Synopsis of geometrical observables
Part 2: Many-body formulation

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Based on:
https://www.cond-mat.de/events/correl20/manuscripts/resta.pdf

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Outline

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Band insulators and band metals

- Most geometry and topology is addressed at the independent-particle level (Hartree Fock or Kohn-Sham)
- In crystalline solids the physics is embedded in the geometry of the occupied Bloch manifold
- For both **band insulators** and **band metals** the formal expressions are Fermi-volume integrals of **reciprocal-space differential forms**

In mathematical speak:

- the **Berry connection** is a Chern-Simons 1-form
- the **Berry curvature** (a 2-form) is called first Chern form

References about **band-structure** geometry and topology:

- D. Vanderbilt, *Berry Phases in Electronic Structure Theory* (Cambridge University Press, 2018)
- R. Resta, Lecture Notes, http://www-dft.ts.infn.it/~resta/gtse/draft.pdf

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Band insulators and band metals

- Geometrical/topological observables come in two very different classes:
  - **Class (i)** Observables whose bulk value is only defined modulo 2π (in dimensionless units)
  - **Class (ii)** Observables whose bulk value is single-valued
- All of the known class (ii) observables are rooted in a 2-form
- Those in class (ii) are rooted in a 1-form and a 3-form

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Synopsis (band insulators and band metals)

Class (i)

Chern-Simons 1-form	Polarization (insulators only)
Chern-Simons 3-form	Axion term in magnetoelectrics (insulators only)

Class (ii)

Time-reversal odd (antisymmetric 2-forms)	**Time-reversal even** (symmetric 2-forms)
Anomalous Hall conductivity metals and insulators	Souza-Wilkens-Martin sum rule insulators only
Circular dichrois sum rule metals and insulators	**??**
Orbital magnetization metals and insulators	Drude weight metals only

From geometry to topology

Class (i)

Chern-Simons 1-form	Polarization Topological $\mathbb{Z}_2$ with I-symmetry
Chern-Simons 3-form	Axion term in magnetoelectrics $\mathbb{Z}_2$ with either T- or I-symmetry

Class (ii)

Time-reversal odd (antisymmetric 2-forms)	**Time-reversal even** (symmetric 2-forms)
Anomalous Hall conductivity Topological $\mathbb{Z}$ in 2d insulators: QAHE	SWM sum rule
Circular dichroism sum rule	
Orbital magnetization	Drude weight

From band structure to many-body physics

- Some—**not all**—geometrical/topological observables can be defined for correlated many-electron system
- There is no **k**-vector to speak of: a **different Hilbert space** is needed

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- Why sum rules are **ground-state** properties?

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The simplest geometrical property: Distance

Two state vectors $|\Psi_1\rangle$ and $|\Psi_2\rangle$ in the **same** Hilbert space

$$D_{12}^2 = -\ln |\langle \Psi_1 | \Psi_2 \rangle|^2$$

- D_{12}^2 clearly **gauge-invariant**
- $D_{12}^2 = 0$ if the two quantum states coincide apart for an irrelevant phase
- $D_{12}^2 = \infty$ if the two states are orthogonal
- **Caveat:** It is a **pseudo**distance

A second geometrical property: Connection

$$D_{12}^2 = -\ln |\langle \Psi_1 | \Psi_2 \rangle|^2 = -\ln \langle \Psi_1 | \Psi_2 \rangle - \ln \langle \Psi_2 | \Psi_1 \rangle$$

- The two terms are **not** gauge-invariant
- Each of the two terms is a complex number
- What is the meaning of Im ln $\langle \Psi_1 | \Psi_2 \rangle$?

$$\langle \Psi_1 | \Psi_2 \rangle = |\langle \Psi_1 | \Psi_2 \rangle| e^{i\varphi_{12}}$$

$$-\text{Im ln } \langle \Psi_1 | \Psi_2 \rangle = \varphi_{12}, \qquad \varphi_{21} = -\varphi_{12}$$

- The connection fixes the **phase difference**
- The connection is **arbitrary**
- Given that it is arbitrary, **why bother?**

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Metric, connection, curvature

- $|\Psi_{\boldsymbol{\kappa}}\rangle$ a **differentiable** function of $\boldsymbol{\kappa}$

- Quantum metric $g_{\alpha\beta}(\boldsymbol{\kappa})$:

$$D^2_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = g_{\alpha\beta}(\boldsymbol{\kappa}) d\kappa_\alpha d\kappa_\beta$$

- Berry connection $\mathcal{A}_\alpha(\boldsymbol{\kappa})$:

$$\varphi_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = \mathcal{A}_\alpha(\boldsymbol{\kappa}) d\kappa_\alpha$$

- Berry curvature $\Omega_{\alpha\beta}(\boldsymbol{\kappa})$ (curl of the connection):

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) d\kappa_\alpha d\kappa_\beta = [\partial_{\kappa_\alpha} \mathcal{A}_\beta(\boldsymbol{\kappa}) - \partial_{\kappa_\beta} \mathcal{A}_\alpha(\boldsymbol{\kappa})] d\kappa_\alpha d\kappa_\beta$$

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Metric, connection, curvature

- Quantum metric **gauge-invariant 2-form**:

$$g_{\alpha\beta}(\boldsymbol{\kappa}) = \text{Re}\, \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle - \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \Psi_{\boldsymbol{\kappa}} \rangle \langle \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$$

- Berry connection **(gauge-dependent 1-form)**:

$$\mathcal{A}_\alpha(\boldsymbol{\kappa}) = i \langle \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} \rangle$$

- Berry curvature **(gauge-invariant 2-form)**:

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = i(\langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle - \langle \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} \rangle)$$

$$= -2\, \text{Im}\, \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$$

- One more **gauge-invariant 2-form**:

$$\langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | (H_{\boldsymbol{\kappa}} - E_{\boldsymbol{\kappa}}) | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$$

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Kohn's Hamiltonian

- N electrons in a cubic box of volume L^d
- Eventually $N \to \infty$, $L \to \infty$, N/L^d constant

- Hamiltonian with a "flux" (a gauge transformation):

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i=1}^{N} |\mathbf{p}_i + \hbar \boldsymbol{\kappa}|^2 + \hat{V}$$

- $\hat{V}$ includes one-body and two-body terms
- Crystalline and noncrystalline systems
- Thermodynamic limit **after** taking $\boldsymbol{\kappa}$-derivatives

Geometrical forms

- All forms evaluated on the **ground state** at $\boldsymbol{\kappa} = 0$
- All forms **real** and **extensive**

- Connection:
  $\mathcal{A}_\alpha(\boldsymbol{\kappa}) = i\langle \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} \rangle$
- Metric:
  $g_{\alpha\beta}(\boldsymbol{\kappa}) = \text{ Re } \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle - \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | \Psi_{\boldsymbol{\kappa}} \rangle \langle \Psi_{\boldsymbol{\kappa}} | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$
- Curvature:
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- One more 2-form:
  $\mathcal{G}_{\alpha\beta}(\boldsymbol{\kappa}) = \langle \partial_{\kappa_\alpha} \Psi_{\boldsymbol{\kappa}} | (\hat{H}_{\boldsymbol{\kappa}} - E_{0\boldsymbol{\kappa}}) | \partial_{\kappa_\beta} \Psi_{\boldsymbol{\kappa}} \rangle$

Two different Hilbert spaces

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m}\sum_{i=1}^{N} |\mathbf{p}_i + \hbar\boldsymbol{\kappa}|^2 + \hat{V}$$

- OBC: the flux is easily "gauged away"
  - Eigenvalues $\boldsymbol{\kappa}$-independent
  - $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle, \qquad \hat{\mathbf{r}} = \sum_{i=1}^{N}\mathbf{r}_i$
  - $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle$ obeys Schrödinger Eq. and OBCs at **any** $\boldsymbol{\kappa}$

- Born-von-Kàrmàn PBCs violate gauge invariance
  - The coordinates $r_{i\alpha}$ are actually **angles** $\varphi_{i\alpha} = 2\pi r_{i\alpha}/L$
  - The position $\hat{\mathbf{r}} = \sum_{i=1}^{N}\mathbf{r}_i$ is a **forbidden** operator
  - $E_{0\boldsymbol{\kappa}}$ **does** depend on $\boldsymbol{\kappa}$.
  - $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$ **does not** obey PBCs (for a generic $\boldsymbol{\kappa}$)

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A lattice of special κ vectors

