The insulating state of matter: A geometrical theory

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The Physics of Correlated Insulators, Metals, and Superconductors
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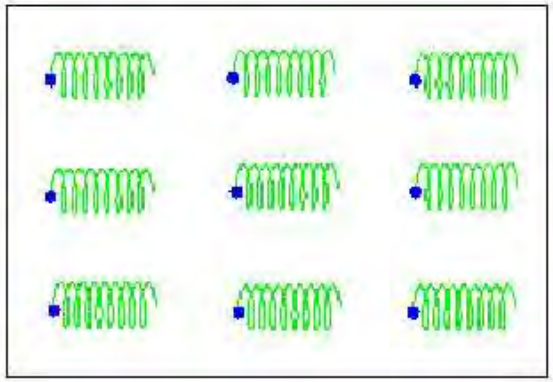
Acknowledgments

- Many, many discussions over the years with **Ivo Souza** in San Sebastian

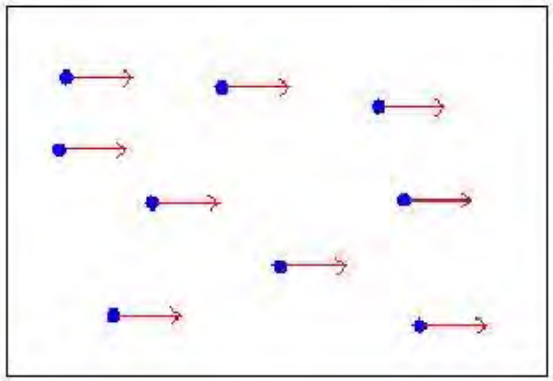
- Recent work in collaboration with my former students:
  Raffaello Bianco (PhD)
  Antimo Marrazzo (undergraduate)

Before quantum mechanics
(Discovery of the electron: J.J. Thomson 1897)



Insulator

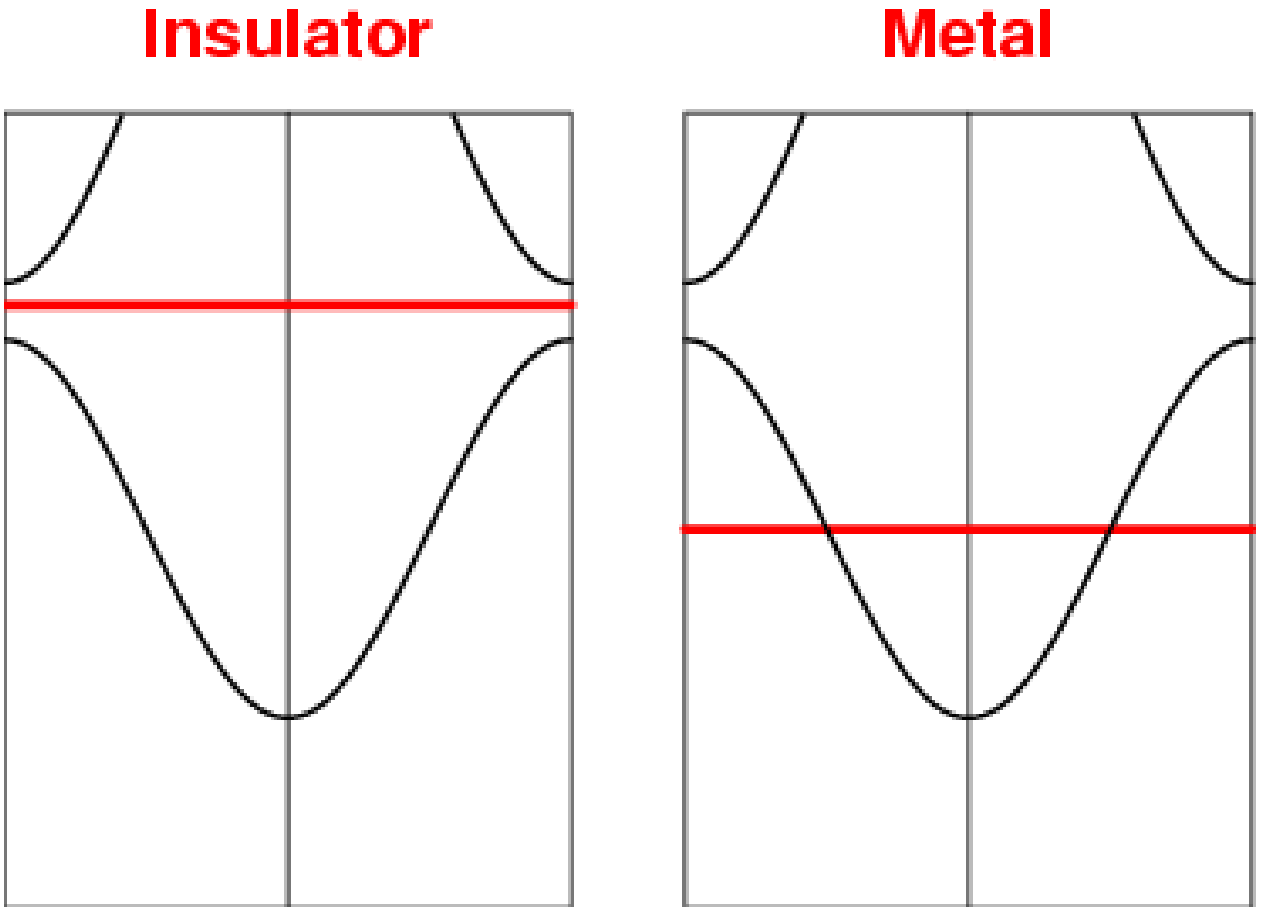
(Lorentz, 1909)



Metal

(Drude, 1900)

Soon after quantum mechanics
(Bloch 1928, Wilson 1931)



A more general theory is needed: why?

