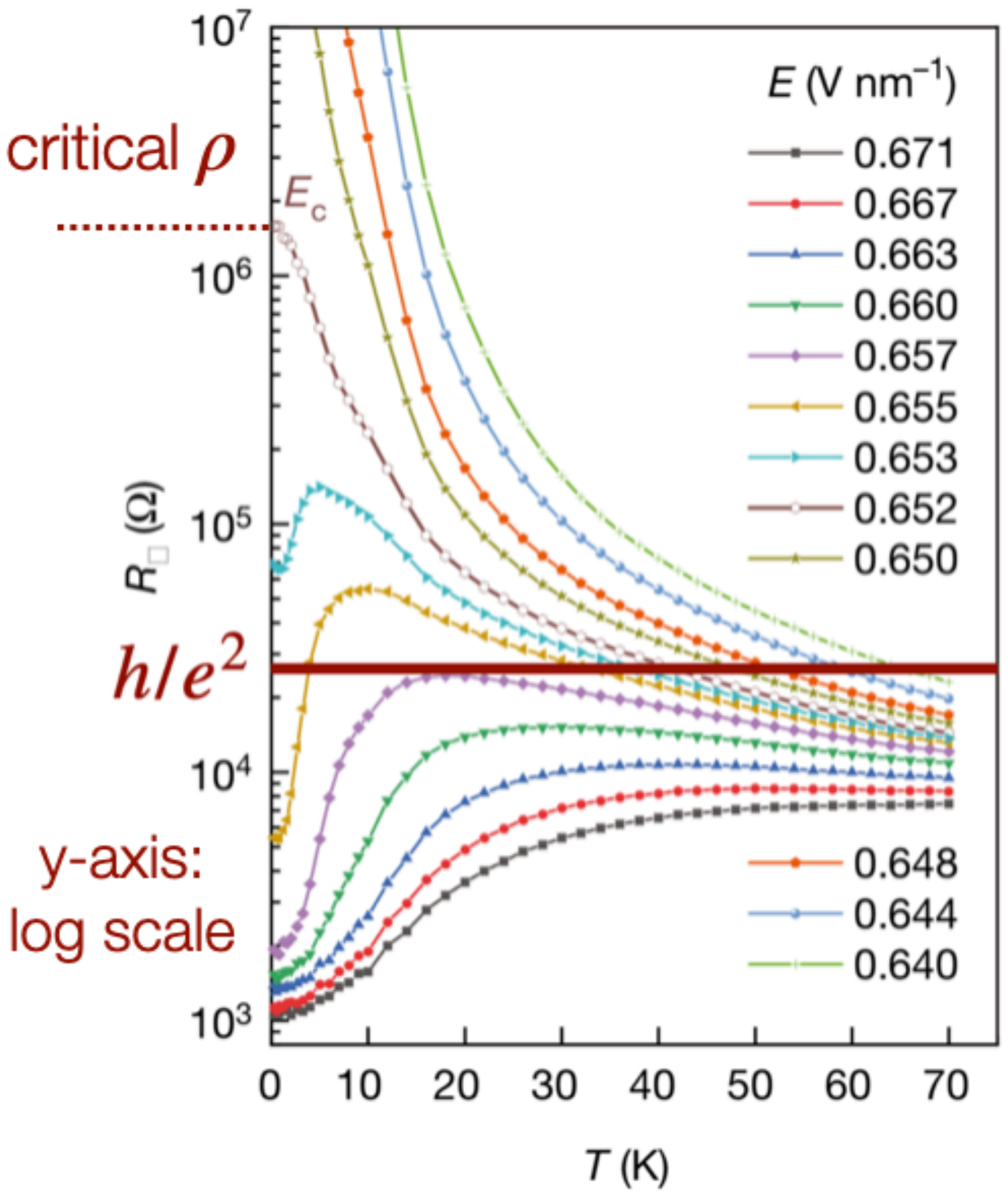




- bandwidth tuned by the interlayer displacement field ⇒ continuous metal-insulator transition
- The conclusion of the experimental paper: it is potentially an interaction-driven transition, and disorder only plays a “perturbative role”.
- Half-band filling density (two orders) ≫ disorder density
- A different perspective: disorder plays an important role in another theory in Kim et al. arXiv:2204.10865

Continues metal-insulator transition in heterobilayer $MoTe_2/WSe_2$

Continuous MIT at half-filling:



If this is an interaction-driven continuous MIT, the critical ρ is much larger than the expected value within the current theoretical understanding.