- If the κ components are **integer multiples** of $2\pi/L$ then:
  - $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$ obeys Schrödinger Eq. and PBCs
  - It is an eigenstate of $\hat{H}_{\boldsymbol{\kappa}}$ with eigenvalue E_0
  - Is it the **ground eigenstate?????**

- Set $\boldsymbol{\kappa}_1 = \left(\frac{2\pi}{L}, 0, 0\right)$:

$$\mathfrak{z}_N^{(x)} = \langle\tilde{\Psi}_{0\boldsymbol{\kappa}_1}|\Psi_0\rangle = \langle\Psi_0|\,\mathrm{e}^{i\frac{2\pi}{L}\sum_i x_i}\,|\Psi_0\rangle = \langle\Psi_0|\,U\,|\Psi_0\rangle$$

- U many-body unitary operator
- $\mathfrak{z}_N^{(x)}$ complex number, $|\mathfrak{z}_N^{(x)}| \leq 1$
- Polarization and Resta-Sorella theory of the insulating state both rooted in $\mathfrak{z}_N^{(x)}$ (in the large-N limit)

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Discretized connection and metric

- Phase difference between $|\tilde{\Psi}_{0\boldsymbol{\kappa}_1}\rangle$ and $|\Psi_0\rangle$:

$$\gamma_x^{(\mathrm{el})} = \mathrm{Im}\,\ln\langle\Psi_0|\,\mathrm{e}^{i\frac{2\pi}{L}\sum_i x_i}\,|\Psi_0\rangle = \mathrm{Im}\,\ln\,\mathfrak{z}_N^{(x)}$$

  - **Single-point Berry phase** (electronic term)
  - Discretized connection in a **specific gauge**:

$$\gamma_x^{(\mathrm{el})} \simeq \boldsymbol{\mathcal{A}}(0)\cdot\Delta\boldsymbol{\kappa} = \mathcal{A}_x(0)\frac{2\pi}{L}$$

- Quantum distance between $|\tilde{\Psi}_{0\boldsymbol{\kappa}_1}\rangle$ and $|\Psi_0\rangle$:

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Center of charge (1d & quasi-1d systems)

According e.g. to **Kittel textbook** **P** is nonzero when "....the **center** of positive charge does not coincide with the **center** of negative charge"

- N spinless electrons in a segment of lenght L:

$$\Psi_0 = \Psi_0(x_1, x_2, \ldots x_j, \ldots x_N),$$

- Periodic boundary conditions:

$$\Psi_0 = \Psi_0(x_1, x_2, \ldots x_j, \ldots x_N) = \Psi_0(x_1, x_2, \ldots x_j + L, \ldots x_N)$$

- Nuclei of charge eZ_ℓ at sites X_ℓ
- **Centers of charge:**

$$\sum_\ell Z_\ell X_\ell - \langle \Psi_0 | \sum_j x_j \, | \Psi_0 \rangle$$

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Center of charge, better

R. Resta, Phys. Rev. Lett. 1998

- Within PBCs coordinates are actually **angles**
- The two "centers" must be defined **modulo** L
- Their **difference** must be origin-invariant

$$\sum_\ell Z_\ell X_\ell - \langle \Psi_0 | \sum_j x_j \, | \Psi_0 \rangle$$

$$\longrightarrow \frac{L}{2\pi} \mathrm{Im\ ln}\ \ e^{i\frac{2\pi}{L}\sum_\ell Z_\ell X_\ell} + \frac{L}{2\pi} \mathrm{Im\ ln}\ \ \langle \Psi_0 | e^{-i\frac{2\pi}{L}\sum_j x_j} | \Psi_0 \rangle$$

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$$P = -\frac{e}{2\pi} \mathrm{Im\ ln}\ \ \langle \Psi_0 | e^{i\frac{2\pi}{L}\left(\sum_j x_j - \sum_\ell Z_\ell X_\ell\right)} | \Psi_0 \rangle$$

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The single-point Berry phase

$$\gamma = \mathrm{Im}\,\ln \mathcal{Z}_N + \gamma^{(\mathrm{nucl})} \quad = \quad \mathrm{Im}\,\ln \langle \Psi_0 | e^{i\frac{2\pi}{L}\left(\sum_j x_j - \sum_\ell Z_\ell X_\ell\right)} | \Psi_0 \rangle$$

$$P \quad = \quad -e\frac{\gamma}{2\pi} \quad \text{defined modulo } e$$

- γ is the Berry phase in disguise
- γ includes the nuclear contribution
- The electronic term is the **discretized connection** in a specific gauge
- P is a **multivalued** bulk observable: "modulo" ambiguity fixed after terminations are specified

- Matrix element real in centrosymmetric systems: γ is a $\mathbb{Z}_2$ topological invariant

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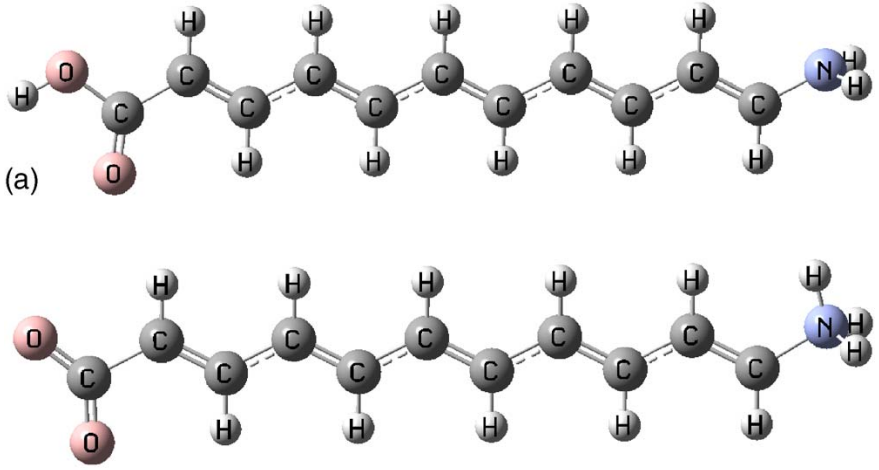
Polarization is a multivalued observable
(K. Kudin, R. Car, & R. Resta, J. Chem Phys. 2007)



Centrosymmetric “bulk”

Two different asymmetric terminations

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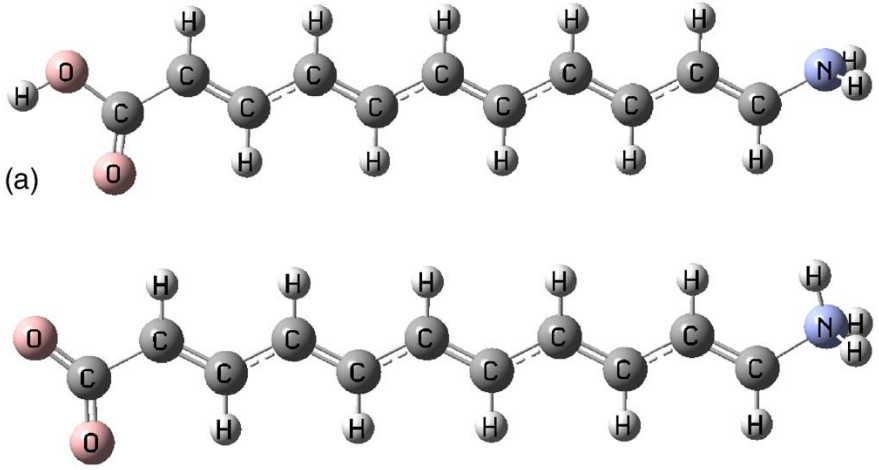
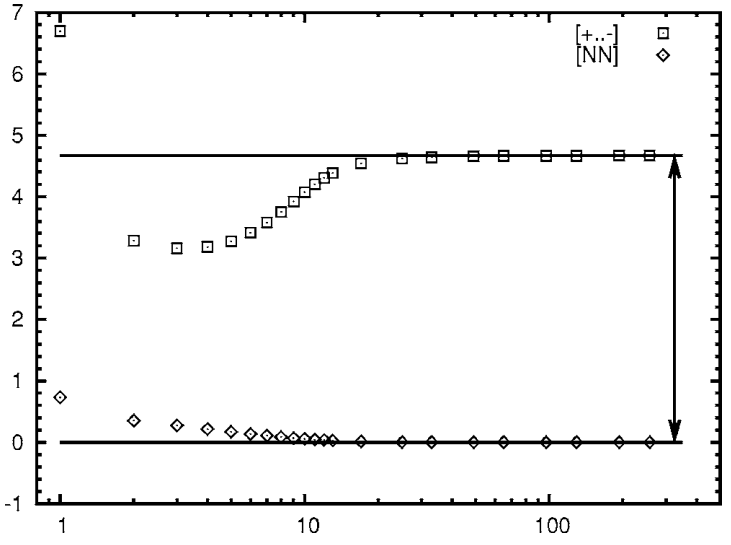


Centrosymmetric “bulk”

Two different asymmetric terminations

dipole/length = P

Polyacetylene is $\mathbb{Z}_2$-even



dipole per monomer

Outline

$\mathbb{Z}_2$ classification of centrosymmetric polymers

$\mathbb{Z}_2$-even: $P = 0 \mod e$

Alternant polyacetilene, model molecular crystal.....