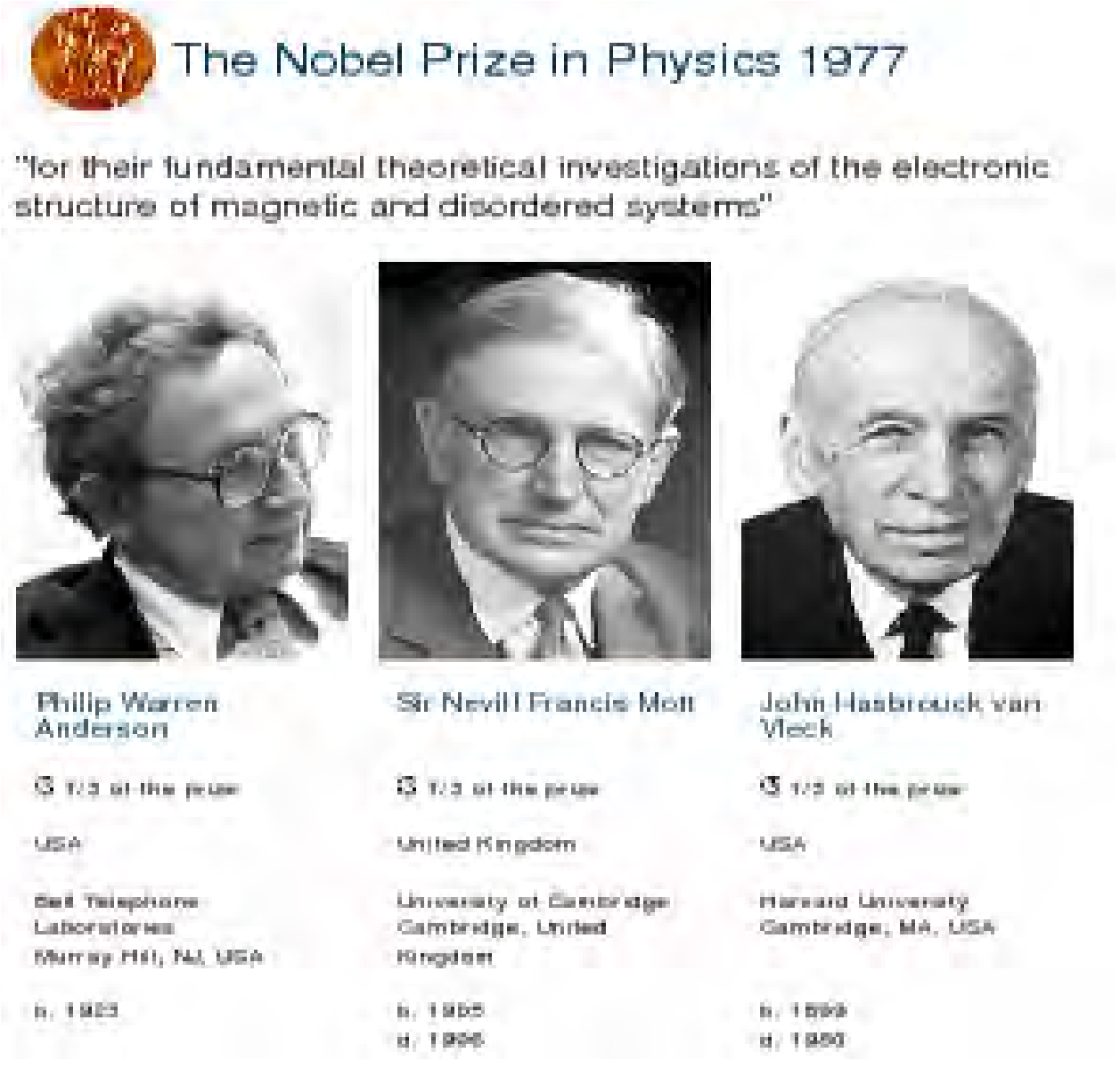
- Bloch theorem applies to **noninteracting** electrons in a periodic **crystalline** potential.
  "Noninteracting" means that the Bloch theorem applies to a **mean-field theory**.

- Some insulators are obviously noncrystalline
  (i.e. liquid or amorphous).
- In some crystalline materials the electron-electron interaction must be dealt with **explicitly**
  (i.e beyond mean-field theory).

"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**.

Exotic insulators first discovered by theoreticians
(late 1950s)



A very ambitious title indeed!

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.

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

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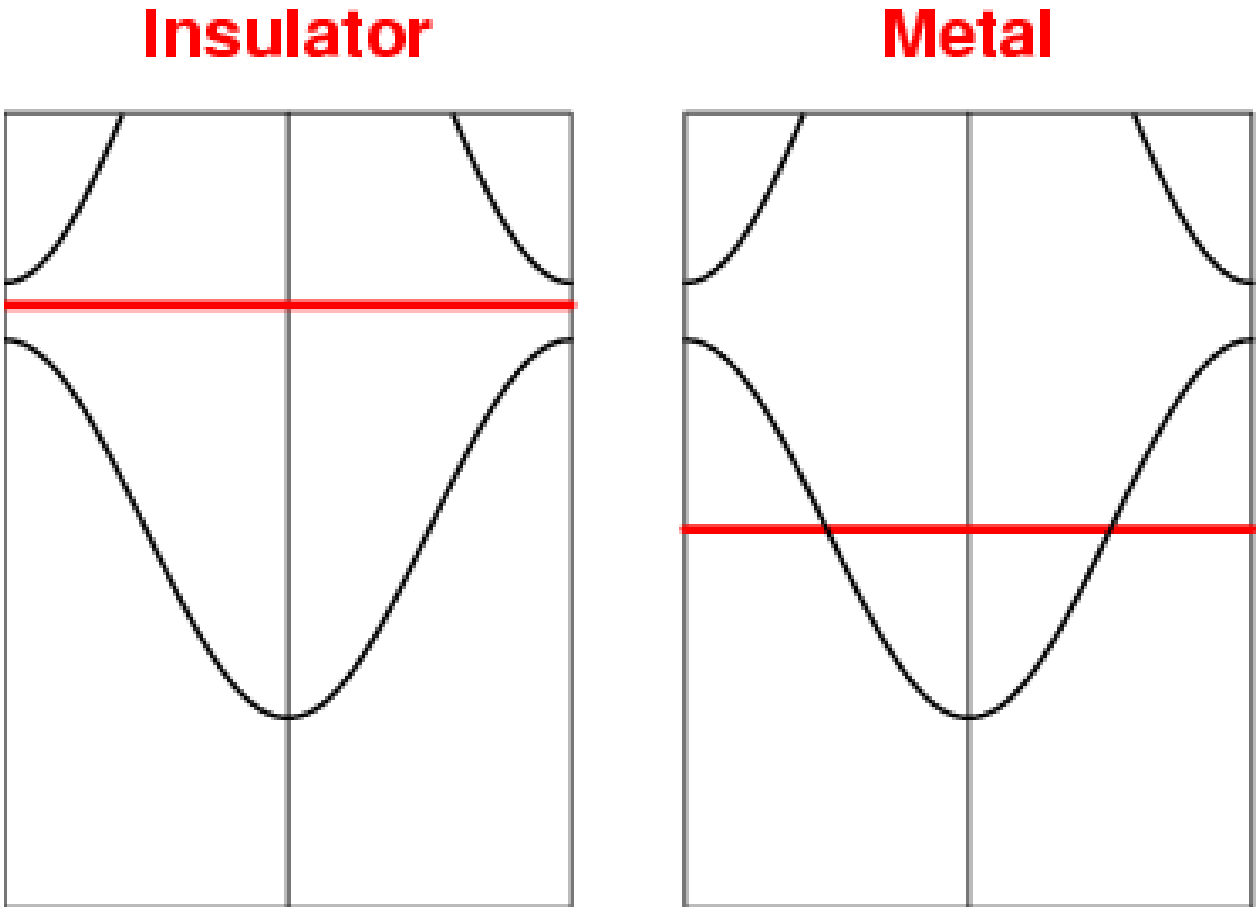
- **Kohn's revolutionary message (1):**
  The insulating behavior reflects a certain type of organization of the electrons in their **ground state**.

