The insulating state of matter: A geometrical theory

Raffaele Resta

CNR-IOM Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche,
and Donostia International Physics Center, San Sebastián, Spain

Lisbon, June 29th, 2020

Review paper

Geometry and topology in many-body physics

Raffaele Resta
Istituto Officina dei Materiali IOM-CNR, Trieste, Italy
and Donostia International Physics Center, San Sebastián, Spain

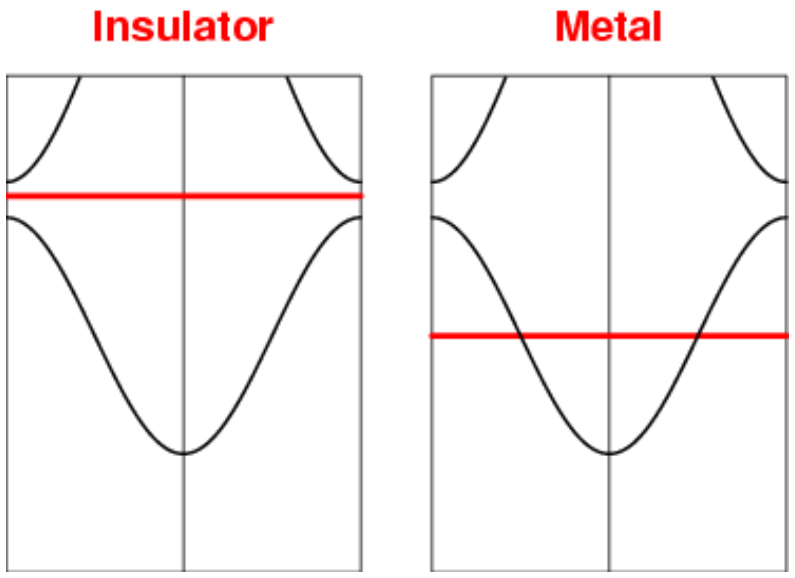
- Posted **yesterday** at ArXiv.org

- To appear in:
  Topology, Entanglement, and Strong Correlations
  Modeling and Simulation, Vol. 10
  Verlag des Forschungszentrum Jülich, 2020
  Editors: Eva Pavarini and Erik Koch

Outline

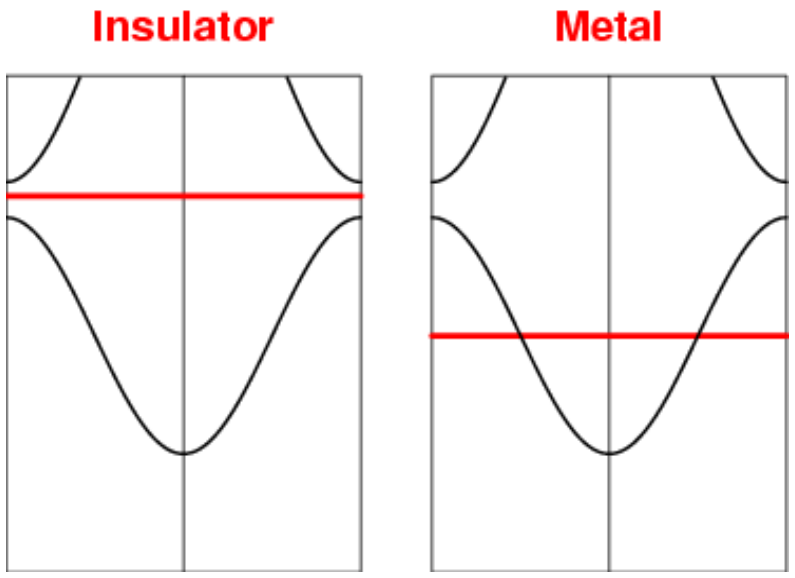
Outline

The textbook picture
(Bloch 1928, Wilson 1931)



- Bloch theorem applies to **noninteracting** electrons in a periodic **crystalline** potential.
- "Noninteracting" means in a mean field
- **Main message:**
  The insulating state requires a spectral gap

The textbook picture
(Bloch 1928, Wilson 1931)



- Bloch theorem applies to **noninteracting** electrons in a periodic **crystalline** potential.
- "Noninteracting" means in a mean field
- **Main message:**
  The insulating state requires a spectral gap

“Exotic” insulators

- In some materials, the insulating character is **dominated** by disorder: **Anderson insulators**.
- In some materials, the insulating character is **dominated** by electron-electron interaction: **Mott insulators**.
- Other kinds of exotic insulators exist.
  Example: a two-dimensional electron fluid in the quantum-Hall regime.
- 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, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, 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
- **What Kohn did not provide:**
  - A "marker" (quantitative probe) for the insulating state

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, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, 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
- **What Kohn did not provide:**
  - A "marker" (quantitative probe) for the insulating state

Kohn's theory revisited since 1999

VOLUME 82, NUMBER 2 PHYSICAL REVIEW LETTERS 11 JANUARY 1999

Electron Localization in the Insulating State

Raffaele Resta
Istituto Nazionale di Fisica della Materia (INFM), Strada Costiera 11, I-34014 Trieste, Italy
and Dipartimento di Fisica Teorica, Università di Trieste, I-34014 Trieste, Italy

Sandro Sorella
Istituto Nazionale di Fisica della Materia (INFM), Via Beirut 4, I-34014 Trieste, Italy
and Scuola Internazionale Superiore di Studî Avanzati (SISSA), Via Beirut 4, 34014, Trieste Italy
(Received 11 August 1998)

- **In the original paper:**
  Theory of the insulating state and theory of polarization based on the same formalism
- **More recent findings:**
  Even dc conductivity stems from the same formalism

Conductivity vs. polarization

- **Phenomenologically:**
  - **Metal:** Has a **nonzero** dc conductivity
  - **Insulator:** Has a **zero** dc conductivity (at zero temperature)

- **But also**
  - **Metal:** Macroscopic electrical polarization is trivial: It is **not** a bulk effect.
  - **Insulator:** Macroscopic polarization is **non**trivial: It is a bulk effect, material dependent.

- **Change of paradigm** about polarization in the 1990s: Polarization is a geometrical ground state observable

Conductivity vs. polarization

- **Phenomenologically:**
  - **Metal:** Has a **nonzero** dc conductivity
  - **Insulator:** Has a **zero** dc conductivity (at zero temperature)

- **But also**
  - **Metal:** Macroscopic electrical polarization is trivial: It is **not** a bulk effect.
  - **Insulator:** Macroscopic polarization is **non**trivial: It is a bulk effect, material dependent.

- **Change of paradigm** about polarization in the 1990s: Polarization is a geometrical ground state observable

Outline

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?**

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 $\mathrm{Im} \ln \langle \Psi_1 | \Psi_2 \rangle$?

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

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

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

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 $\mathrm{Im} \ln \langle \Psi_1 | \Psi_2 \rangle$?