Shan, Mak et al. Nature 597, 350–354 (2021)

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Metal-insulator transition (half-filling) with large critical resistivity

- "Standard construction" in Senthil 2008
- $c_{\boldsymbol{r},\alpha} = b_{\boldsymbol{r}} f_{\boldsymbol{r},\alpha}$, $\alpha = \uparrow\downarrow$
- One emergent $U(1)$ gauge field a
- f: spinon fermi surface
- b: 3D XY transition

- New construction: $c_{\boldsymbol{r},\alpha} = b_{\alpha,\boldsymbol{r}} f_{\boldsymbol{r},\alpha}$, $\alpha = \uparrow\downarrow$
- (time-reversal symmetry, no $SU(2)$ rotation)
- Two emergent $U(1)$ gauge fields $a_\uparrow, a_\downarrow$
- f: spinon fermi surface
- $b_\uparrow, b_\downarrow$: 3D XY transitions simultaneously (by time-reversal symmetry)
- $\Rightarrow$ **charge fractionalization** $\Rightarrow$ **Large electrical resistivity at critical point**

Metal-insulator transition (half-filling) with large critical resistivity

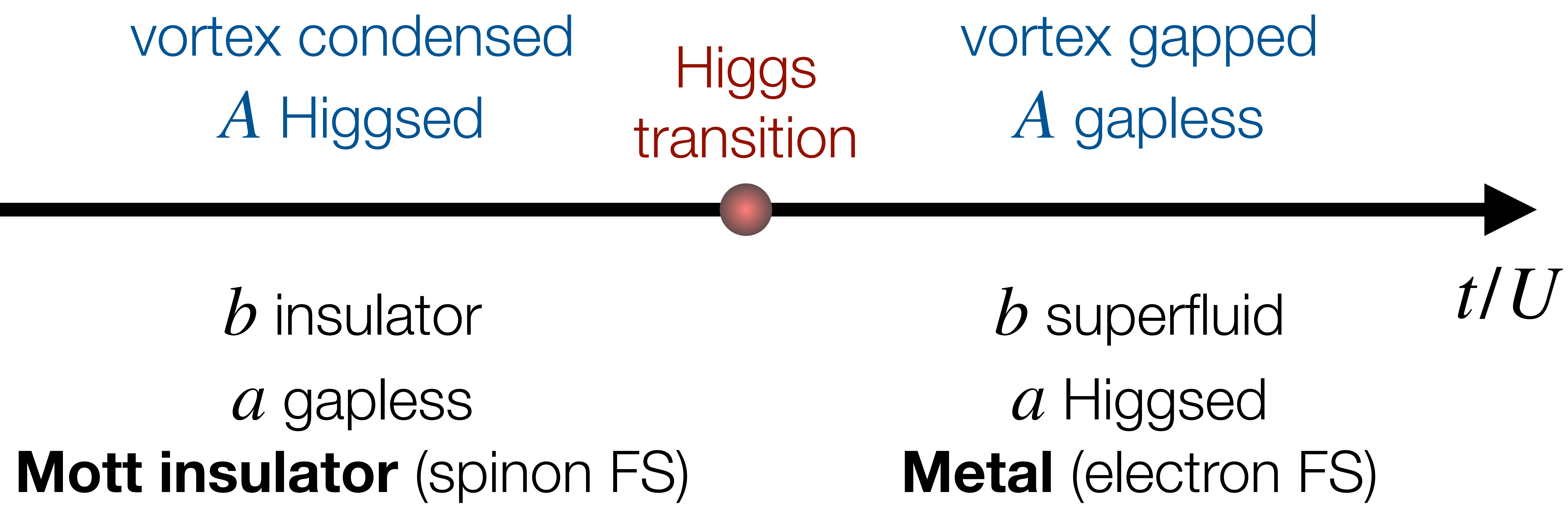
- “Standard construction” in Senthil 2008
- $c_{\boldsymbol{r},\alpha} = b_{\boldsymbol{r}} f_{\boldsymbol{r},\alpha},\ \alpha = \uparrow\downarrow$
- Electron c at half-filling
- $\Rightarrow$ b at integer filling
- the Mott insulator of b trivially gapped