Property of the ground state or of the excitations?



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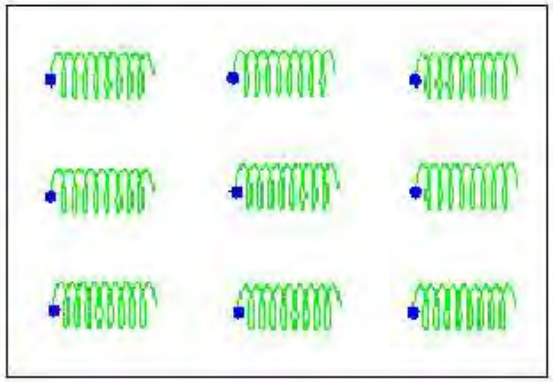
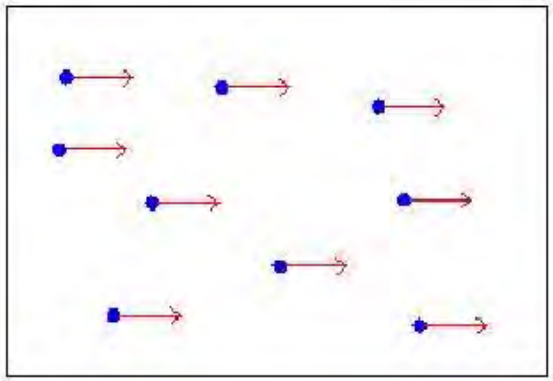
- **Kohn's revolutionary message (2):**
  Insulating characteristics are a strict consequence of **electronic localization** (in an appropriate sense) and do not require an energy gap.

Kohn's theory vindicates classical physics: Electrons localized/delocalized in insulators/metals



Insulator

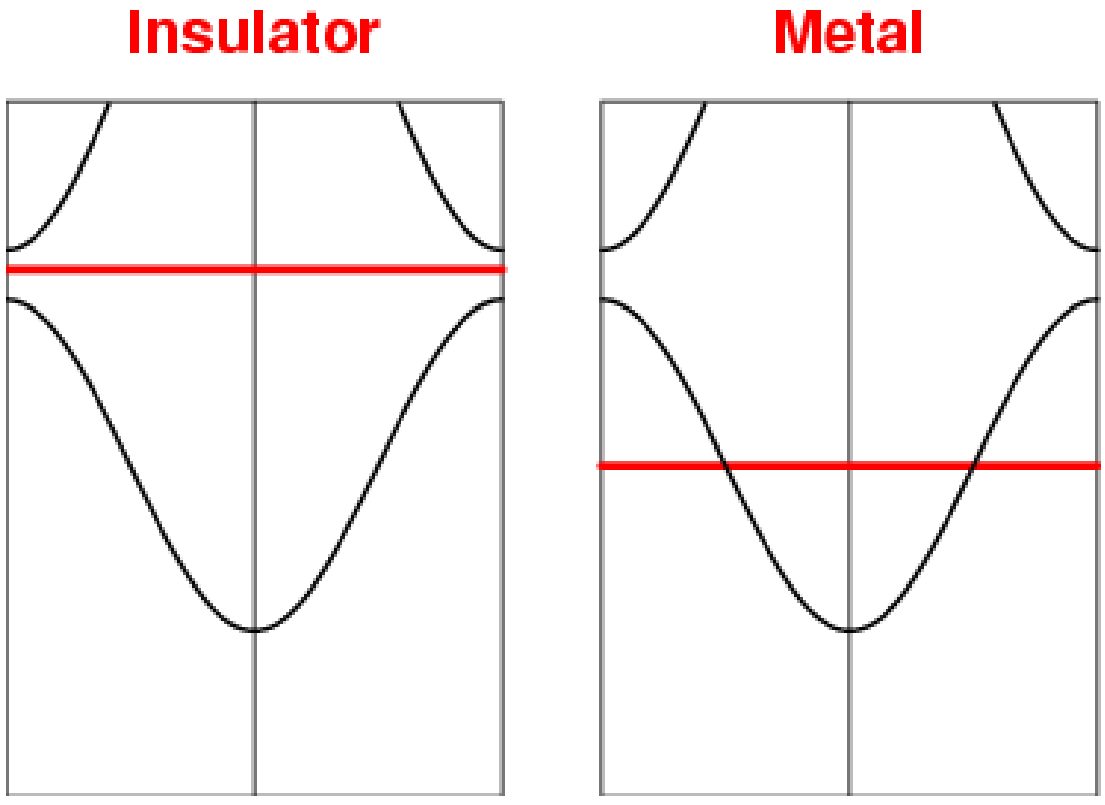
(Lorentz, 1909)



Metal

(Drude, 1900)

Which "appropriate sense"?
(Simple example: a band insulator)



What Kohn did not provide:

A "marker" for the insulating/metallic state of matter

The old paradigm: Before 1992
(Feynman Lectures in Physics, Vol. 2)