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

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

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

Sir Michael

M.V. Berry,
“Quantal phase factors accompanying adiabatic changes”,
Proc. R. Soc. Lond. 1984

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):

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

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):

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

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):

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

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**:

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

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**:

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

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

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 $\boldsymbol{\kappa}$)

A lattice of special $\boldsymbol{\kappa}$ vectors

- 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

- 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, $|\mathfrak{z}_N^{(x)}| \leq 1$
- Theory of polarization and RS theory of the insulating state both rooted in $\mathfrak{z}_N^{(x)}$ (in the large-N limit)

A lattice of special $\boldsymbol{\kappa}$ vectors

- 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

- 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, $|\mathfrak{z}_N^{(x)}| \leq 1$
- Theory of polarization and RS theory of the insulating state both rooted in $\mathfrak{z}_N^{(x)}$ (in the large-N limit)

A lattice of special $\boldsymbol{\kappa}$ vectors

- 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

- 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, $|\mathfrak{z}_N^{(x)}| \leq 1$
- Theory of polarization and RS theory of the insulating state both rooted in $\mathfrak{z}_N^{(x)}$ (in the large-N limit)

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 $|\Psi_0\rangle$:

$$D^2_{0,\boldsymbol{\kappa}_1} = -\ln|\langle\tilde{\Psi}_{0\boldsymbol{\kappa}_1}|\Psi_0\rangle|^2 = -\ln|\mathfrak{z}_N^{(x)}|^2$$

  - Discretized metric:

$$-\ln|\mathfrak{z}_N^{(x)}|^2 \simeq g_{xx}(0)(\Delta\kappa_x)^2 = g_{xx}(0)\left(\frac{2\pi}{L}\right)^2$$

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 $|\Psi_0\rangle$:

$$D^2_{0,\boldsymbol{\kappa}_1} = -\ln |\langle\tilde{\Psi}_{0\boldsymbol{\kappa}_1}|\Psi_0\rangle|^2 = -\ln |\mathfrak{z}_N^{(x)}|^2$$

  - Discretized metric:

$$-\ln |\mathfrak{z}_N^{(x)}|^2 \simeq g_{xx}(0)(\Delta\kappa_x)^2 = g_{xx}(0)\left(\frac{2\pi}{L}\right)^2$$

Outline

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:**

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

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:**

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

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

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

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

- Polarization:

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

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

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

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

- Polarization:

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

The single-point Berry phase

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

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

- γ is the Berry phase in disguise
- γ includes the nuclear contribution
- 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

The single-point Berry phase

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

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

- γ is the Berry phase in disguise
- γ includes the nuclear contribution
- 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

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

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

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

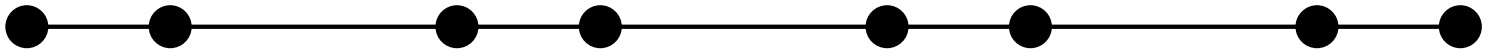
Alternant polyacetilene, model molecular crystal.....

$\mathbb{Z}_2$-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

Simple tight-binding Hamiltonians

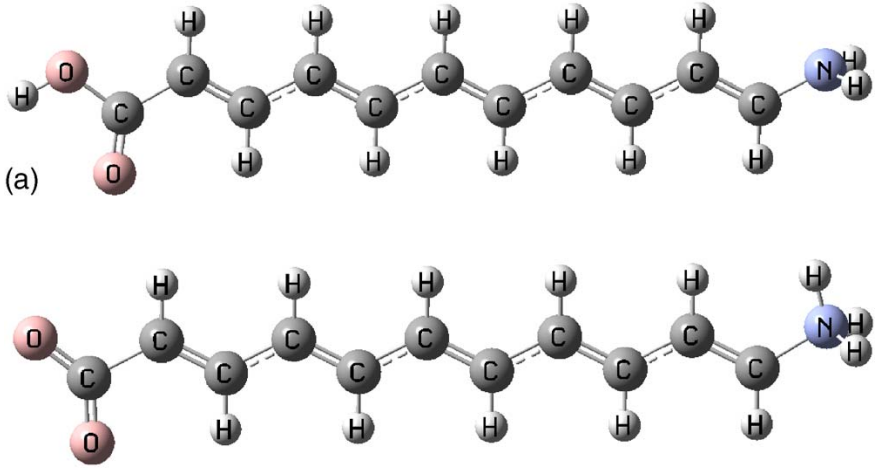


$\mathbb{Z}_2$-even: Onsite ϵ_i constant, alternating hoppings t and t'

$\mathbb{Z}_2$-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!**

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

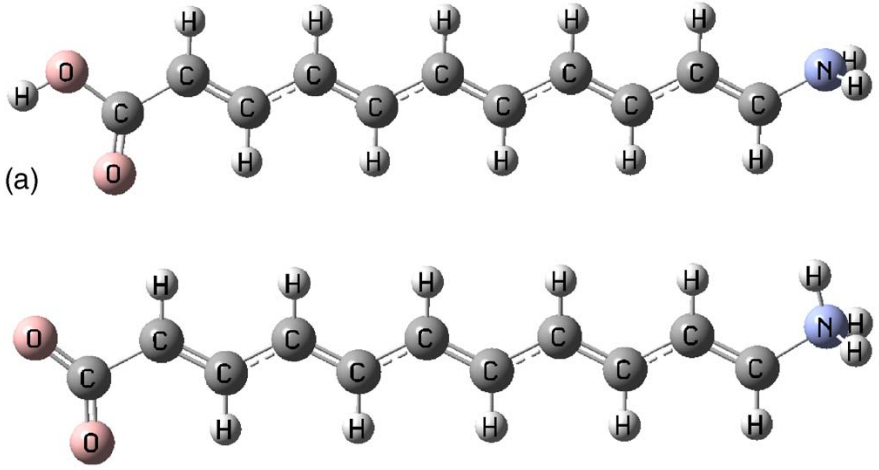


Centrosymmetric “bulk”

Two different asymmetric terminations

Polarization is a multivalued observable

(K. Kudin, R. Car, & R. Resta, J. Chem Phys. 2007)

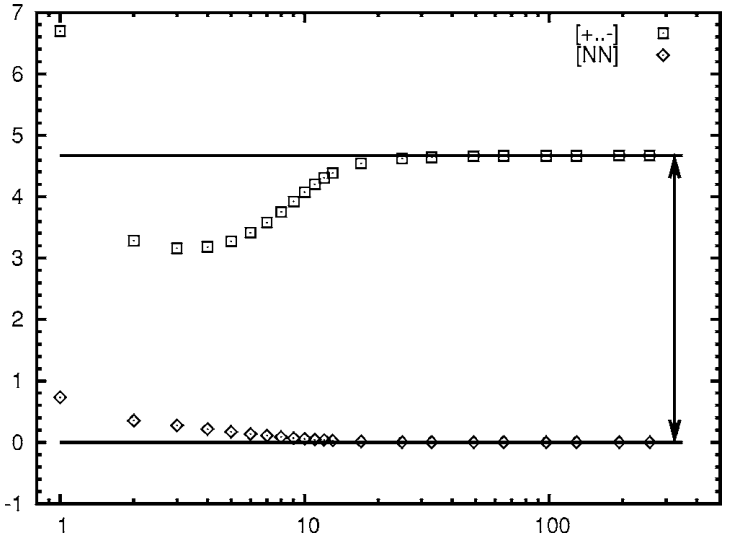


Centrosymmetric “bulk”