$\mathbb{Z}_2$-odd: $P = e/2 \mod e$

Model ionic crystal.....

- $\mathbb{Z}_2$ invariant **topological**:
  - Independent e.g. of ionicity difference
  - Independent of the theory level (tight-binding, first-principle...)
  - Robust by continuous deformation of the wavefunction

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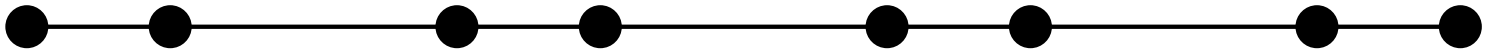
Simple tight-binding Hamiltonians



$\mathbb{Z}_2$-even: Onsite ϵ_i constant, alternating hoppings t and t'

$\mathbb{Z}_2$-odd: Constant hopping t, alternating ϵ_i

- $\mathbb{Z}_2$ invariant protected by **centrosymmetry**
- When joining the two with a continuous & centrosymmetric deformation of the Hamiltonian **the gap closes!**

Outline

Model 1d ionic crystal

$$\gamma = \mathrm{Im}\,\ln\ \langle\Psi_0|e^{i\frac{2\pi}{L}\left(\sum_j x_j - \sum_\ell Z_\ell X_\ell\right)}|\Psi_0\rangle = \pi \pmod{2\pi}$$

- Tight-binding Hamiltonian:

$$H = \sum_j [\ (-1)^j \Delta\, c_j^\dagger c_j - t\ c_j^\dagger c_{j+1} - t\ c_{j+1}^\dagger c_j\ ]$$

- $\mathbb{Z}_2$-odd: $P = e/2 \mod e$

Tight binding 1d binary crystal again

- Introducing spin:

$$H = \sum_{j\sigma} [\ (-1)^j \Delta\, c^\dagger_{j\sigma} c_{j\sigma} - t(c^\dagger_{j\sigma} c_{j+1\sigma} + \text{H.c.})\ ]$$

- Introducing Hubbard on-site repulsion:

$$H = \sum_{j\sigma} [\ (-1)^j \Delta\, c^\dagger_{j\sigma} c_{j\sigma} - t(c^\dagger_{j\sigma} c_{j+1\sigma} + \text{H.c.})] \ + \ U \sum_j n_{j\uparrow} n_{j\downarrow}.$$

The $t = 0$ case has an obvious exact solution

The $\mathbb{Z}_2$ invariant

$$P = -\frac{e}{2\pi} \mathrm{Im}\, \ln \langle \Psi_0 | e^{i\frac{2\pi}{L}\left(\sum_j x_j - \sum_\ell z_\ell x_\ell\right)} | \Psi_0 \rangle$$

- Matrix element real in inversion-symmetric systems:
  - $\langle \Psi_0 | U | \Psi_0 \rangle > 0 \Longrightarrow \mathbb{Z}_2$-even
  - $\langle \Psi_0 | U | \Psi_0 \rangle < 0 \Longrightarrow \mathbb{Z}_2$-odd

- Topological invariant "protected" by inversion symmetry
- Parity may switch only crossing $\mathfrak{z}_N = 0$: metallic state!

$$|\langle \Psi_0 | e^{i\frac{2\pi}{L}\left(\sum_j x_j - \sum_\ell z_\ell x_\ell\right)} | \Psi_0 \rangle| = |\langle \Psi_0 | e^{i\frac{2\pi}{L}\sum_j x_j} | \Psi_0 \rangle| = |\mathfrak{z}_N| = 0$$

$$\Rightarrow \qquad \lambda^2 = -\frac{1}{N}\left(\frac{L}{2\pi}\right)^2 \mathrm{Im}\, \ln |\mathfrak{z}_N|^2 \to \infty$$

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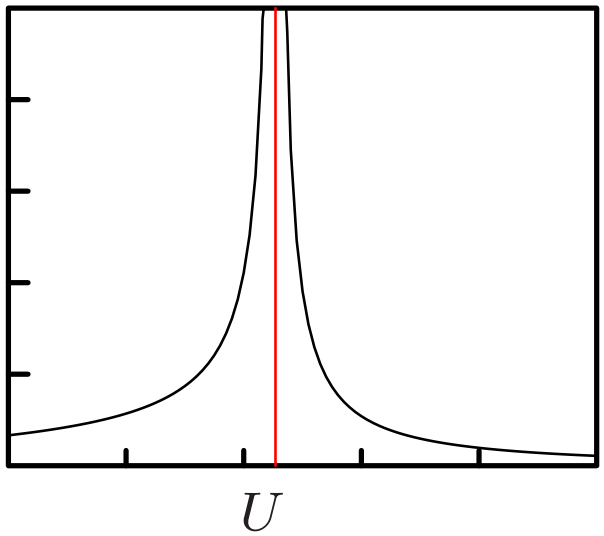
Topological insulator-insulator transition

- Plot of λ^2 (intensive quantity) at half filling:



After:
R. Resta & S. Sorella,
PRL 1999

- **Metallic** only for a special U value
- On the left it is a **band-like insulator**
- On the right it is a **Mott-like insulator**
- **Topological transition:** From $\mathbb{Z}_2$-odd to $\mathbb{Z}_2$-even

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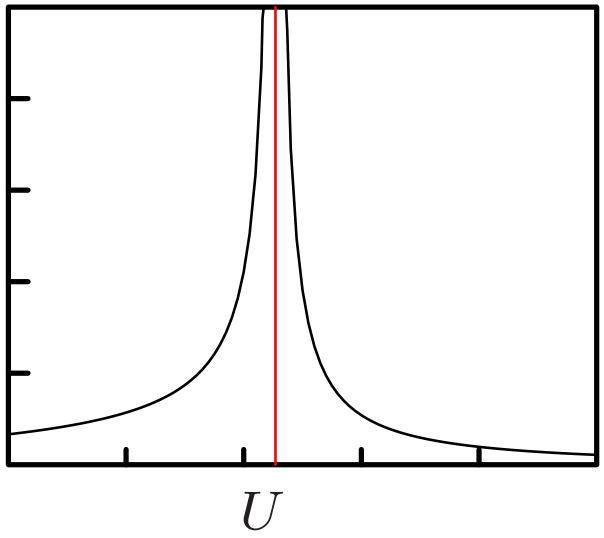

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Outline

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“Exotic” insulators

- In some materials, the insulating character is dominated by disorder: **Anderson insulators**
- In some materials, the insulating character dominated by electron-electron interaction: **Mott insulators**
- Other kinds of exotic insulators exist.
  Example: a two-dimensional electron fluid in the quantum-Hall regime: **Quantum Hall insulators**
- The nonexotic textbook insulators will be called in the following **band insulators**

Which property characterizes all insulators? (band insulators & exotic insulators)

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \Sigma_{-\infty}^{\infty} \Phi_M$, which are localized in disconnected regions of the many-particle configuration space and have essentially vanishing overlap. This property is the analog of localization for a single particle and leads directly to the electrical properties characteristic of insulators. An Appendix deals with a soluble model exhibiting a transition between an insulating and a conducting state.