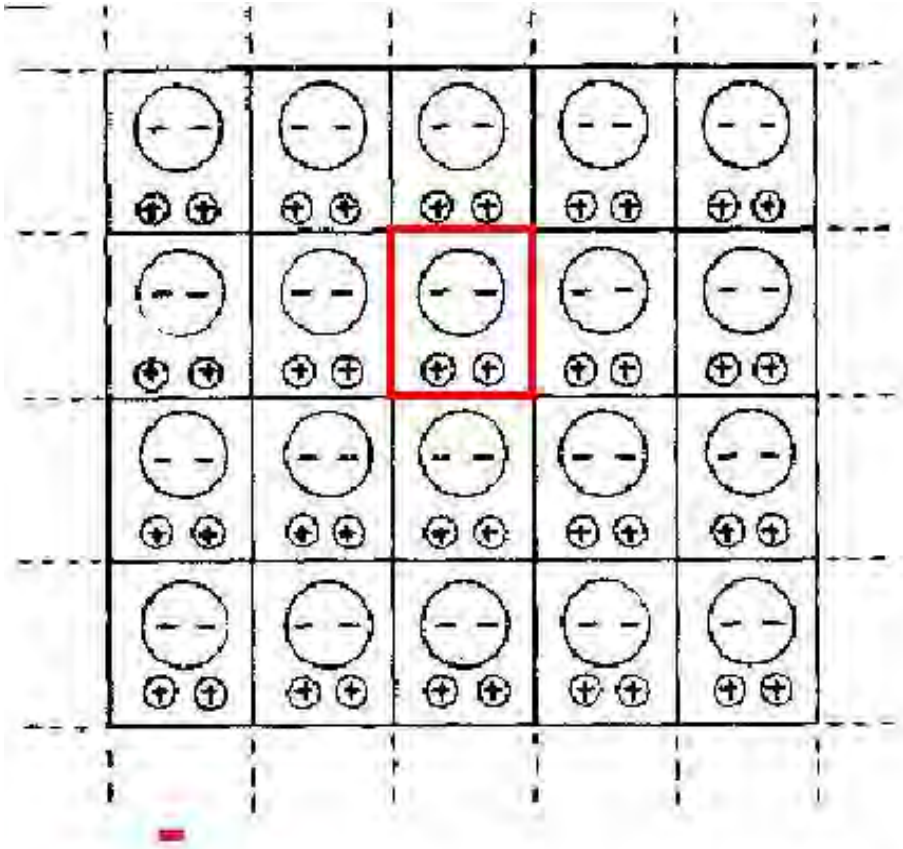


Fig. 11–8. A complex crystal lattice can have a permanent intrinsic polarization P.

The old paradigm: Before 1992
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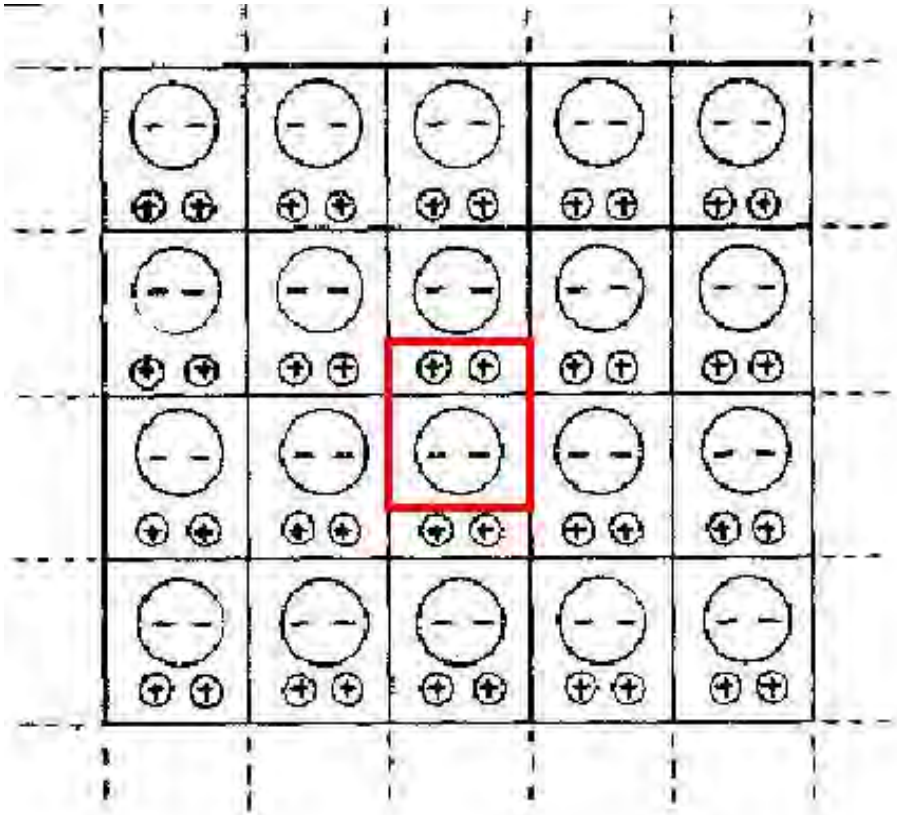


Fig. 11–8. A complex crystal lattice can have a permanent intrinsic polarization P.

The "Modern theory of polarization"

A genuine change of paradigm, based on a geometric phase (Berry phase)

- Macroscopic polarization has **nothing to do** with the periodic charge of a polarized dielectric
  (contrary to common statements in most textbooks).
- Polarization can be expressed as a **geometric phase** (Berry phase) of the electronic wavefunction.
- Nowadays, the Berry phase is computed as a standard option within all the **electronic-structure codes** on the market.
- Nonetheless, the popular **textbooks** (Kittel, Ashcroft-Mermin...) are slow to catch up and are still plagued with erroneous concepts and definitions.

Outline

Center of charge

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 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 positive & negative charge:**

$$\sum_\ell Z_\ell X_\ell - 2 \langle \Psi_0 | \sum_j x_j | \Psi_0 \rangle$$

Center of charge, much better

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

$$\sum_\ell Z_\ell X_\ell - 2\,\langle\Psi_0|\sum_j x_j\,|\Psi_0\rangle$$

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

- Polarization, including **disordered** & **correlated** insulators:

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

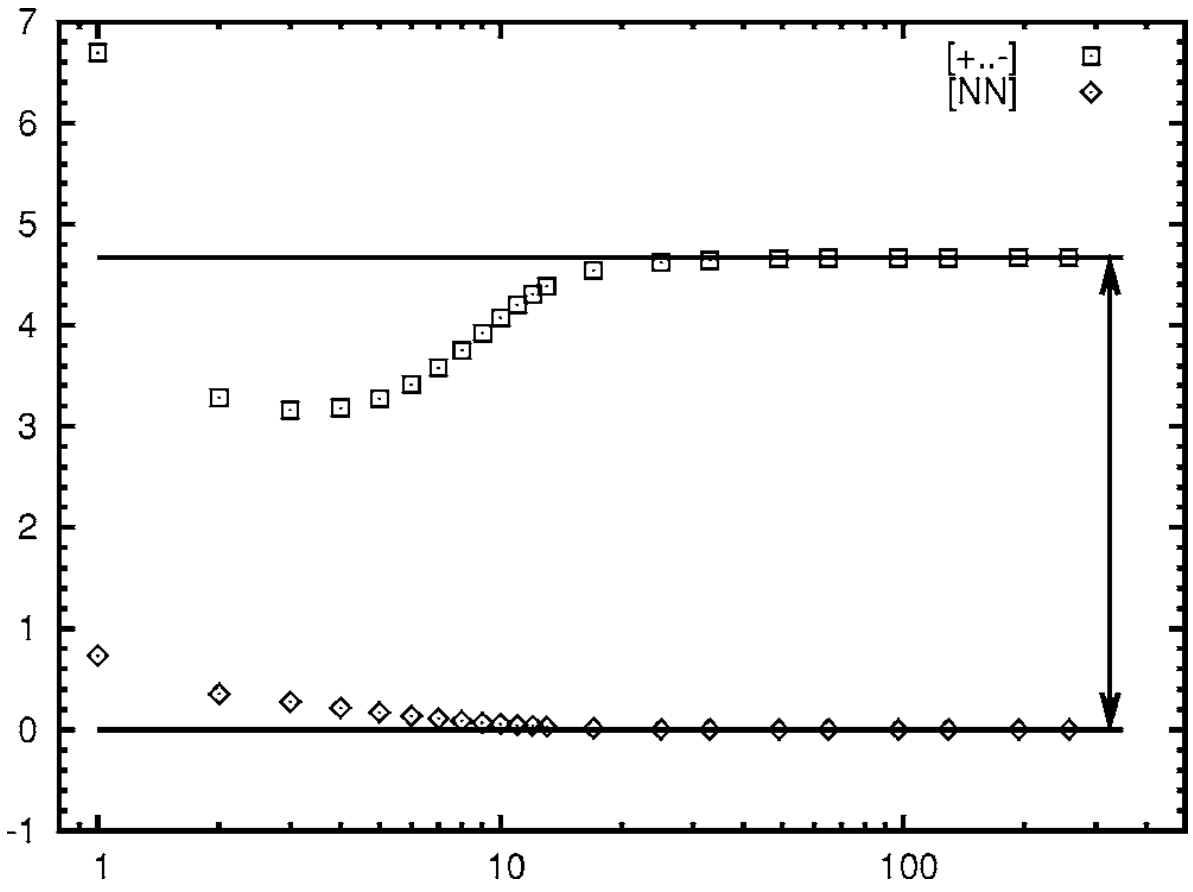
- γ is the Berry phase in disguise

Polyacetilene, different terminations

- In this centrosymmetric polymer is $P = 0$?
- Polarization defined modulo e

$$P = \frac{e}{2\pi}\gamma$$

Dipole per monomer
(Kudin, Car, & Resta, JCP 2007)



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

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

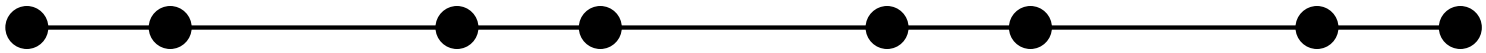
Alternant polyacetilene, model molecular crystal.....

$\mathbb{Z}_2$-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'

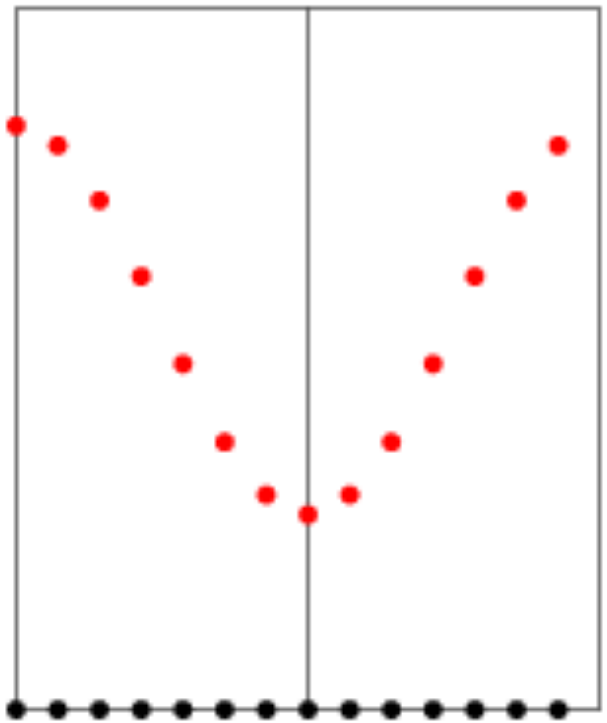
$\mathbb{Z}_2$-odd: Constant hopping t, alternating ϵ_i

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

Outline

Crystalline system of independent electrons

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 occupied orbitals in the insulating state ($N = M$)

Electronic term when $|\Psi_0\rangle$ is a Slater determinant

$$\mathfrak{z}_N = \langle \Psi_0 | \exp\left(i\frac{2\pi}{L} \sum_{j=1}^{N} x_j \right) |\Psi_0\rangle = \langle \Psi_0 | \tilde{\Psi}_0 \rangle$$

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

Theorem: $\langle \Psi_0 | \tilde{\Psi}_0 \rangle = \det S$

Single band case:

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

The connection matrix is very sparse in the band case

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

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

$$\mathcal{Z}_N = \det S = \prod_{j=1}^{N} S(q_j, q_{j-1})$$

King-Smith & Vanderbilt Berry phase

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

Insulating case: Discretization of King-Smith & Vanderbilt γ

$$\gamma = i \int_{\mathrm{BZ}} dk \, \langle \psi_k | \frac{d}{dk} \psi_k \rangle = \lim_{N \to \infty} \mathrm{Im} \, \ln \prod_{j=1}^{M} S(q_j, q_{j-1}) = \lim_{N \to \infty} \mathrm{Im} \, \ln \, \mathfrak{z}_N$$

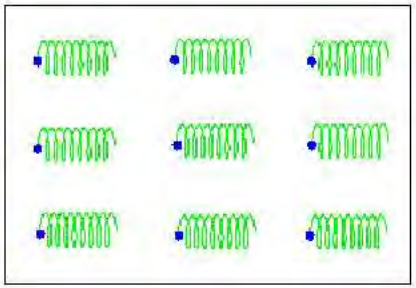
Outline

What is the relationship between polarization and the insulating state?