Two different asymmetric terminations

dipole/length = P

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



dipole per monomer

Outline

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

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

Outline

Definition

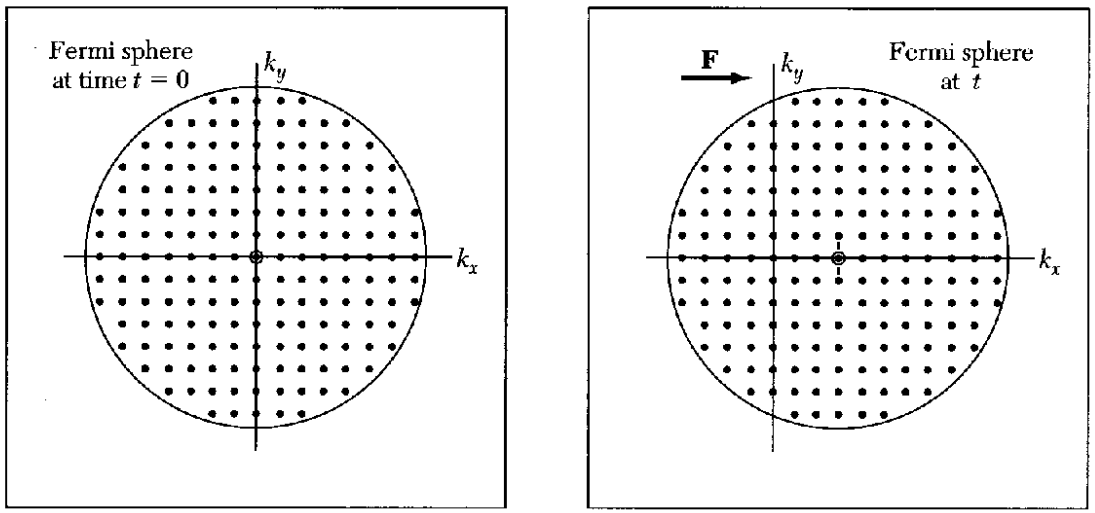
- Charge transport in a metal is a balance between free acceleration and dissipation (Ohm's law)
- QM addresses the **free-acceleration** side of the problem
- The **Drude weight** D (a.k.a. adiabatic **charge stiffness**) measures the inverse inertia of the many-electron system
- $D = 0$ in insulators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

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

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

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

- Spectral weight transferred from D to the regular term

- f-sum rule

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

Drude weight (Kohn's formula)

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

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

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

- Spectral weight transferred from D to the regular term

- f-sum rule

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

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 $1/L$:

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

Why RS discriminate insulators from metals (cont'd)

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

To lowest order in $1/L$:

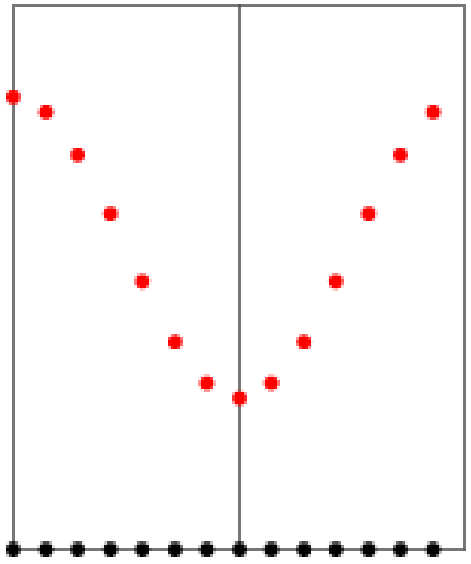
$$\begin{aligned}
|\mathfrak{z}_N| &= |\, \langle \Psi_0 | \, \mathrm{e}^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_0 \rangle \,| \simeq 0, \quad D \neq 0 \\
|\mathfrak{z}_N| &= |\, \langle \Psi_0 | \, \mathrm{e}^{i\boldsymbol{\kappa}_1 \cdot \hat{\mathbf{r}}} \, | \Psi_0 \rangle \,| \simeq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

Outline

Outline

Bloch orbitals in 1d (insulator)

Before the thermodynamic limit: N and L **finite**



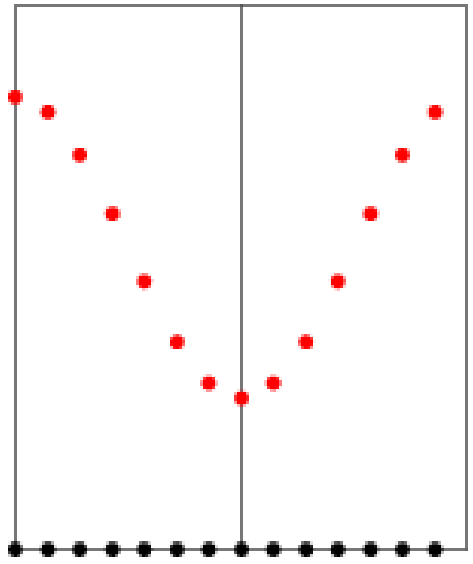
PBCs over 14 cells: $L = Ma$, $M = 14$ in this drawing:

14 Bloch vectors in the Brillouin zone
14 orbitals in a band

The ground state $|\Psi_0\rangle$ is a Slater determinant:
14 Bloch orbitals (spinless electrons); Bloch vectors k_j

Bloch orbitals in 1d (insulator)

Before the thermodynamic limit: N and L **finite**



PBCs over 14 cells: $L = Ma$, $M = 14$ in this drawing:

14 Bloch vectors in the Brillouin zone
14 orbitals in a band

The ground state $|\Psi_0\rangle$ is a Slater determinant:
14 Bloch orbitals (spinless electrons); Bloch vectors k_j

P when $|\Psi_0\rangle$ is a Slater determinant

$$\mathfrak{z}_N = \langle\Psi_0|e^{i\frac{2\pi}{L}\sum_j x_j}|\Psi_0\rangle = \langle\Psi_0|U|\Psi_0\rangle = \langle\Psi_0|\tilde{\Psi}_0\rangle$$

Even $|\tilde{\Psi}_0\rangle$ is a Slater determinant

Theorem: $\langle\Psi|\tilde{\Psi}\rangle = \det S$

Single band case:

$$S(k_j, k_{j'}) = \langle\psi_{k_j}|\tilde{\psi}_{k_{j'}}\rangle = \int_0^L dx\ \psi^*_{k_j}(x) e^{i\frac{2\pi}{L}x}\psi_{k_{j'}}(x).$$

P when $|\Psi_0\rangle$ is a Slater determinant

$$\mathfrak{z}_N = \langle\Psi_0|e^{i\frac{2\pi}{L}\sum_j x_j}|\Psi_0\rangle = \langle\Psi_0|U|\Psi_0\rangle = \langle\Psi_0|\tilde{\Psi}_0\rangle$$

Even $|\tilde{\Psi}_0\rangle$ is a Slater determinant

Theorem: $\langle\Psi|\tilde{\Psi}\rangle = \det S$

Single band case:

$$S(k_j, k_{j'}) = \langle\psi_{k_j}|\tilde{\psi}_{k_{j'}}\rangle = \int_0^L dx\ \psi^*_{k_j}(x)e^{i\frac{2\pi}{L}x}\psi_{k_{j'}}(x).$$

P when $|\Psi_0\rangle$ is a Slater determinant

$$\mathfrak{z}_N = \langle\Psi_0|e^{i\frac{2\pi}{L}\sum_j x_j}|\Psi_0\rangle = \langle\Psi_0|U|\Psi_0\rangle = \langle\Psi_0|\tilde{\Psi}_0\rangle$$

Even $|\tilde{\Psi}_0\rangle$ is a Slater determinant

Theorem: $\langle\Psi|\tilde{\Psi}\rangle = \det S$

Single band case:

$$S(k_j, k_{j'}) = \langle\psi_{k_j}|\tilde{\psi}_{k_{j'}}\rangle = \int_0^L dx\ \psi^*_{k_j}(x)e^{i\frac{2\pi}{L}x}\psi_{k_{j'}}(x).$$

The (connection) matrix is very sparse

$$S = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \blacksquare \\ \blacksquare & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \blacksquare & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \blacksquare & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \blacksquare & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \blacksquare & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \blacksquare & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \blacksquare & 0 \end{pmatrix}$$