- New construction: $c_{\boldsymbol{r},\alpha} = b_{\alpha,\boldsymbol{r}} f_{\boldsymbol{r},\alpha},\ \alpha = \uparrow\downarrow$
- Electron c at half-filling
- $\Rightarrow$ $b_\uparrow$ at half-filling, and $b_\downarrow$ at half-filling
- Lieb-Schultz-Mattis (LSM) theorem $\Rightarrow$ the Mott insulator of $b_\uparrow, b_\downarrow$ can NOT be trivially gapped.
- (1) topological order;
- (2) density-wave state (that spontaneously breaks translation symmetry).

Y. Xu, XW, Z.-X. Luo, M. Ye, C.-M. Jian, and C. Xu,
(arXiv:2106.14910) PRX 12, 021067 (2022)

Critical theory of $b_\uparrow$ (or $b_\downarrow$) at fractional filling: dual vortex theory

Dual theory: vortex of b + dynamical $U(1)$ gauge field A (dual to Goldstone of superfluid of b)



- Case 1: the condensation of N-vortex (bound state) at $\boldsymbol{k} = 0$ gives $\mathbb{Z}_N$ topological order.
- Case 2: the condensation of vortex at finite momentum $\boldsymbol{k} \neq 0$ breaks translation symmetry.

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Case 1: $\mathbb{Z}_N$ topological order

- The critical theory of N-vortex (bound state) condensation for $b_\uparrow$ (or $b_\downarrow$)
- $\mathscr{L} = |(\partial_\mu - \mathtt{i}NA_\mu)\psi|^2 + r|\psi|^2 + u|\psi|^4 + \frac{\mathtt{i}}{2\pi} A \wedge d(a + eA_{ext}) + \ldots$
- The chargon sector (3D XY* universality) is dynamically decoupled from the spinon fermi-surface.

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- The chargon sector (3D XY* universality) is dynamically decoupled from the spinon fermi-surface.
- **Charge fractionalization** (both critical point and Mott insulator): the charge carrier is the anyon $\tilde{\psi}$ of the $\mathbb{Z}_N$ topological order, with $e_* = e/N$. We find $\tilde{\psi}$ has universal DC resistivity $\tilde{\rho} \approx 7.93h/e_*^2$. The total species of $\tilde{\psi}$ is 2 ($b_\uparrow$ and $b_\downarrow$) $\Rightarrow$ the universal chargon contribution $\rho_b = \tilde{\rho}/2$.
- **Large critical resistivity** $\rho = \rho_f + \rho_b$ **where** $\rho_b \approx 3.96N^2\frac{h}{e^2} \sim N^2\frac{h}{e^2}$ (although $\rho_f < \frac{h}{e^2}$).