- **Kohn's revolutionary message:**

  The insulating behavior reflects a certain type of organization of the electrons in their **ground state**

  Spectral gap **not** required

Basic postulate

R. Resta & S. Sorella, Phys. Rev. Lett. **82**, 370 (1999)

- Electronic term in polarization

$$P^{(\mathrm{el})} = -\frac{e}{2\pi}\,\mathrm{Im}\,\ln \lim_{N\to\infty} \mathcal{Z}_N$$

- It is impossible to **define** polarization whenever

$$\lim_{N\to\infty} \mathcal{Z}_N = 0$$

all insulators: $\lim_{N\to\infty} |\mathcal{Z}_N| = 1$ **all metals:** $\lim_{N\to\infty} \mathcal{Z}_N = 0$

A quantitative probe of the insulating character

$$\lambda^2 = -\lim_{N\to\infty} \frac{1}{N}\left(\frac{L}{2\pi}\right)^2 \ln|\mathfrak{z}_N|^2 = \lim_{N\to\infty} \frac{1}{N} g_{xx}(0)$$

- Intensive quantity (tensor in $3d$)
- λ^2 is finite in all insulators
- λ^2 diverges in all metals

- Very general: **all kinds** of insulators:
  - Correlated insulator
  - Independent electrons, crystalline
    a.k.a. "band insulator"
  - Independent electrons, disordered
  - Quantum Hall insulator

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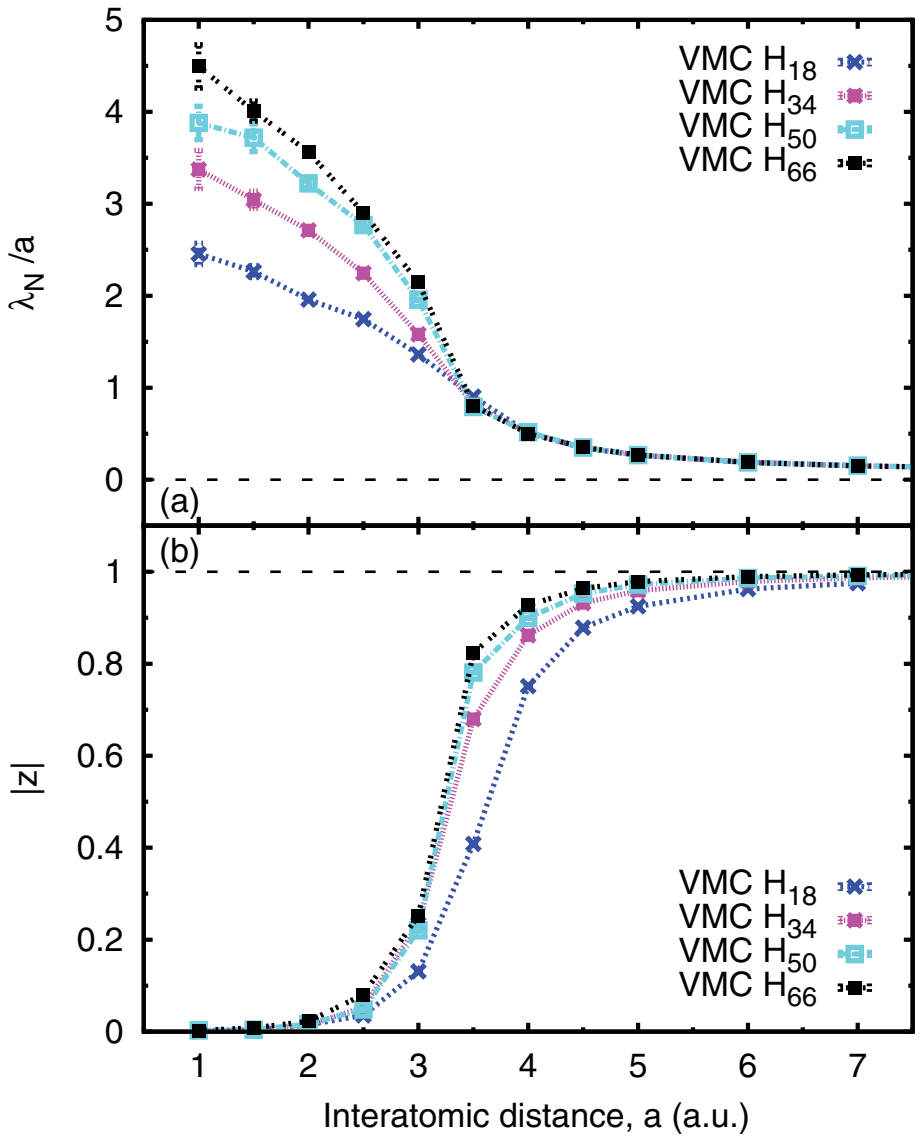
Mott metal-insulator transition in H_N chains

Stella, Attaccalite, Sorella & Rubio, PRB 2011



Paradigmatic system for the Mott transition

$$\lambda_N^2 = -\frac{1}{N}\left(\frac{L}{2\pi}\right)^2 \ln |z_N|^2$$

Transition: $\simeq$ 3.5 bohr

Outline

Definition

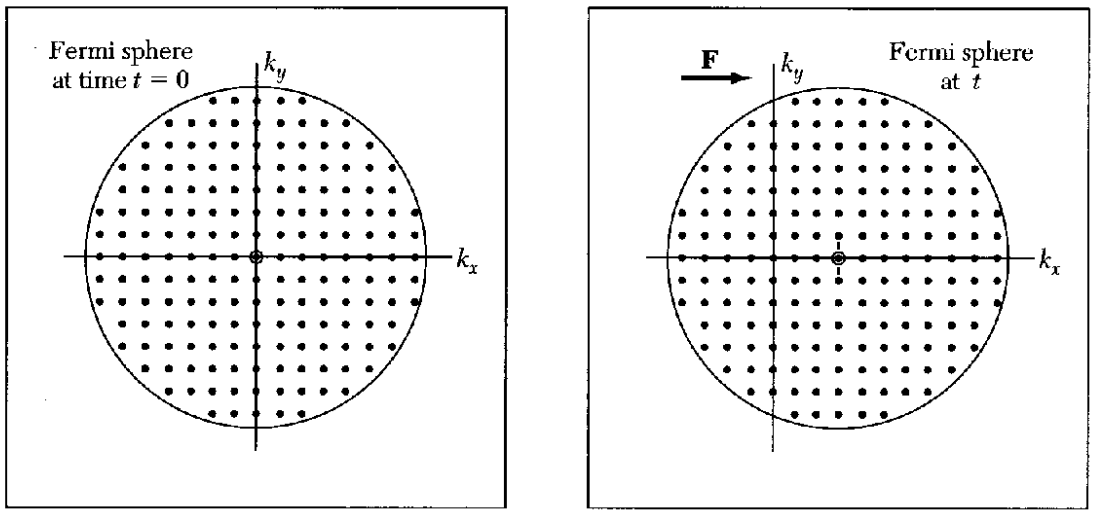
- Charge transport in a metal is a balance between free acceleration and dissipation (Ohm's law)
- QM addresses the **free-acceleration** side of the problem
- The **Drude weight** D (a.k.a. adiabatic **charge stiffness**) measures the inverse inertia of the many-electron system
- $D = 0$ in insulators
- It is a **ground-state** property
  (also retrieved from the Kubo formula for conductivity)

Free electrons

- Classical physics (Ashcroft-Mermin, Ch.1)

$$\sigma(\omega) = D_{\text{free}} \left[\delta(\omega) + \frac{i}{\pi\omega} \right], \qquad D_{\text{free}} = \pi e^2 \frac{n}{m}$$

- Quantum physics (Kittel ISSP, Ch. 6):



- In an **E** field the velocity grows linearly with time
  $D_{\text{free}} = \pi e^2 \frac{n}{m}$ **same** as in the classical case

Longitudinal conductivity (zero T, no dissipation)

- In a real metal:

$$\begin{aligned}\sigma^{(+)}_{\alpha\beta}(\omega) &= D_{\alpha\beta}\left[\delta(\omega)+\frac{i}{\pi\omega}\right]+\sigma^{(\text{regular})}_{\alpha\beta}(\omega)\\ &= \sigma^{(\text{Drude})}_{\alpha\beta}(\omega)+\sigma^{(\text{regular})}_{\alpha\beta}(\omega)\end{aligned}$$

- The insulating state requires **both**:
  - $D_{\alpha\beta}=0$
  - Re $\sigma^{(\text{regular})}_{\alpha\beta}(\omega)$ goes to zero for $\omega\to 0$
- The metallic state requires **either**:
  - $D_{\alpha\beta}>0$ (in crystalline systems, including correlation)
  - Re $\sigma^{(\text{regular})}_{\alpha\beta}(0)>0$ (only allowed in noncrystalline systems)

Drude weight (Kohn's formula, 1964)

$$D_{\alpha\beta} = \pi e^2 \left(\frac{n}{m}\right)_{\text{effective}} = \frac{\pi e^2}{\hbar^2 L^d} \left.\frac{\partial^2 E_{0\boldsymbol{\kappa}}}{\partial\kappa_\alpha \partial\kappa_\beta}\right|_{\boldsymbol{\kappa}=0} \qquad \text{(PBCs)}$$