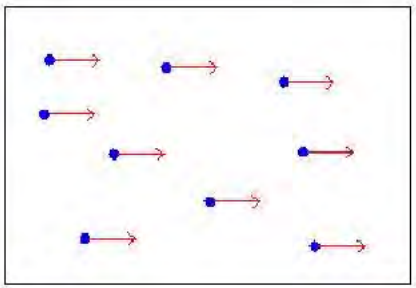
- **Phenomenologically:**
  - **Metal:** Has a **nonzero** dc conductivity
  - **Insulator:** Has a **zero** dc conductivity (at zero temperature)

- **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.

Under the action of a dc electrical field



Insulator
(Lorentz, 1909)



Metal
(Drude, 1900)

- **Insulator:** Electrons do not flow freely (they polarize instead)
- **Metal:** Electrons flow freely over macroscopic distances (hindered by scattering)

The relationship between localization and polarization

VOLUME 82, NUMBER 2 PHYSICAL REVIEW LETTERS 11 JANUARY 1999

Electron Localization in the Insulating State

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(Received 11 August 1998)

The insulating state of matter is characterized by the excitation spectrum, but also by qualitative features of the electronic ground state. The insulating ground wave function in fact (i) sustains macroscopic polarization, and (ii) is *localized*. We give a sharp definition of the latter concept and we show how the two basic features stem from essentially the same formalism. Our approach to localization is exemplified by means of a two-band Hubbard model in one dimension. In the noninteracting limit, the wave function localization is measured by the spread of the Wannier orbitals.

- Macroscopic polarization and electron localization in the insulating state stem from the same formalism
- They are two aspects of the same phenomenon

A marker for the insulating state of matter

- Electronic term in polarization

$$P^{(\mathrm{el})} = \frac{e}{2\pi} \mathrm{Im}\ \log \lim_{N\to\infty} \mathfrak{z}_N$$

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

$$\lim_{N\to\infty} \mathfrak{z}_N = 0$$

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

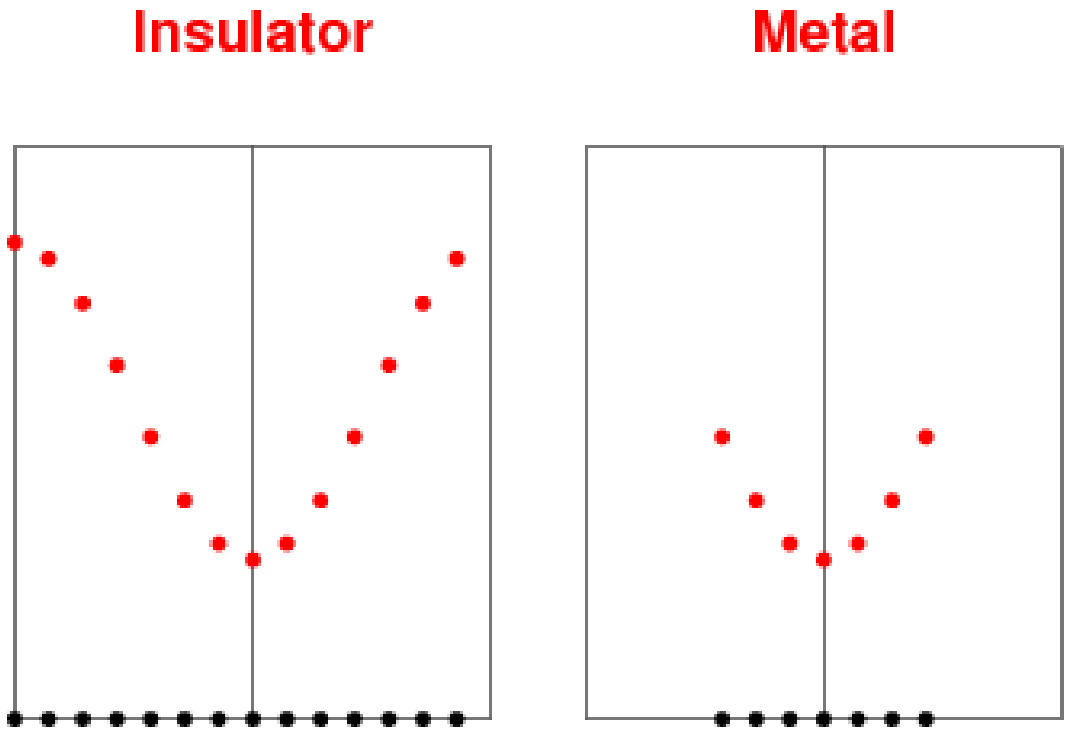
RS localization length

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

- λ is finite in all insulators
- λ 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 (not shown here)

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 $|\Psi_0\rangle$.