The matrix element vanishes unless $k_{j'} = k_j - 2\pi/L$, that is $j' = j-1$: the determinant **factors**.

$$\mathcal{Z}_N = \det S = \prod_{j=1}^{M} S(k_j, k_{j-1})$$

The Berry phase

Periodic factor in a Bloch orbital: $\psi_k(x) = \mathrm{e}^{ikx} u_k(x)$

$$
\begin{aligned}
S(k_j, k_{j-1}) &= \int_0^L dx\ \psi^*_{k_j}(x) \mathrm{e}^{i\frac{2\pi}{L}x} \psi_{k_{j-1}}(x) \\
&= \int_0^L dx\ u^*_{k_j}(x) u_{k_{j-1}}(x) \\
&= \langle u_{k_j} | u_{k_{j-1}} \rangle \\
\gamma^{(\mathrm{el})} &= \mathrm{Im}\ \ln \prod_{j=1}^{M} S(k_j, k_{j-1}) = -\mathrm{Im}\ \ln \prod_{j=1}^{M} \langle u_{k_{j-1}} | u_{k_j} \rangle
\end{aligned}
$$

King-Smith & Vanderbilt discretized formula (1993):

$$
\gamma^{(\mathrm{el})} = \int_{\mathrm{BZ}} dk\ \mathcal{A}(\mathbf{k}) = i \int_{\mathrm{BZ}} dk\ \langle u_k | \frac{d}{dk} u_k \rangle = -\lim_{M\to\infty} \mathrm{Im}\ \ln \prod_{j=1}^{M} \langle u_{k_{j-1}} | u_{k_j} \rangle
$$

The Berry phase

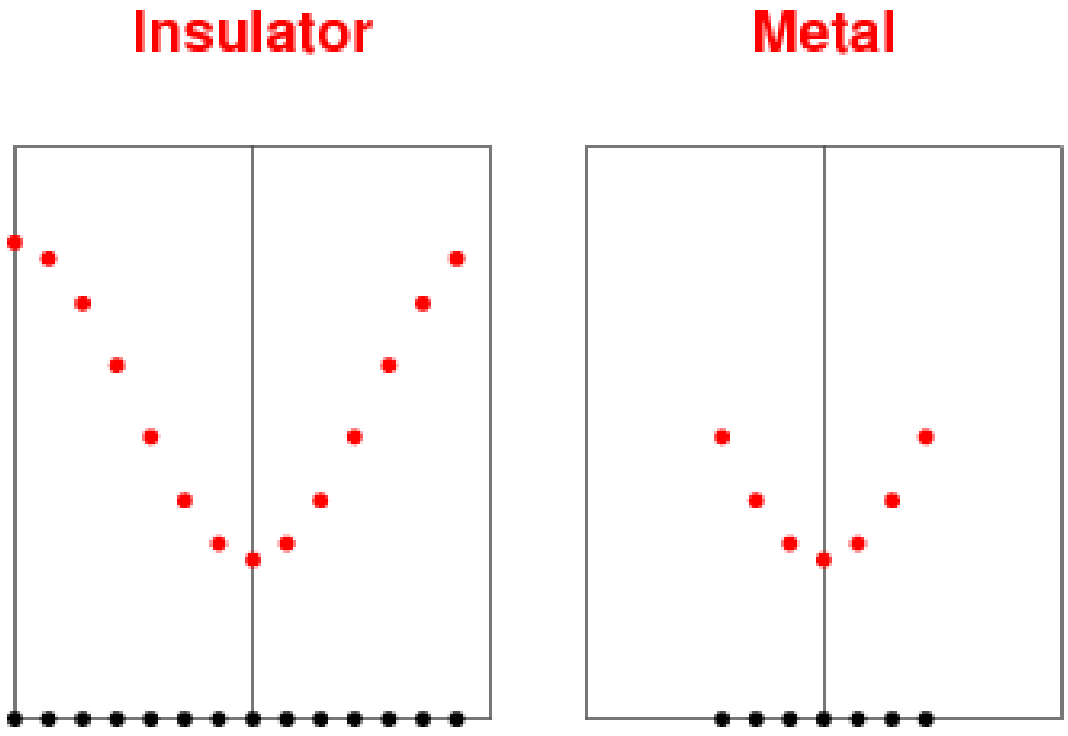
Periodic factor in a Bloch orbital: $\psi_k(x) = \mathrm{e}^{ikx} u_k(x)$

$$
\begin{aligned}
S(k_j, k_{j-1}) &= \int_0^L dx\ \psi^*_{k_j}(x) \mathrm{e}^{i\frac{2\pi}{L}x} \psi_{k_{j-1}}(x) \\
&= \int_0^L dx\ u^*_{k_j}(x) u_{k_{j-1}}(x) \\
&= \langle u_{k_j} | u_{k_{j-1}} \rangle \\
\gamma^{(\mathrm{el})} &= \mathrm{Im}\ \ln \prod_{j=1}^{M} S(k_j, k_{j-1}) = -\mathrm{Im}\ \ln \prod_{j=1}^{M} \langle u_{k_{j-1}} | u_{k_j} \rangle
\end{aligned}
$$

King-Smith & Vanderbilt discretized formula (1993):

$$
\gamma^{(\mathrm{el})} = \int_{\mathrm{BZ}} dk\ \mathcal{A}(\mathbf{k}) = i \int_{\mathrm{BZ}} dk\ \langle u_k | \frac{d}{dk} u_k \rangle = -\lim_{M\to\infty} \mathrm{Im}\ \ln \prod_{j=1}^{M} \langle u_{k_{j-1}} | u_{k_j} \rangle
$$

Band insulators vs. band metals



PBCs over 14 cells: $L = Ma$, $M = 14$ in this drawing:
14 Bloch vectors in the Brillouin zone.

14 occupied orbitals in the insulating state ($N = M$),
7 occupied orbitals in the metallic state ($N = M/2$).

Crystalline system of independent electrons

Before the thermodynamic limit: N and L **finite**

- $|\Psi_0\rangle$ is written as a determinant of occupied Bloch orbitals, in **both** the insulating and the metallic case.

- **Key difference:**
  The whole band is used to build the insulating $|\Psi_0\rangle$, while only one half of the band is used for the metallic $|\Psi_0\rangle$.