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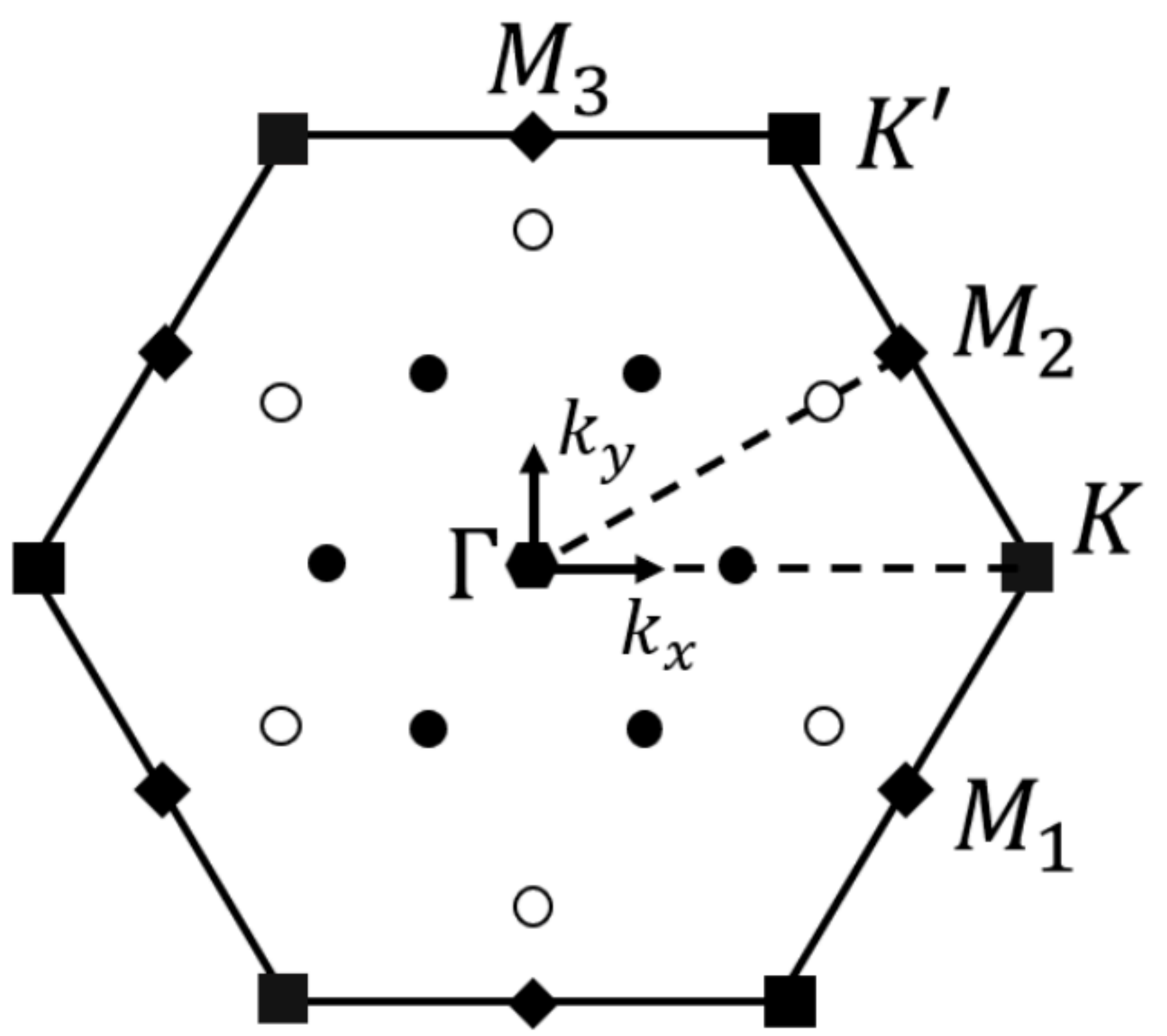
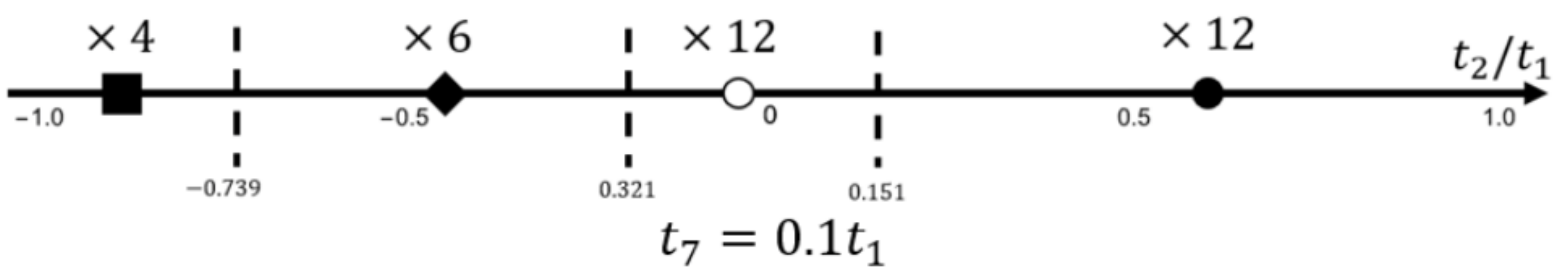
Case 2: density-wave state