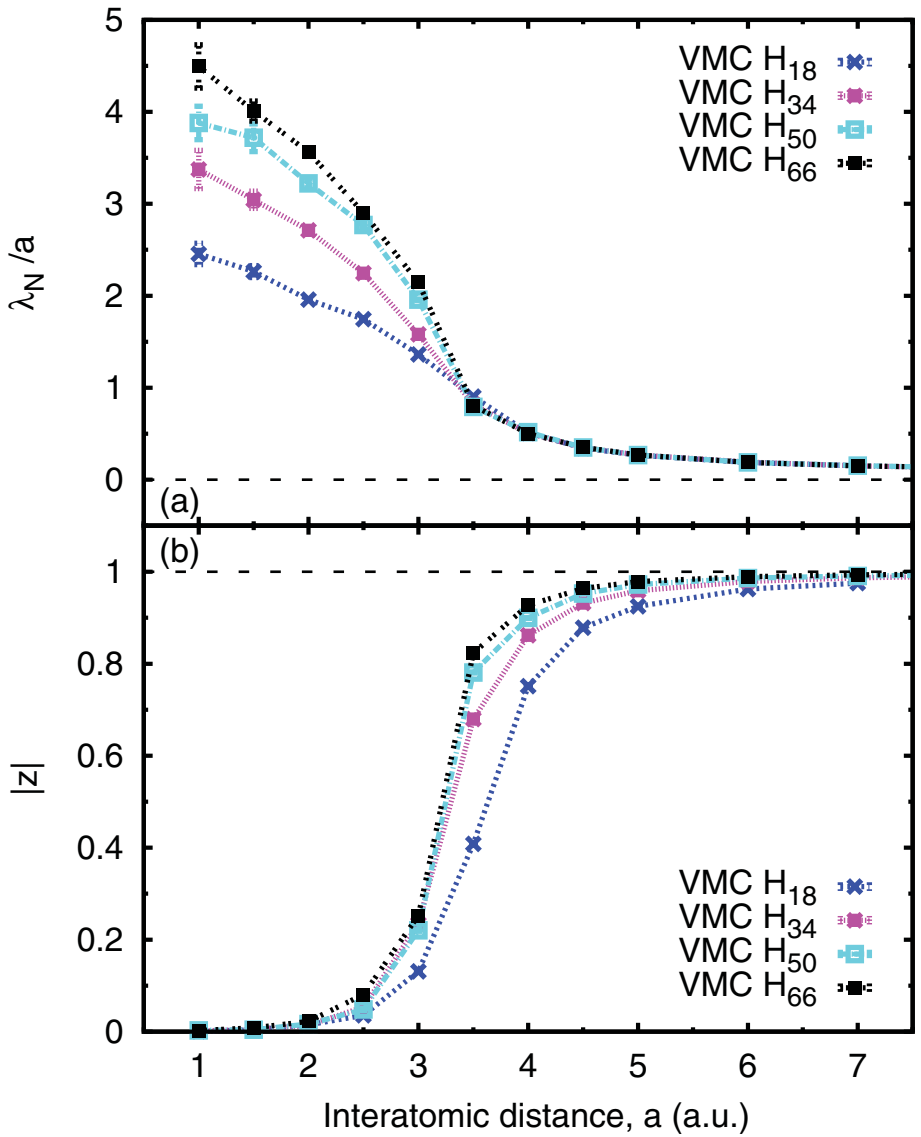
Insulators vs. metal

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

The connection matrix has **zero determinant** in the metallic case!

Implementation: Mott transition in H_N chains

Stella, Attaccalite, Sorella & Rubio, PRB 2011



localization length

(tensor in 3d)

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

Outline

Longitudinal conductivity (zero T)

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

- Both terms obtain from Kubo formulas
  (may include disorder & correlation, but **not** dissipation)
- The Drude weight $D_{\alpha\beta}$ is actually a **ground-state** property:
  it measures the inertia of the electrons in the adiabatic limit

- The insulating state requires **both**:
  - $D_{\alpha\beta}=0$
  - Re $\sigma^{(\mathrm{regular})}_{\alpha\beta}(\omega)$ goes to zero for $\omega\to 0$

Drude weight according to Kohn (1964)

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

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m} \sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}}$$

- Thermodynamic limit **after** taking derivatives
- PBCs violate gauge invariance in the conventional sense: E_0 **does** depend on $\boldsymbol{\kappa}$.

- Drude weight

$$D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^d} \left. \frac{\partial^2 E_0(\boldsymbol{\kappa})}{\partial\kappa_\alpha \partial\kappa_\beta} \right|_{\boldsymbol{\kappa}=0}$$

Why RS discriminate insulators from metals

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m}\sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}}, \qquad \widehat{\mathbf{r}} = \sum_{\mathbf{i}} \mathbf{r_i}$$

- $|\tilde{\Psi}_0(\boldsymbol{\kappa})\rangle = \mathrm{e}^{-i\boldsymbol{\kappa}\cdot\hat{\mathbf{r}}}|\Psi_0(0)\rangle$ obeys Schrödinger Eq.
- It **does not** obey PBCs
- Except for a commensurate $\boldsymbol{\kappa}_0$
- Does $|\tilde{\Psi}_0(\boldsymbol{\kappa}_0)\rangle$ coincide with the genuine $|\Psi_0(\boldsymbol{\kappa}_0)\rangle$?
  - **Yes** (modulo a phase) if $D = 0$
  - **No** (it is orthogonal to it) if $D \neq 0$

Why RS discriminate insulators from metals (cont'd)

$$\begin{aligned}
\langle\tilde{\Psi}_0(\boldsymbol{\kappa}_0)|\Psi_0(\boldsymbol{\kappa}_0)\rangle &= \langle\Psi_0(0)|\,\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}\,|\Psi_0(\boldsymbol{\kappa}_0)\rangle = 0, \quad D \neq 0 \\
\langle\tilde{\Psi}_0(\boldsymbol{\kappa}_0)|\Psi_0(\boldsymbol{\kappa}_0)\rangle &= \langle\Psi_0(0)|\,\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}\,|\Psi_0(\boldsymbol{\kappa}_0)\rangle = \mathrm{e}^{i\gamma}, \quad D = 0
\end{aligned}$$

$$\begin{aligned}
|\mathcal{Z}_N| &= |\,\langle\Psi_0(0)|\,\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}\,|\Psi_0(0)\rangle\,| = \mathcal{O}(1/L), \quad D \neq 0 \\
|\mathcal{Z}_N| &= |\,\langle\Psi_0(0)|\,\mathrm{e}^{i\boldsymbol{\kappa}_0\cdot\hat{\mathbf{r}}}\,|\Psi_0(0)\rangle\,| = 1 - \mathcal{O}(1/L), \quad D = 0
\end{aligned}$$

Outline

Outline

Quantum metric (Provost & Vallée, 1980)

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

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m}\sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}} \qquad \widehat{\mathbf{r}} = \sum_{\mathbf{i}} \mathbf{r_i}$$

- OBCs **do not** violate gauge invariance: E_0 is $\boldsymbol{\kappa}$-independent

- 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)

The modern theory (OBCs)

$$\hat{H}(\boldsymbol{\kappa}) = \frac{1}{2m}\sum_{i=1}^{N} |\mathbf{p_i} + \hbar\boldsymbol{\kappa}|^2 + \widehat{\mathbf{V}} \qquad \widehat{\mathbf{r}} = \sum_{\mathbf{i}} \mathbf{r_i}$$

- **Basic tenet of the modern theory:**
  The OBCs metric $\tilde{g}_{\alpha\beta}$ in the thermodynamic limit
  - Diverges in all metals
  - Converges in all insulators

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

Physical meaning of the OBCs quantum metric tensor

- Second moment of the exchange-correlation hole:

$$\tilde{g}_{\alpha\beta} = \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' \, (\mathbf{r} - \mathbf{r}')_\alpha (\mathbf{r} - \mathbf{r}')_\beta [\, n(\mathbf{r}) n(\mathbf{r}') - n^{(2)}(\mathbf{r}, \mathbf{r}') \,]$$