Insulators vs. metal

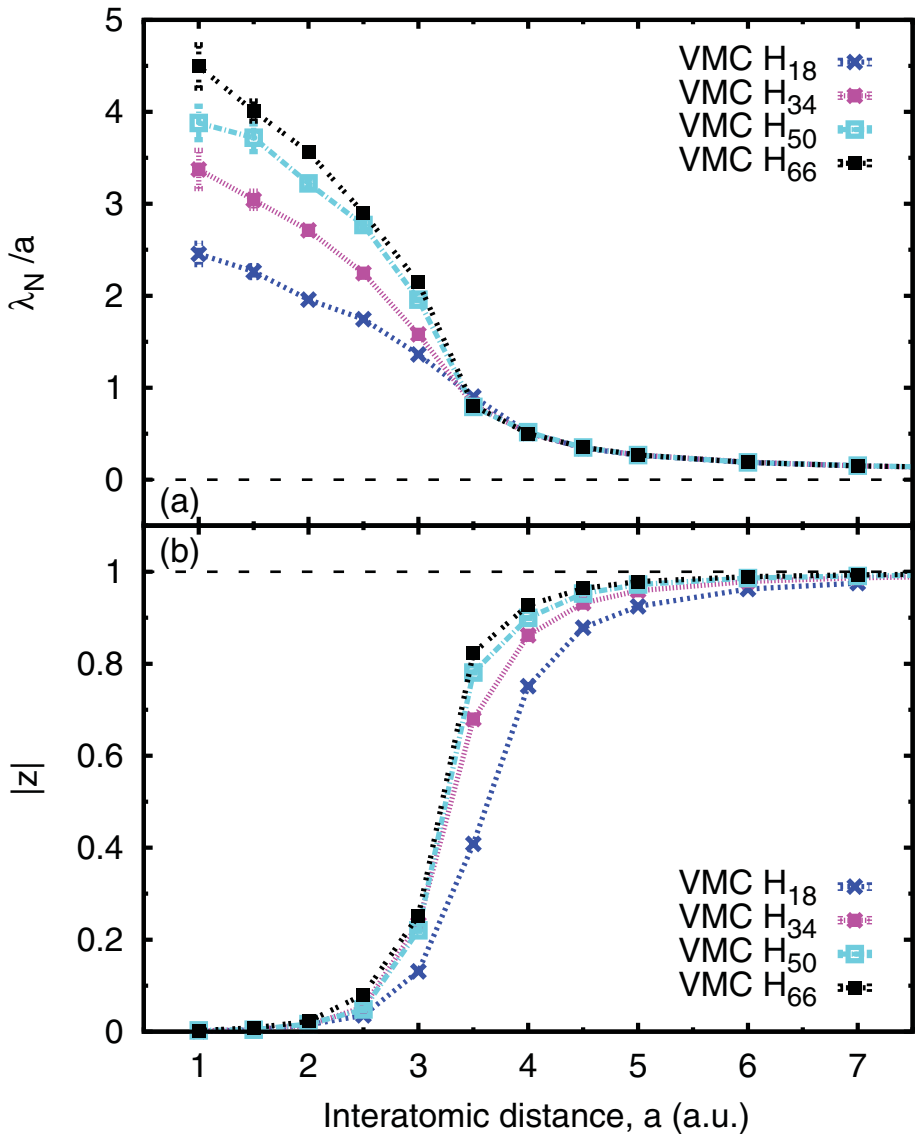
$$S = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \blacksquare \\ \blacksquare & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \blacksquare & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \blacksquare & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \blacksquare & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \blacksquare & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \blacksquare & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \blacksquare & 0 \end{pmatrix}$$

- **Zero determinant** in the metallic case!
- In a band metal $\lambda^2 = \infty$ **even at finite** N
- In a band insulator $\lambda^2 \propto$ Wannier fct's quadratic spread Ω_{I}

Outline

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

Model 1d ionic crystal

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

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

$$H = \sum_j [\ (-1)^j \Delta\ |j\rangle\langle j| - t\ |j+1\rangle\langle j| - t\ |j\rangle\langle j+1|\ ]$$

- In second quantization notations:

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

Model 1d ionic crystal

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

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

$$H = \sum_j [\ (-1)^j \Delta\ |j\rangle\langle j| - t\ |j+1\rangle\langle j| - t\ |j\rangle\langle j+1|\ ]$$

- In second quantization notations:

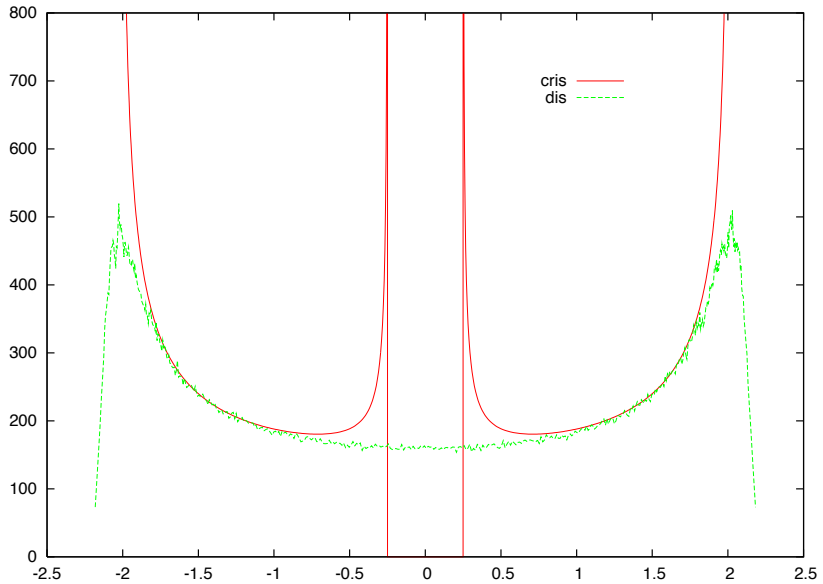
$$H = \sum_j [\ (-1)^j \Delta\ c_j^\dagger c_j - t\ c_j^\dagger c_{j+1} - t\ c_{j+1}^\dagger c_j\ ]$$

Model 1d ionic crystal

- Band structure:

$$\epsilon(k) = \pm\sqrt{\Delta^2 + 4t^2 \cos^2 ka/2}$$

- Insulator at half filling
- Density of states $\mathcal{D}(\epsilon)d\epsilon$: **Red plot**



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 $\mathbb{Z}_2$ invariant

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

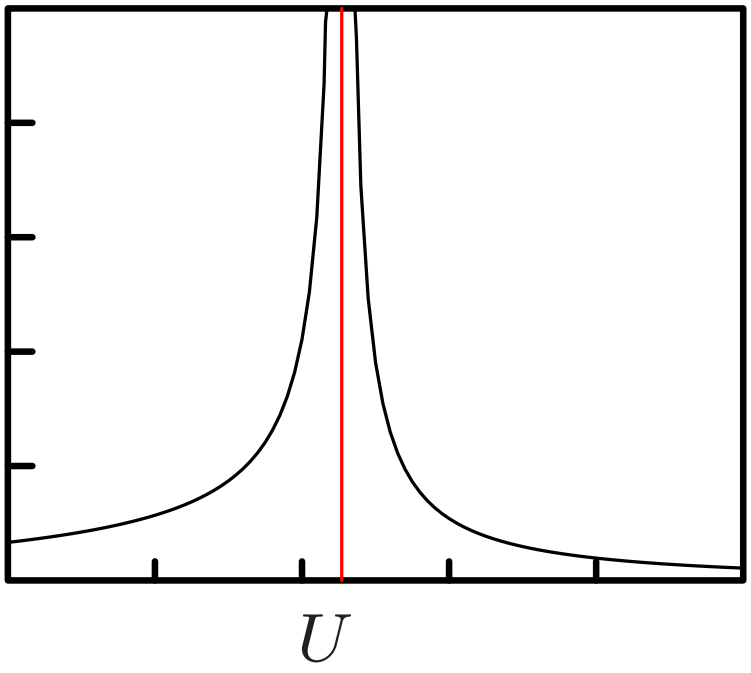
- Matrix element real in inversion-symmetric systems:
  - $\langle \Psi_0 | U | \Psi_0 \rangle > 0 \Longrightarrow \mathbb{Z}_2$-even
  - $\langle \Psi_0 | U | \Psi_0 \rangle < 0 \Longrightarrow \mathbb{Z}_2$-odd

- Topological invariant "protected" by inversion symmetry
- Parity may switch only crossing a metallic state:

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

Topological insulator-insulator transition

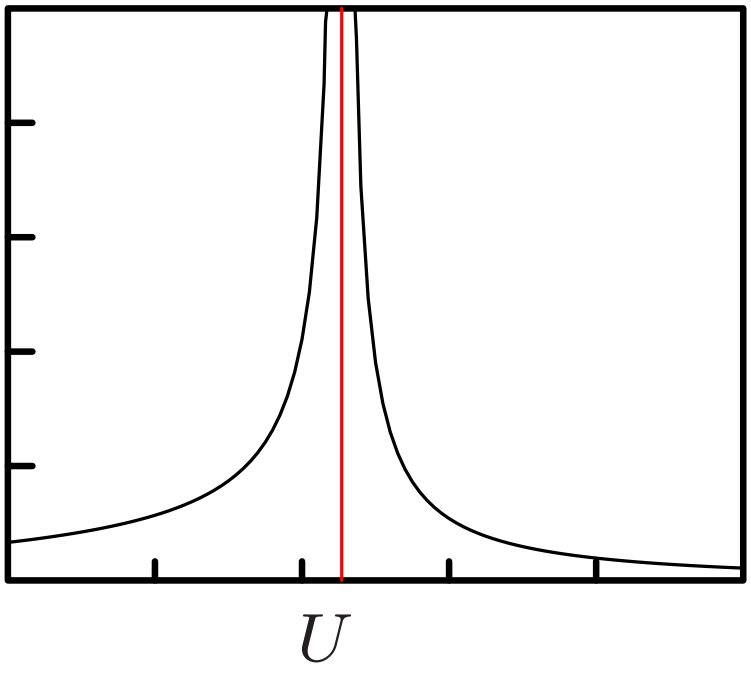
- Plot of λ^2 at half filling:



- **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

Topological insulator-insulator transition

- Plot of λ^2 at half filling:



- **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

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:

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

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:

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

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

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

Outline

Tight binding 1d binary crystal

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

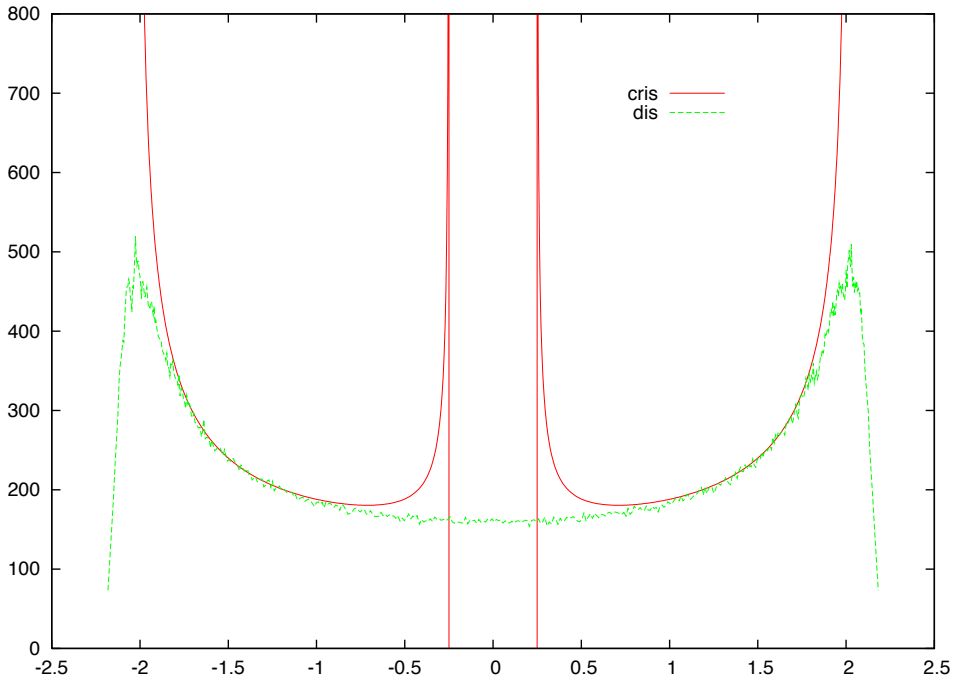
Diagonal disorder: t fixed, $\epsilon_b - \epsilon_a = 2\Delta$ fixed

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

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

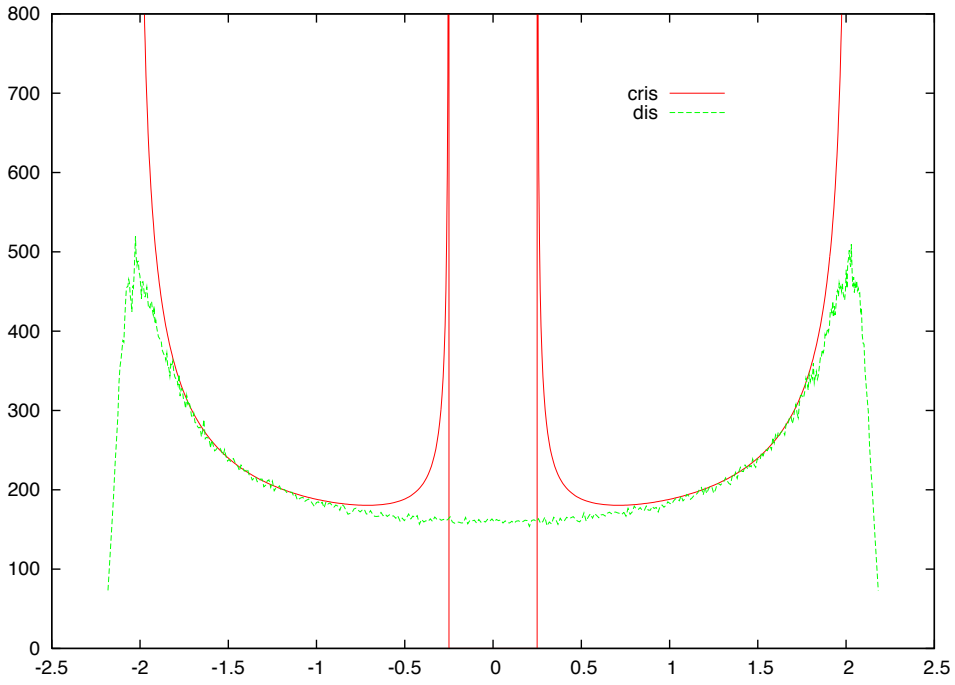
Random choice with equal probability, average over many replicas.

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



- 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)?

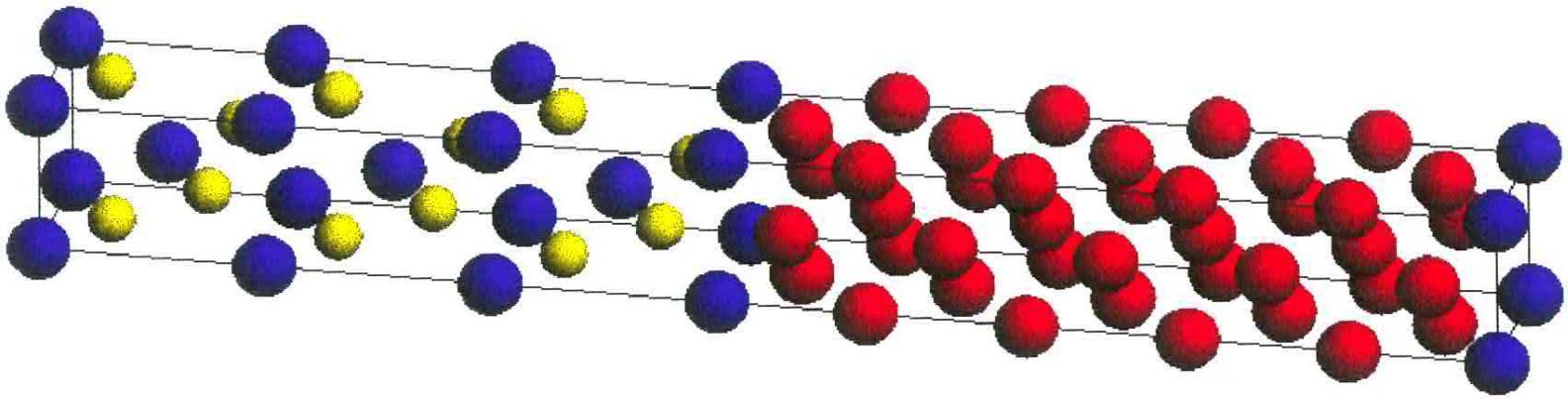
Results of the simulations
(5000 sites, 1000 replicas, 1/2 & 1/4 filling)

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

- 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.