- The vortex band structure: N minima in Brillouin zone ~ $\sum_{I=1}^{N} \psi_I e^{\mathrm{i}\boldsymbol{Q}_I \cdot \boldsymbol{r}}$, where low-energy fields ψ_I
- $$\mathscr{L} = \sum_{I=1}^{N} (|(\partial_\mu - \mathrm{i}A_\mu)\psi_I|^2 + r|\psi_I|^2) + u(\sum_{I=1}^{N} |\psi_I|^2)^2 + \frac{\mathrm{i}}{2\pi} A \wedge d(a + eA_{ext}) + \dots$$





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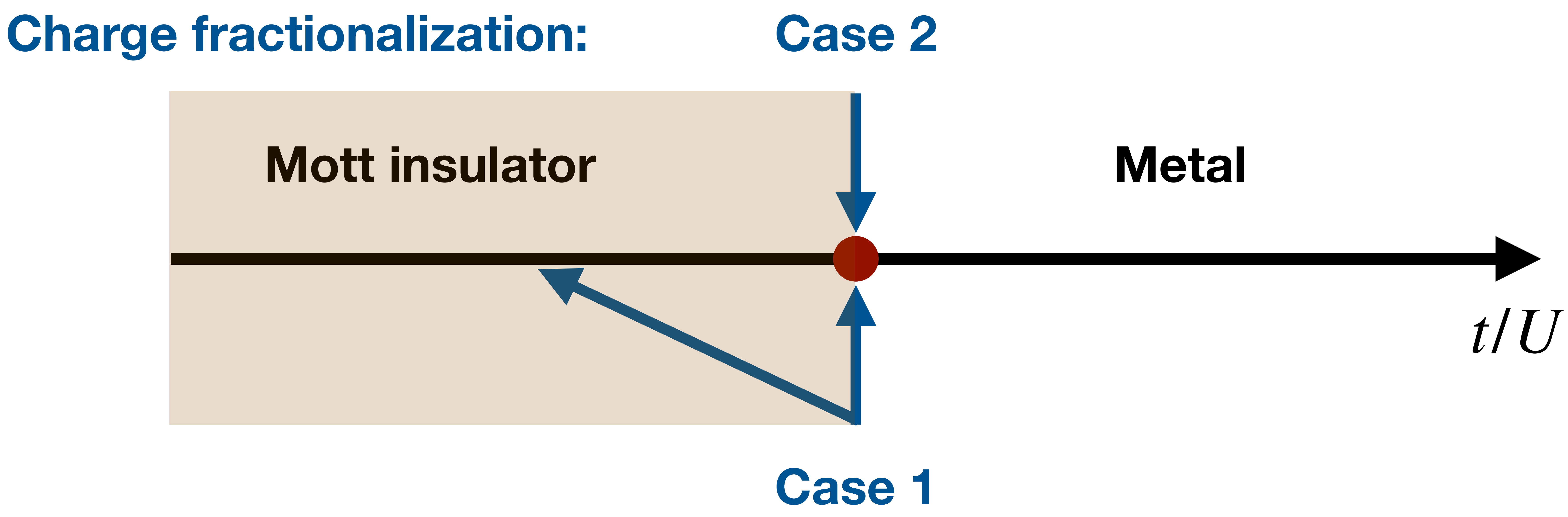
- **Charge fractionalization** at critical point (Landau-forbidden transition in chargon sector): the charge carrier is the vortex $\tilde{\psi}_I$ of each ψ_I with $e_* = e/N$. The total species of $\tilde{\psi}$ is $2N$ ($b_\uparrow$ and $b_\downarrow$). Generalized Ioffe-Larkin rule (for $\sum_{I=1}^{N} e_I = e$): $\rho_b = \frac{h}{e^2}\frac{1}{2}\sum_{I=1}^{N} \tilde{R}^I$, where $\tilde{R}^I = \langle J^I_\omega J^I_{-\omega} \rangle / \omega$.

- **Large critical resistivity** $\rho = \rho_f + \rho_b$ **where** $\rho_b \approx (3.62 + 1.68(N-1))\frac{h}{e^2} \sim N\frac{h}{e^2}$.

Experimental distinctions of two cases



- Case 1: in topological order (Mott insulator), the charge carriers are still deconfined at $T = 0$.
- Case 2: in density wave (Mott insulator), the $U(1)$ gauge field that couples to the fractionalized charge carrier will confine even at $T = 0$, due to the condensation of monopole which carries lattice translation symmetry.