- Equivalent geometrical expression (gauge-invariant 2-form)

$$D_{\alpha\beta} = D_{\text{free}}\delta_{\alpha\beta} - \frac{2\pi e^2}{\hbar^2 L^d} \text{Re} \left\langle \partial_{\kappa_\alpha}\Psi_0 \right| \left(\hat{H} - E_0\right) \left| \partial_{\kappa_\beta}\Psi_0 \right\rangle$$

- Spectral weight transferred from D_{free} to the regular term

- f-sum rule

$$\int_0^\infty d\omega \ \text{Re}\ \sigma_{\alpha\beta}(\omega) = \frac{D_{\alpha\beta}}{2} + \int_0^\infty d\omega \ \text{Re}\ \sigma^{(\text{regular})}_{\alpha\beta}(\omega) = \frac{D_{\text{free}}}{2}\delta_{\alpha\beta}$$

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Why λ^2 discriminate insulators from metals

If the $\boldsymbol{\kappa}$ components are **integer multiples** of $2\pi/L$ then:

- $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$ obeys Schrödinger Eq. and PBCs
- It is an eigenstate of $\hat{H}_{\boldsymbol{\kappa}}$ with eigenvalue E_0

- Does it coincide with the genuine $|\Psi_{0\boldsymbol{\kappa}}\rangle$ (evaluated according to Kohn's prescription)?

  - **Yes** (modulo a phase) if $D = 0$
  - **No** if $D \neq 0$:
    $E_{0\boldsymbol{\kappa}} > E_0$, $\quad |\Psi_{0\boldsymbol{\kappa}}\rangle$ orthogonal to $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle$

Why RS discriminate insulators from metals (cont'd)

$$\begin{aligned}
\langle \tilde{\Psi}_{0\boldsymbol{\kappa}_1} | \Psi_{0\boldsymbol{\kappa}_1} \rangle &= \langle \Psi_0 | \, e^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_{0\boldsymbol{\kappa}_1} \rangle = 0, \quad D \neq 0 \\
\langle \tilde{\Psi}_{0\boldsymbol{\kappa}_1} | \Psi_{0\boldsymbol{\kappa}_1} \rangle &= \langle \Psi_0 | \, e^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_{0\boldsymbol{\kappa}_1} \rangle = e^{i\gamma}, \quad D = 0
\end{aligned}$$

To lowest order in $1/L$:

$$\begin{aligned}
|\mathfrak{z}_N| &= |\langle \Psi_0 | \, e^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_0 \rangle| \simeq 0, \quad D \neq 0 \\
|\mathfrak{z}_N| &= |\langle \Psi_0 | \, e^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_0 \rangle| \simeq 1, \quad D = 0
\end{aligned}$$

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Outline

Kubo formula

- Need to break time-reversal symmetry at $\boldsymbol{\kappa} = 0$:

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i-1}^{N} \left[\mathbf{p}_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i) + \hbar \boldsymbol{\kappa} \right]^2 + \hat{V}$$

- Intrinsic Hall conductivity:

$$\text{Re } \sigma_{\alpha\beta}^{(-)}(0) = \frac{2\hbar e^2}{L^d} \sum_{n \neq 0}{}' \frac{\text{Im } \langle \Psi_0 | \hat{v}_\alpha | \Psi_n \rangle \langle \Psi_n | \hat{v}_\beta | \Psi_0 \rangle}{(E_n - E_0)^2}$$

- $\boldsymbol{\kappa} \cdot \hat{\mathbf{v}}$ expansion:

$$|\partial_{\boldsymbol{\kappa}} \Psi_0 \rangle = \sum_{n \neq 0} |\Psi_n\rangle \frac{\langle \Psi_n | \, \partial_{\boldsymbol{\kappa}} \hat{H} \, | \Psi_0 \rangle}{E_0 - E_n} = \frac{1}{\hbar} \sum_{n \neq 0} |\Psi_n\rangle \frac{\langle \Psi_n | \, \hat{\mathbf{v}} \, | \Psi_0 \rangle}{E_0 - E_n}$$

From Kubo formula to Berry curvature

- Substituting and exploiting completeness:

$$\text{Re}\,\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^d}\Omega_{\alpha\beta}(0)$$

- Many-body Berry curvature (extensive):

$$\Omega_{\alpha\beta}(\boldsymbol{\kappa}) = i(\,\langle\partial_{\kappa_\alpha}\Psi_0|\partial_{\kappa_\beta}\Psi_0\rangle - \langle\partial_{\kappa_\alpha}\Psi_0|\partial_{\kappa_\beta}\Psi_0\rangle\,)$$

- Insulators and metals, $2d$ and $3d$
- Mean-value theorem in $2d$ (in the $L\to\infty$ limit):

$$\frac{1}{L^2}\Omega_{xy}(0) = \frac{1}{L^2}\frac{L^2}{4\pi^2}\int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y\, \Omega_{xy}(\boldsymbol{\kappa})$$

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Many-body Chern number

- In the insulating case (and **only** in the insulating case):

$$|\Psi_{0,\boldsymbol{\kappa}+\boldsymbol{\kappa}_s}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}_s\cdot\hat{\mathbf{r}}}|\Psi_{0\boldsymbol{\kappa}}\rangle, \qquad \boldsymbol{\kappa}_1 = \left(\frac{2\pi}{L}, 0\right), \boldsymbol{\kappa}_2 = \left(0, \frac{2\pi}{L}\right)$$

- The integral is on a torus:

$$\frac{1}{2\pi}\int_0^{\frac{2\pi}{L}} d\kappa_x \int_0^{\frac{2\pi}{L}} d\kappa_y\, \Omega_{xy}(\boldsymbol{\kappa}) = C_1, \qquad \mathrm{Re}\,\sigma^{(-)}_{\alpha\beta}(0) = -\frac{e}{h}C_1$$

Niu, Thouless, and Wu, Phys. Rev. B **31**, 3372 (1985)

Outline

Kohn's Hamiltonian in the OBCs Hilbert space

- Same Hamiltonian with a "flux", but now within **OBCs**:

$$\hat{H}_{\boldsymbol{\kappa}} = \frac{1}{2m} \sum_{i=1}^{N} |\mathbf{p}_i + \hbar\boldsymbol{\kappa}|^2 + \hat{V}$$

  - The operator $\hat{\mathbf{r}} = \sum_i \mathbf{r}_i$ is well defined
  - $|\tilde{\Psi}_{0\boldsymbol{\kappa}}\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0\rangle$ obeys Schrödinger Eq.
  - It also obeys OBCs

- Ergo $\mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0(0)\rangle$ is the ground eigenstate of $\hat{H}_{\boldsymbol{\kappa}}$ with eigenvalue E_0, $\boldsymbol{\kappa}$-independent:

$$|\partial_{\kappa_\alpha}\Psi_0\rangle = i\,\hat{r}_\alpha|\Psi_0\rangle$$

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Many-body quantum metric within OBCs

- Quantum metric tensor (derivatives taken at $\boldsymbol{\kappa} = 0$))

$$\tilde{g}_{\alpha\beta} = \frac{1}{N}\left(\text{Re}\, \langle \partial_{\kappa_\alpha} \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle - \langle \partial_{\kappa_\alpha} \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle \right)$$

- Intensive ground state property, gauge-invariant (dimensions: squared length)

- **Basic tenet of the theory of the insulating state:** The OBCs metric $\tilde{g}_{\alpha\beta}$ in the thermodynamic limit
  - Diverges in all metals
  - Converges in all insulators
  - $\tilde{g}_{xx}$ converges to λ^2 (isotropic case)

Many-body quantum metric within OBCs

$$
\begin{aligned}
\tilde{g}_{\alpha\beta} &= \frac{1}{N}\left(\mathrm{Re}\, \langle \partial_{\kappa_\alpha} \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle - \langle \partial_{\kappa_\alpha} \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_{\kappa_\beta} \Psi_0 \rangle \right) \\
&= \frac{1}{N}\left(\langle \Psi_0 | \hat{r}_\alpha \hat{r}_\beta | \Psi_0 \rangle - \langle \Psi_0 | \hat{r}_\alpha | \Psi_0 \rangle \langle \Psi_0 | \hat{r}_\beta \Psi_0 \rangle \right) \\
&= \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' \, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,]
\end{aligned}
$$