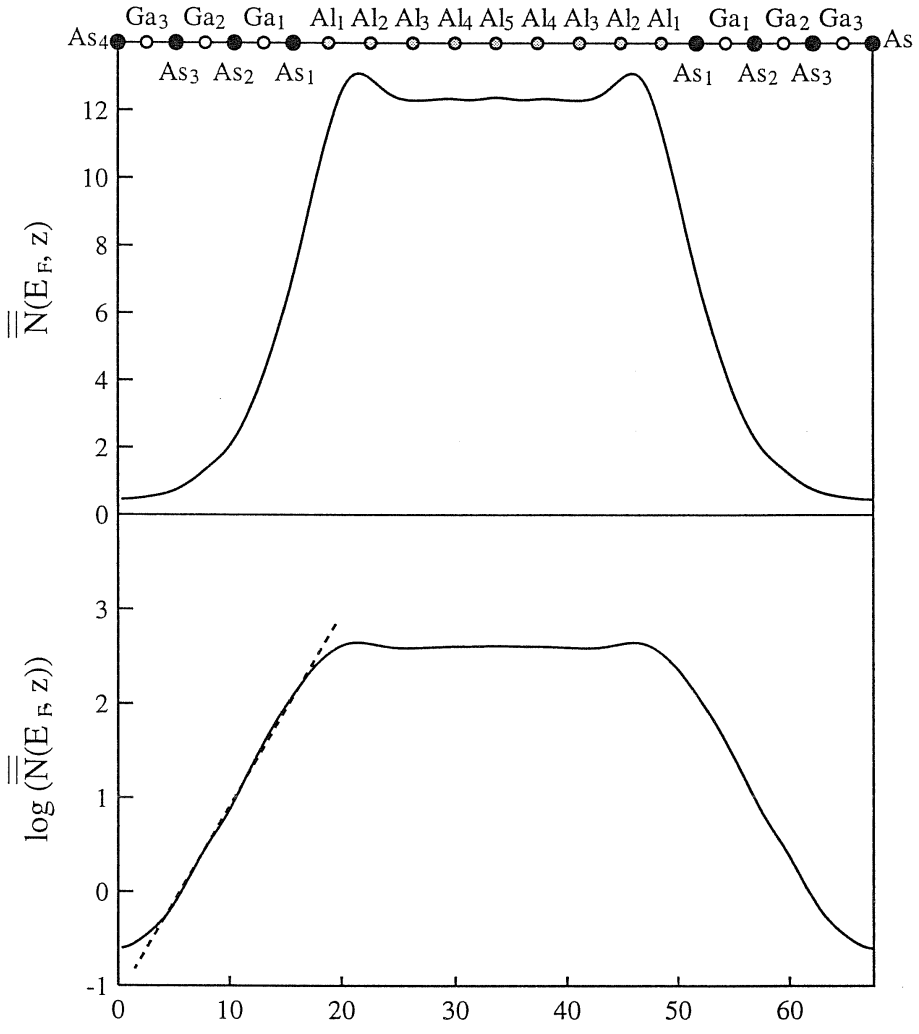
Outline

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

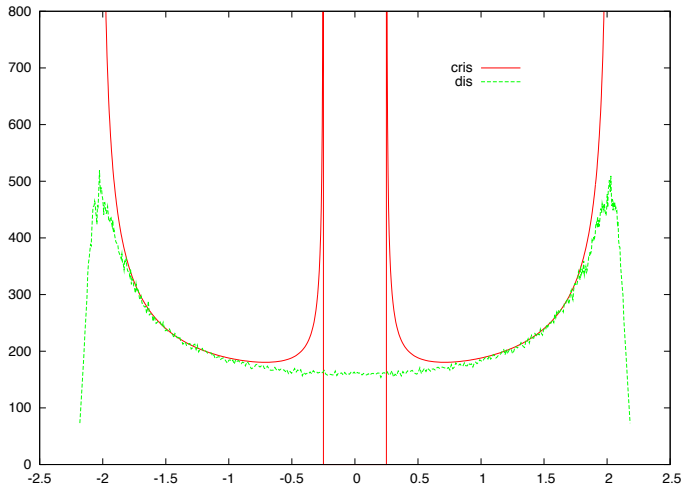
Local density of states at the Fermi level



LDOS (macroscopic average) at the Fermi level

Notice the evanescent states

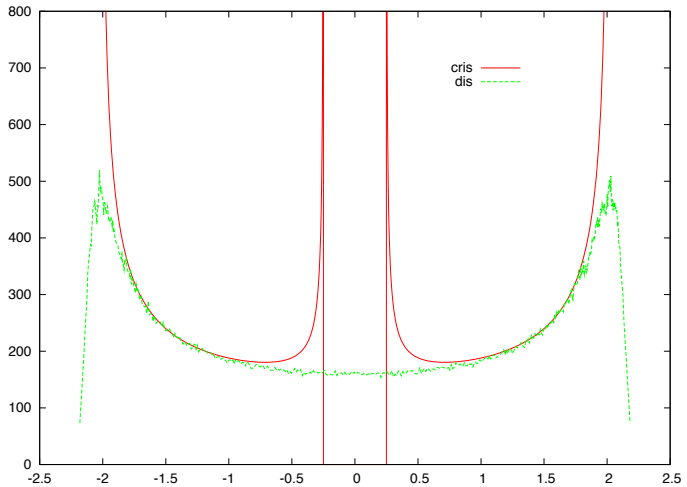
The problem



- 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



- 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**

Simulations for 1d heterojunctions

- Convert into a "localization density"