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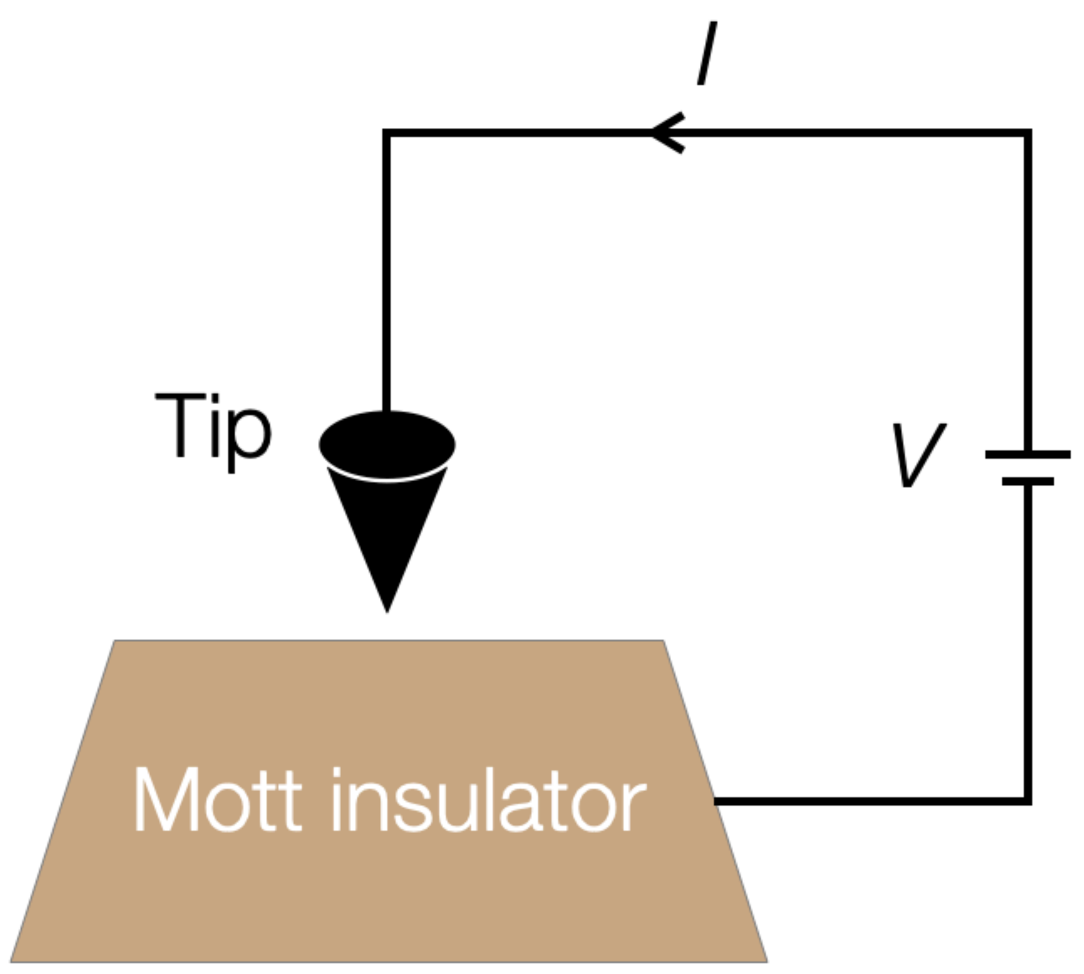