- Exchange-correlation hole (integrates to -1):

$$
n_{xc}(\mathbf{r}, \mathbf{r}') = n^{(2)}(\mathbf{r}, \mathbf{r}') - n(\mathbf{r}) n(\mathbf{r}')
$$

- $\tilde{g}_{\alpha\beta}$ is the second moment of the XC hole, averaged over the sample

Special case: independent electrons

- Isotropic system in dimension d:

$$\tilde{g}_{xx} = \lambda^2 = \frac{1}{2Nd} \int d\mathbf{r} d\mathbf{r}' \, |\mathbf{r} - \mathbf{r}'|^2 [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,]$$

- **Independent electrons:** $n^{(2)}(\mathbf{r}, \mathbf{r}')$ is a function of $\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle$:

$$\begin{aligned} n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') &= 2 \, |\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle|^2 \qquad \text{(spinful)} \\ &= |\langle \mathbf{r} | \, \mathcal{P} \, | \mathbf{r}' \rangle|^2 \qquad \text{(spinless)} \end{aligned}$$

- **Special case:** band insulators and band metals

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- **Special case:** band insulators and band metals

Outline

Tight binding 1d binary crystal

$$H = \sum_j (\epsilon_j |j\rangle\langle j| - t |j+1\rangle\langle j| - t |j\rangle\langle j+1|)$$

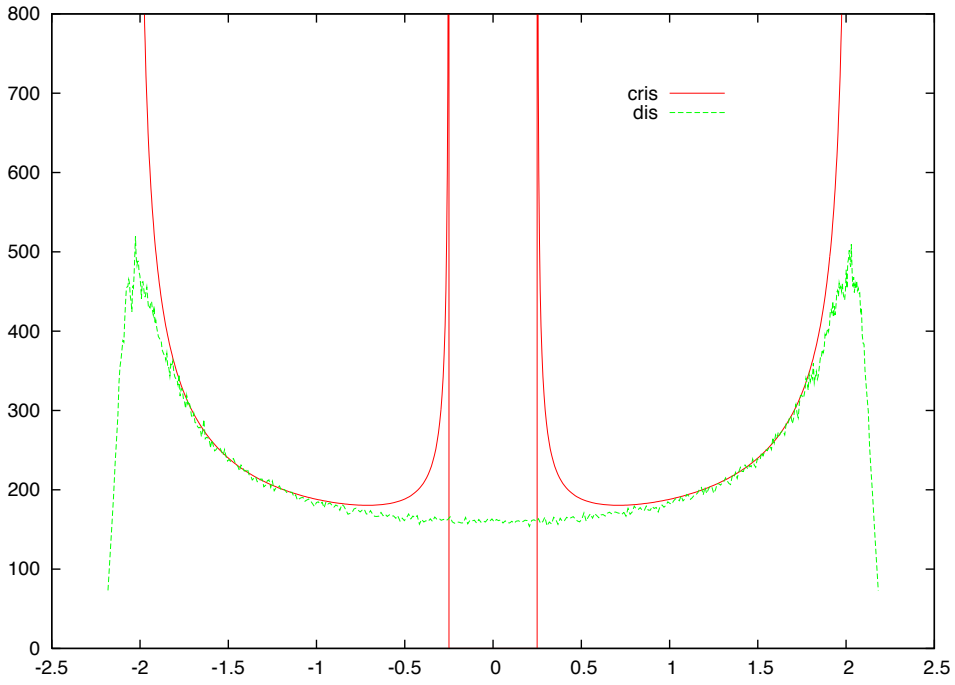
Diagonal disorder: t fixed, $\epsilon_b - \epsilon_a = 2\Delta$ fixed

Crystalline case: $\epsilon_j = (-1)^j \Delta$
ABABABABABABABABABABABABABABABABAB.....

Disordered case: random choice of ± 1 factors
ABAABABBABABBAABABABBABAABABBABABBAA .....

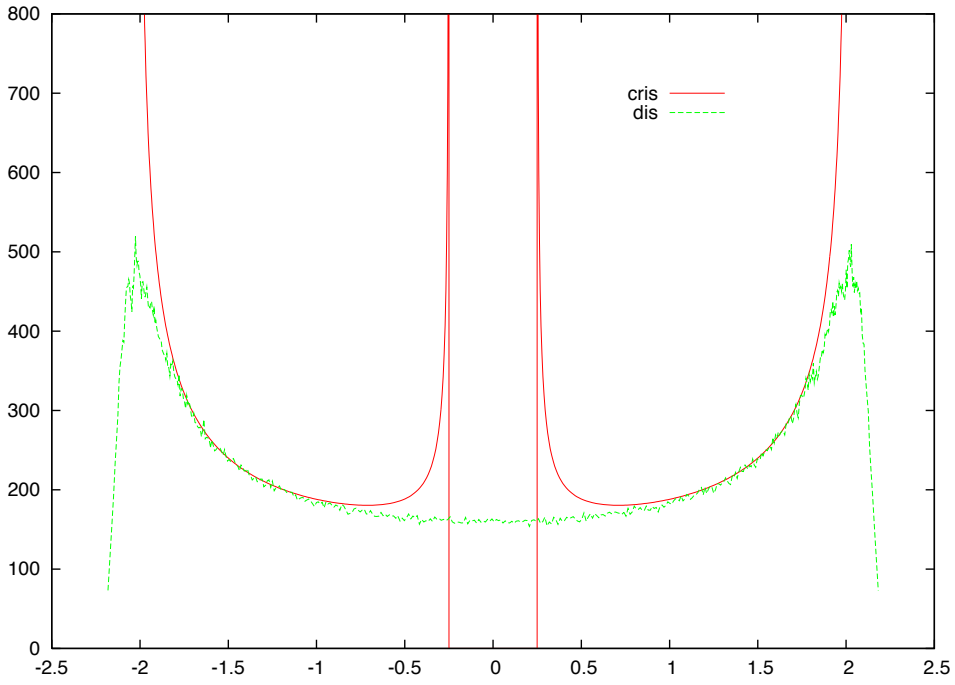
Random choice with equal probability, average over many replicas.

Density of states



- At half filling both (crystalline and disordered) are insulating
- At any other filling the crystalline is conducting and the disordered is insulating.
- What about $\tilde{g}$ (a.k.a. λ^2)?

Density of states



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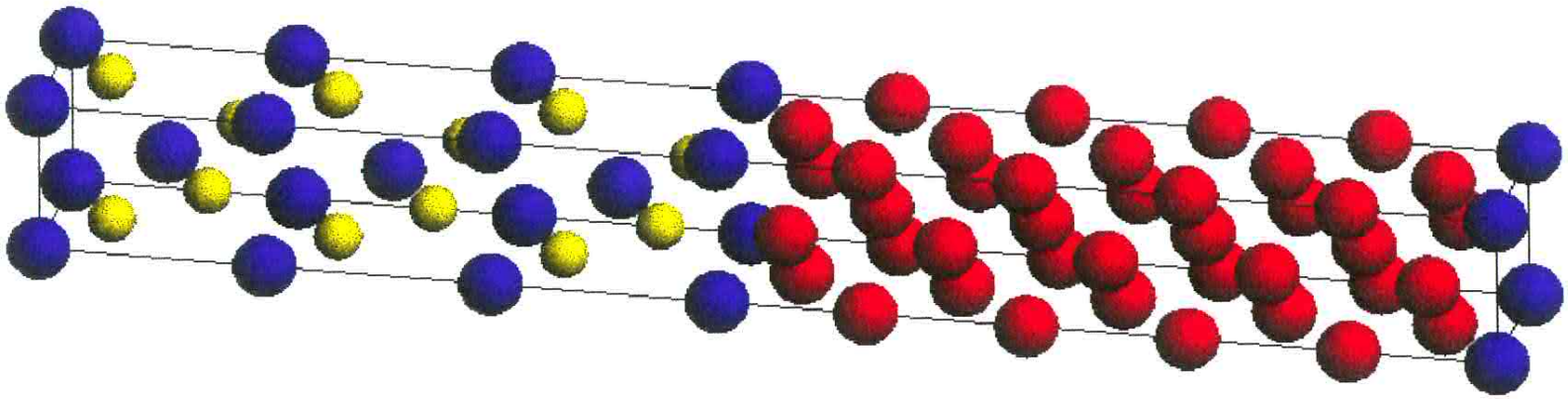
Results of the simulations
(5000 sites, 1000 replicas, 1/2 & 1/4 filling)

$$\tilde{g} = \frac{1}{2N} \int dx dx' \, (x - x')^2 |\langle x | \mathcal{P} | x' \rangle|^2 = \frac{a^2}{2N} \sum_{\ell,\ell'=1}^{N} P^2_{\ell\ell'} (\ell - \ell')^2$$

- In the crystalline case $\tilde{g}$ converges to a finite limit for 1/2 filling, diverges for 1/4 (as expected).
- In the disordered case $\tilde{g}$ always converge (to a very similar value for the two cases).
- The disordered case $\tilde{g}$ is about 20 times larger than the crystalline one. Why?
- The insulating mechanism (band vs. Anderson) is quite different, despite the very similar Hamiltonian.