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

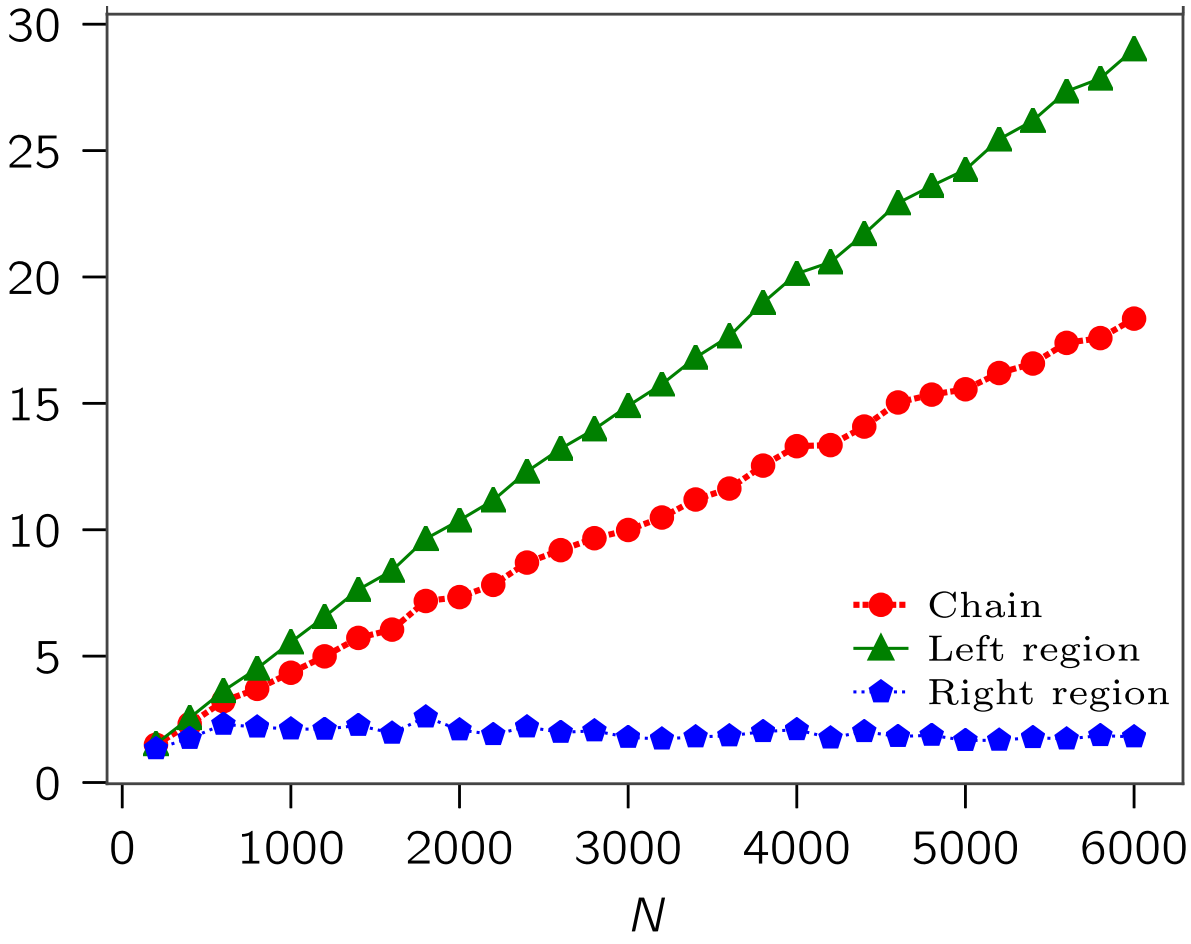
- **Local probe** of the insulating state:

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

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

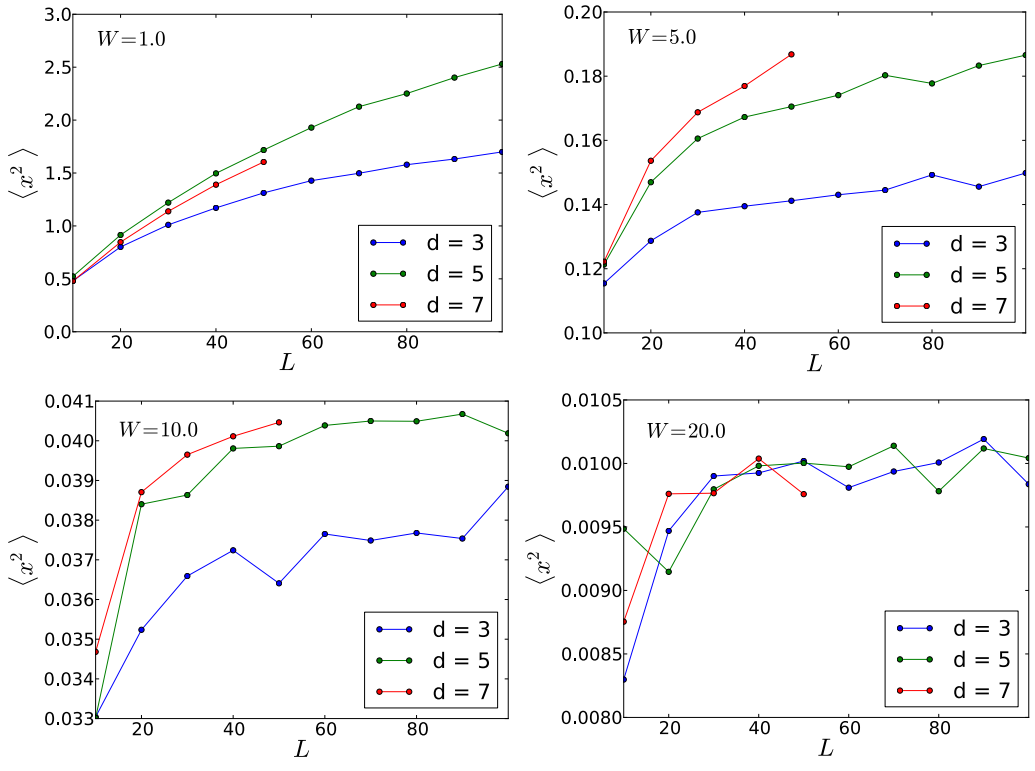
Outline

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**

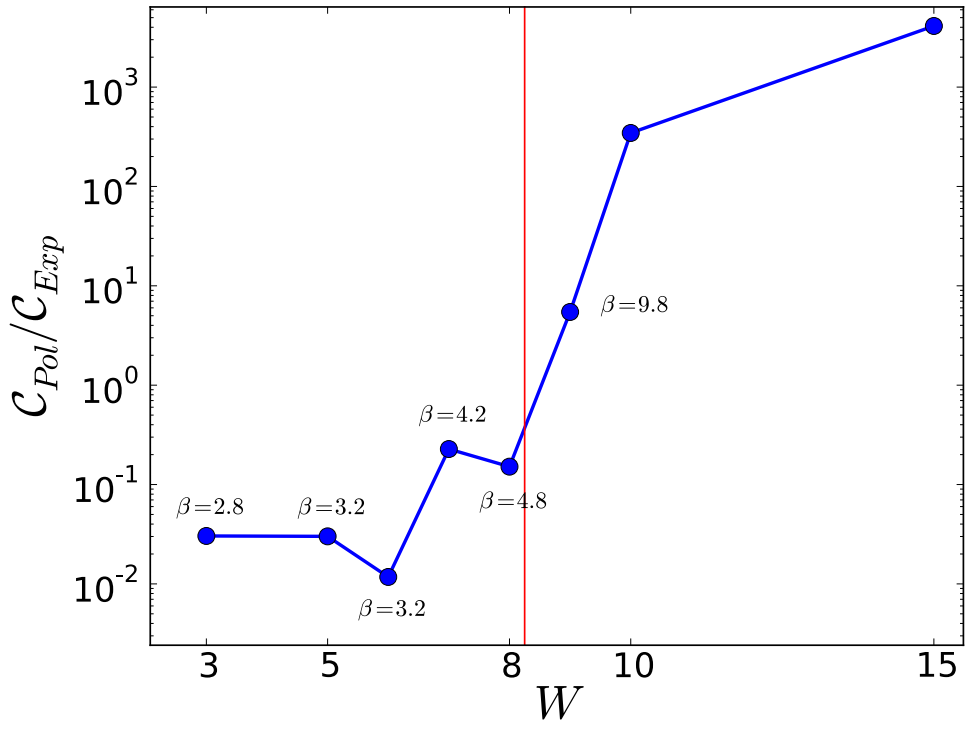
Anderson transition as a ground-state property

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!