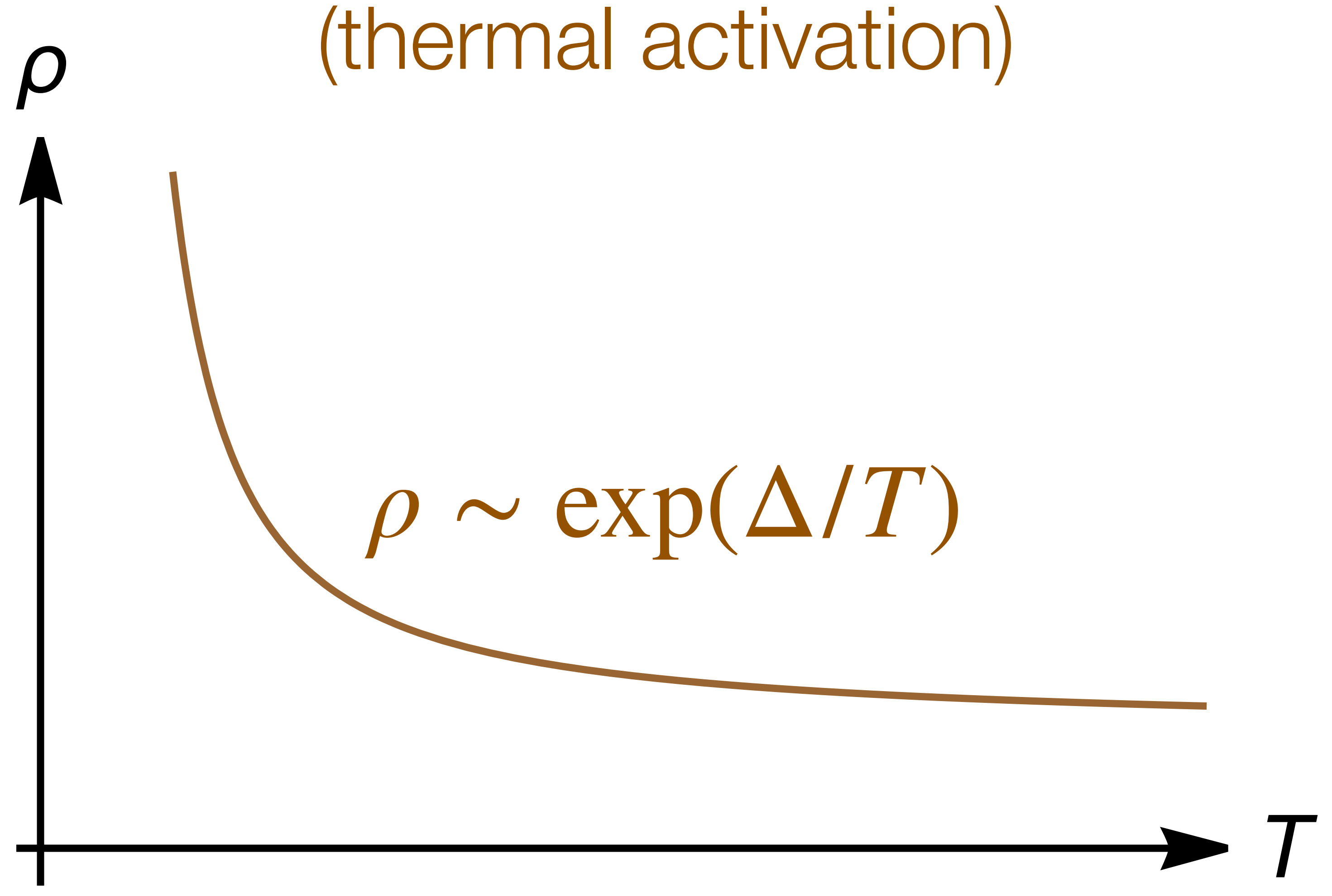
Other predicted physical properties