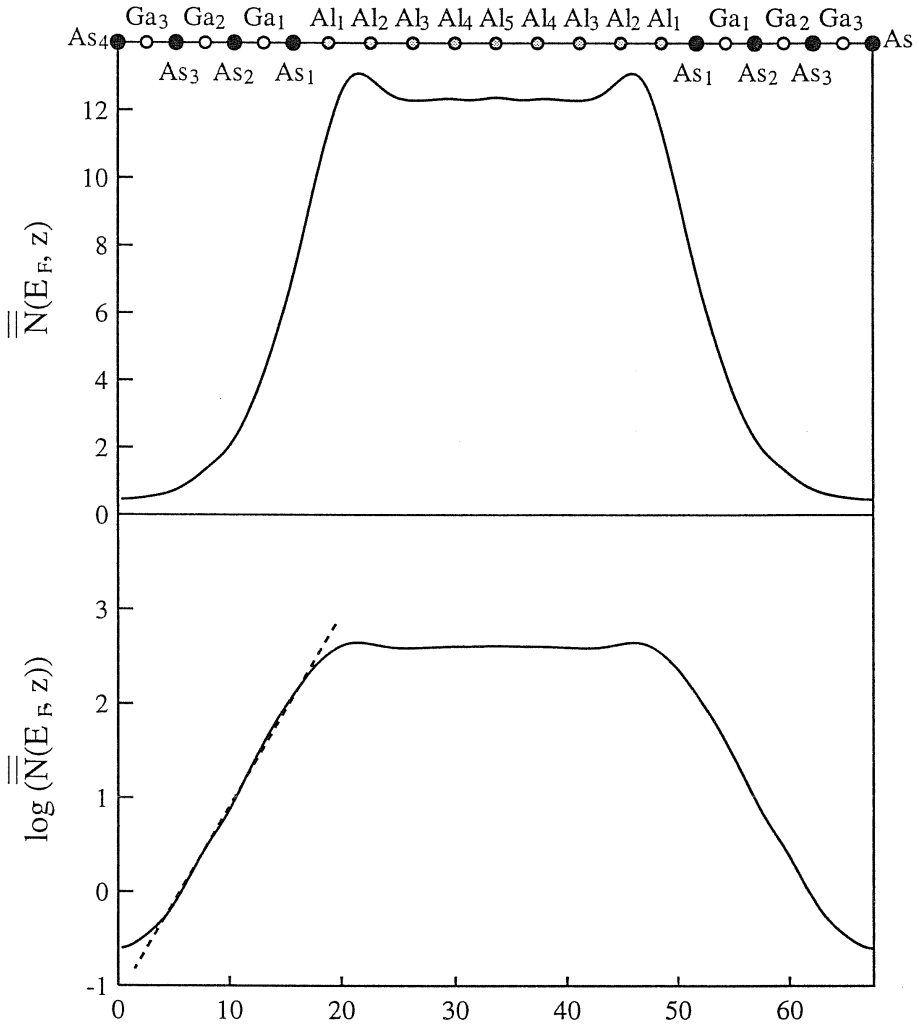
Outline

A metal-semiconductor heterojunction



- (001)Al/GaAs heterojunction
- The **local density of states** at the Fermi level is the obvious **local marker** to discriminate insulating vs. metallic regions

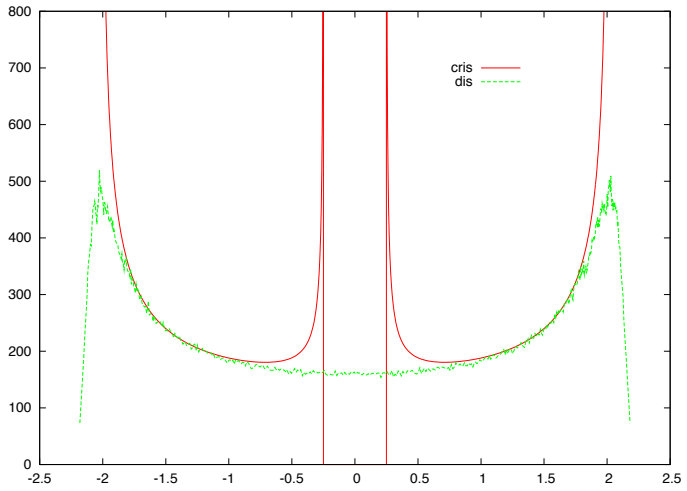
Local density of states at the Fermi level



LDOS (macroscopic average) at the Fermi level

Notice the evanescent states

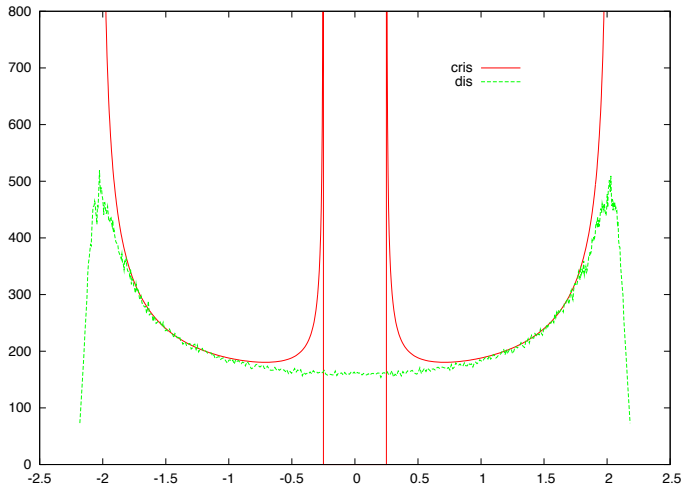
The problem



- The local density of states at the Fermi level cannot work for Anderson insulators: **gapless**

- The OBCs quantum metric
  - Diverges in all metals
  - Converge to a finite value in all insulators
  - It can probe a inhomogeneous system **locally**

The problem



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Simulations for 1d heterojunctions

- Convert into a "localization density"

$$\begin{aligned} \tilde{g} &= \frac{1}{N}\int dx dx' \, (x-x')^2 |\langle x|\,\mathcal{P}\,|x'\rangle|^2 \qquad \text{(spinful)} \\ n\tilde{g} &= \frac{1}{L}\int dx dx' \, (x-x')^2 |\langle x|\,\mathcal{P}\,|x'\rangle|^2 \\ &= -\frac{1}{L}\int_{\text{sample}} dx \, \langle x|\,\mathcal{P}\,[x,\mathcal{P}]\,[x,\mathcal{P}]\,|x\rangle \end{aligned}$$

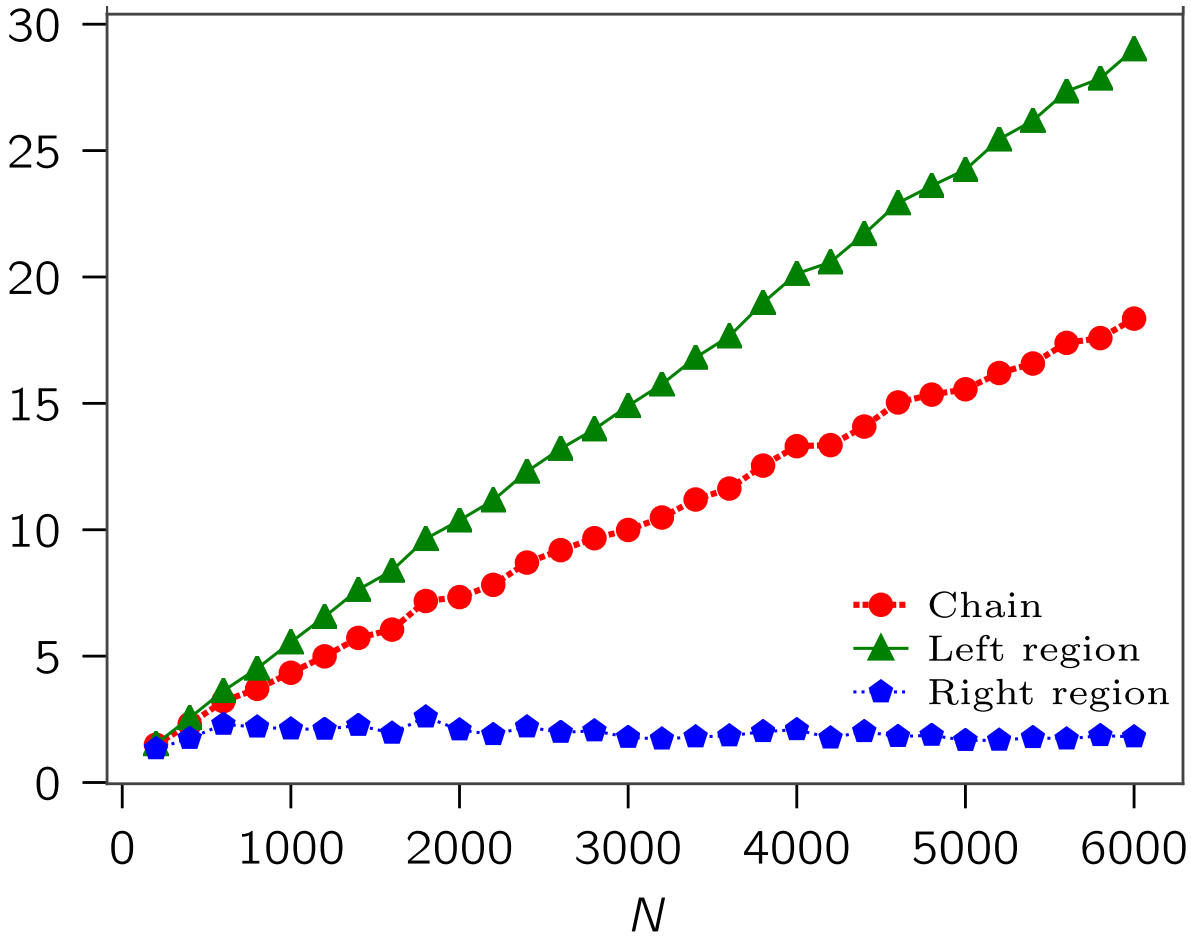
- **Local probe** of the insulating state:

$$\mathcal{L}(x) = -\langle x|\,\mathcal{P}\,[x,\mathcal{P}]\,[x,\mathcal{P}]\,|x\rangle$$

Simulations for 1d heterojunctions

A. Marrazzo and R. Resta, Phys. Rev. Lett. **122**, 166602 (2019)

Local OBCs metric



Left half-chain: Metal

Right half-chain: Anderson insulator

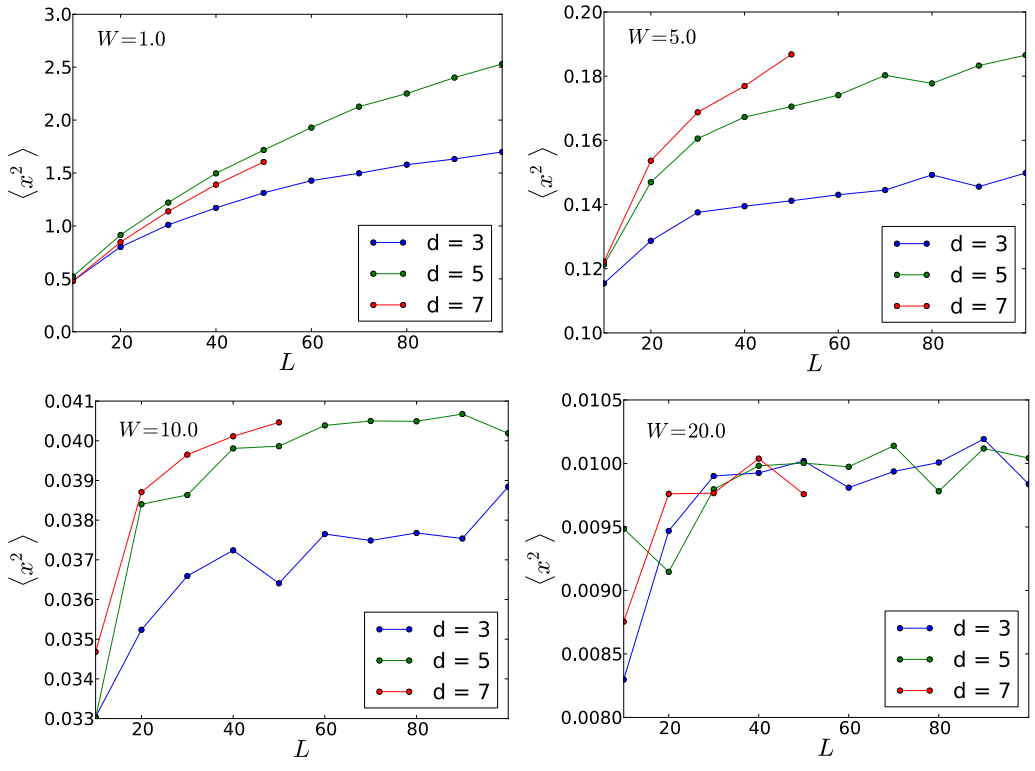
Outline

The benchmark model 3d system

- Need a 3d system to observe the **M-I transition**
- A standard 3d tight-binding Hamiltonian is known from previous literature to undergo the transition at $W_c = 8.25$ (W is the amount of tunable disorder, in appropriate units)
- In our (and others') simulations:
  - Computational samples are long rods of square section
  - Results are averaged over several disorder realizations
- The novelty here: using the quantum metric to detect the transition **in the ground state**

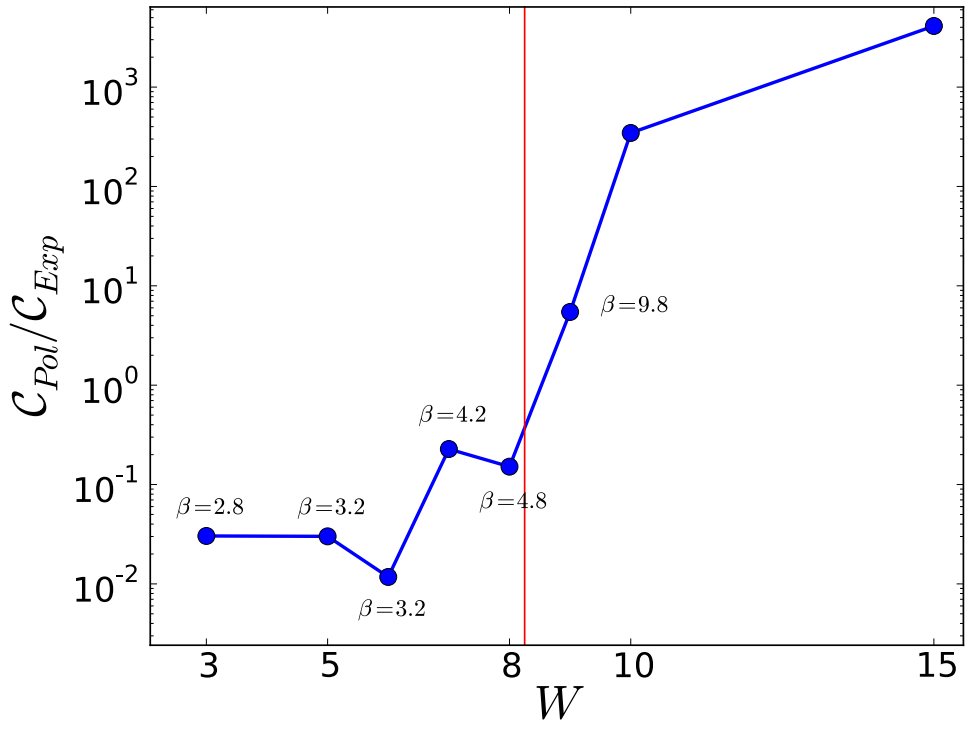
Anderson transition as a ground-state property

T. Olsen, R. Resta, and I. Souza, Phys. Rev. B **95**, 045109 (2017)



Localization length $\lambda = \sqrt{\tilde{g}_{\alpha\alpha}}$ as a function of rod length L
(average over 100 disorder realizations)

A smarter way to estimate W_c (by Thomas Olsen)



Our best estimate: $W_c = 8.5$

We are probing "the organization" of the electrons in their **ground state**

Thank you for your attention!