- In **Mott insulator**, if there are deconfined fractional charges, **tunneling gap** $\approx N$ **transport gap**

Tunneling spectroscopy



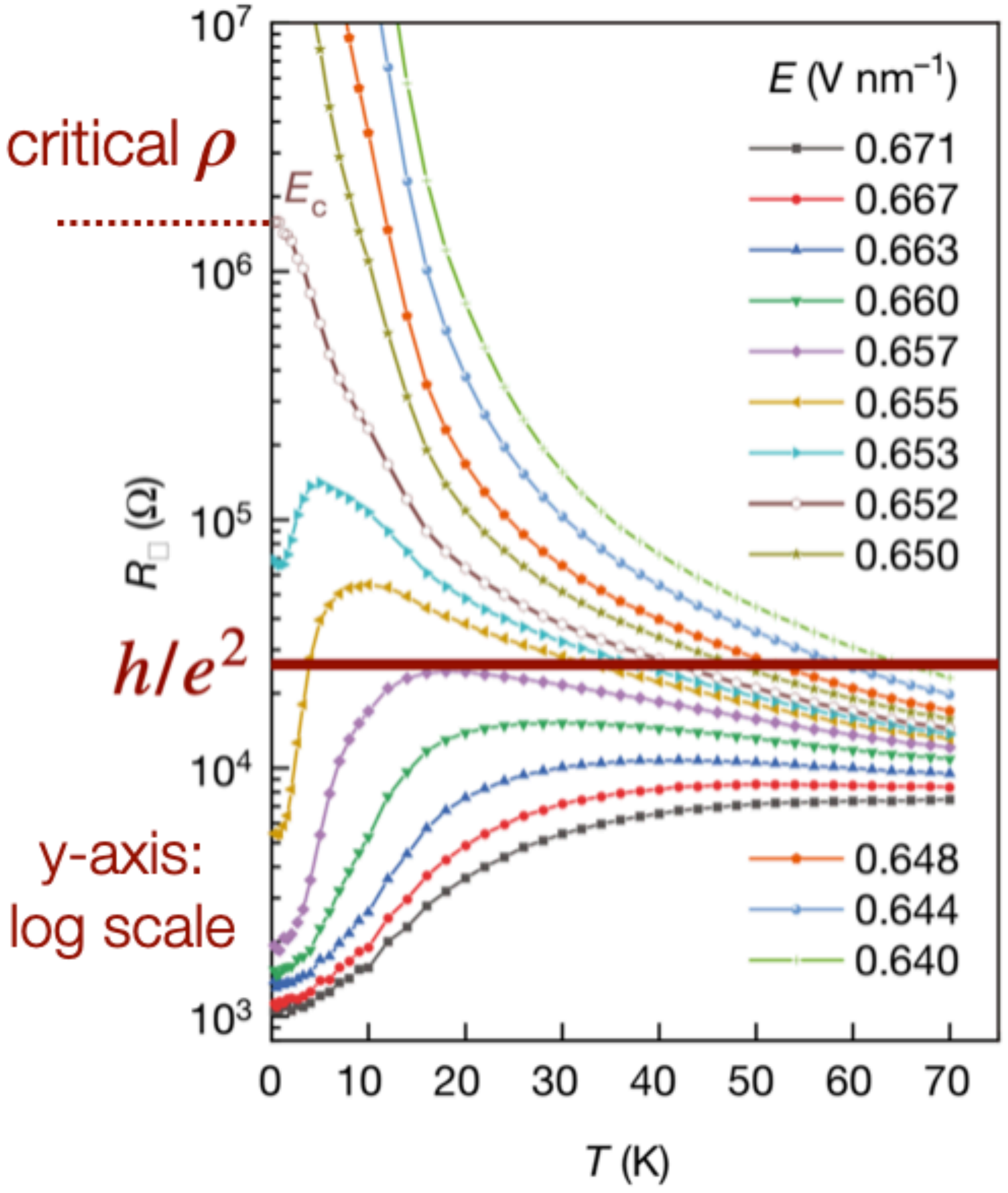
Resistivity at finite-T (thermal activation)



- In **Metal** phase, the electron operator is $c \sim \langle b \rangle f \sim \langle \tilde{\psi}_1 \ldots \tilde{\psi}_N \rangle f$. The **quasi-particle weight** Z will vanish approaching the critical point with scaling $\sqrt{Z} \sim \langle \tilde{\psi}_1 \ldots \tilde{\psi}_N \rangle \sim |g - g_c|^{\beta_N}$, where bandwidth $g \sim t/U$, and critical exponent β_N increases with N (much larger than $\beta_1 = 0.33$ in Senthil 2008).

Big critical resistivity in transition metal dichalcogenides

Continuous MIT at half-filling:



Shan, Mak et al. Nature 597, 350–354 (2021)

Our construction (arXiv:2106.14910) at half-filling (and other fractional fillings): the observed big critical resistivity is potentially explained by **charge fractionalization** at the critical point (two cases: topological order/density wave).

Construction of metal to Wigner crystal transition at 1/6-filling by Musser-Senthil-Chowdhury (arXiv:2111.09894) also involves charge fractionalization at critical point.

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Summary