- Ground-state quantum fluctuation of the dipole:

$$\tilde{g}_{\alpha\beta} = \frac{1}{N} (\langle \Psi_0 | \hat{r}_\alpha \hat{r}_\beta \Psi_0 \rangle - \langle \Psi_0 | \hat{r}_\alpha | \Psi_0 \rangle \langle \Psi_0 | \hat{r}_\beta \Psi_0 \rangle)$$

- $\tilde{g}_{\alpha\beta}$ used as a marker for the insulating/metallic state:
  - Noninteracting crystalline systems:
    - Insulators: $\tilde{g}_{\alpha\beta}$ equals the WF quadratic spread
    - Metals: some simulations prove divergence
  - A few simulations for noninteracting disordered systems
  - **No** simulation so far for correlated systems

Outline

Tight binding 1d binary crystal

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

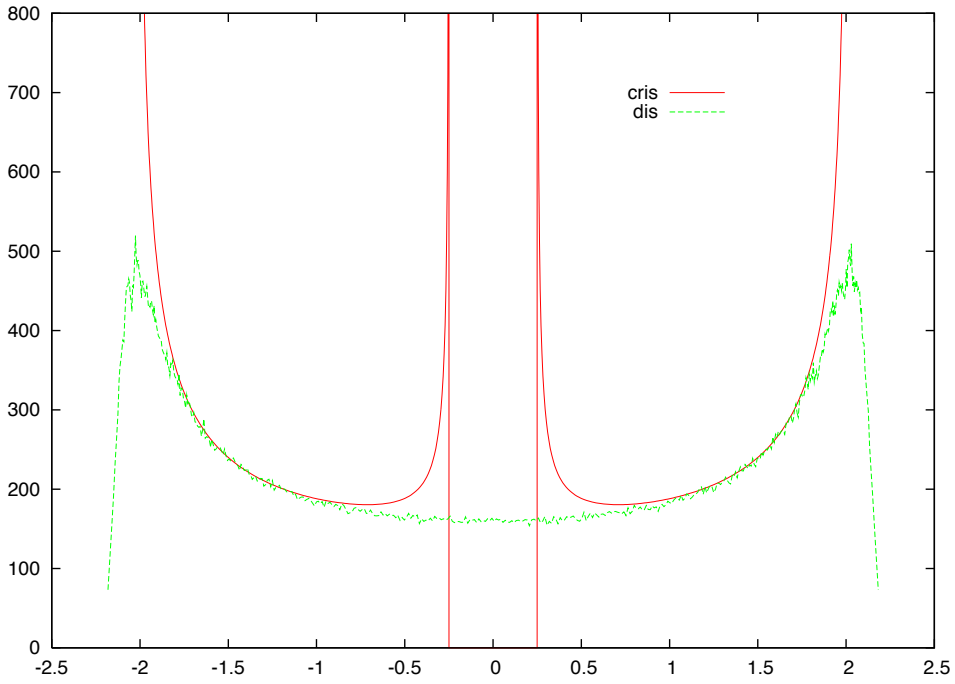
Diagonal disorder: t fixed, $\epsilon_b - \epsilon_a = \Delta$ fixed

Crystalline case:
ABABABABABABABABABABABABABABABABAB.....

Disordered case:
ABAABABBABABBAABABABBABABAABABBABABBAA .....

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 $\tilde{g}$?

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

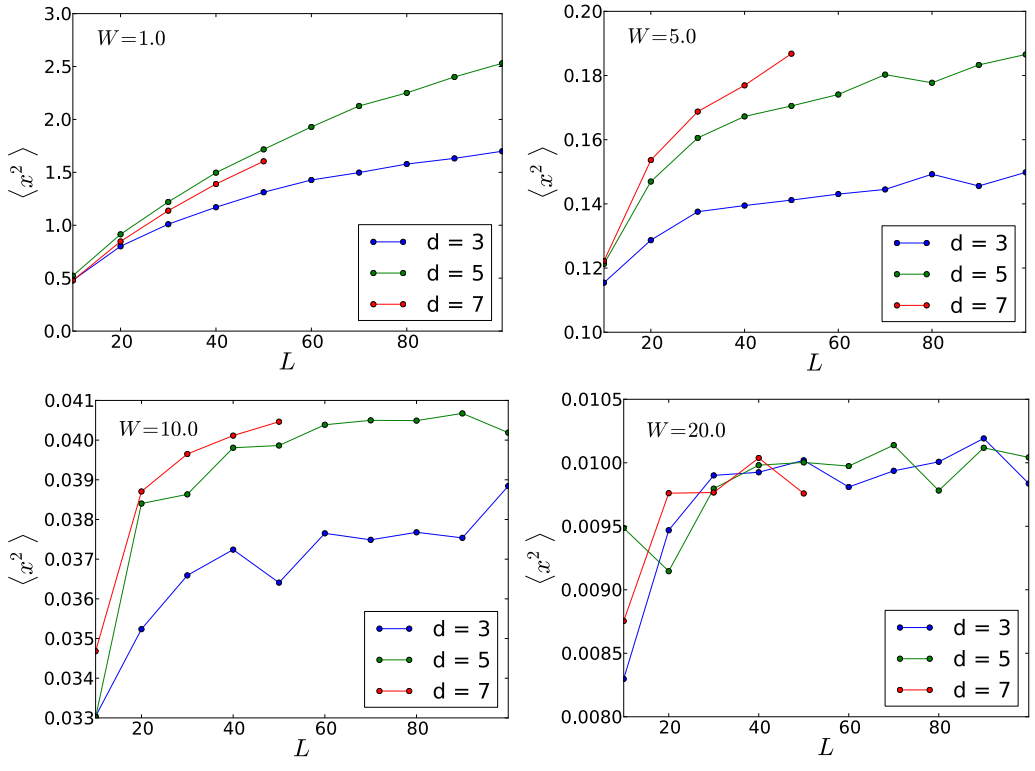
- In the crystalline case $\tilde{g}$ converges to a finite limit for 1/2 filling, diverges for 1/4 (as expected).
- In the disordered case $\tilde{g}$ always converge (to a very similar value for the two cases).
- The disordered case $\tilde{g}$ is about 20 times larger than the crystalline one. Why?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

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: use our marker to detect the transition **in the ground state**

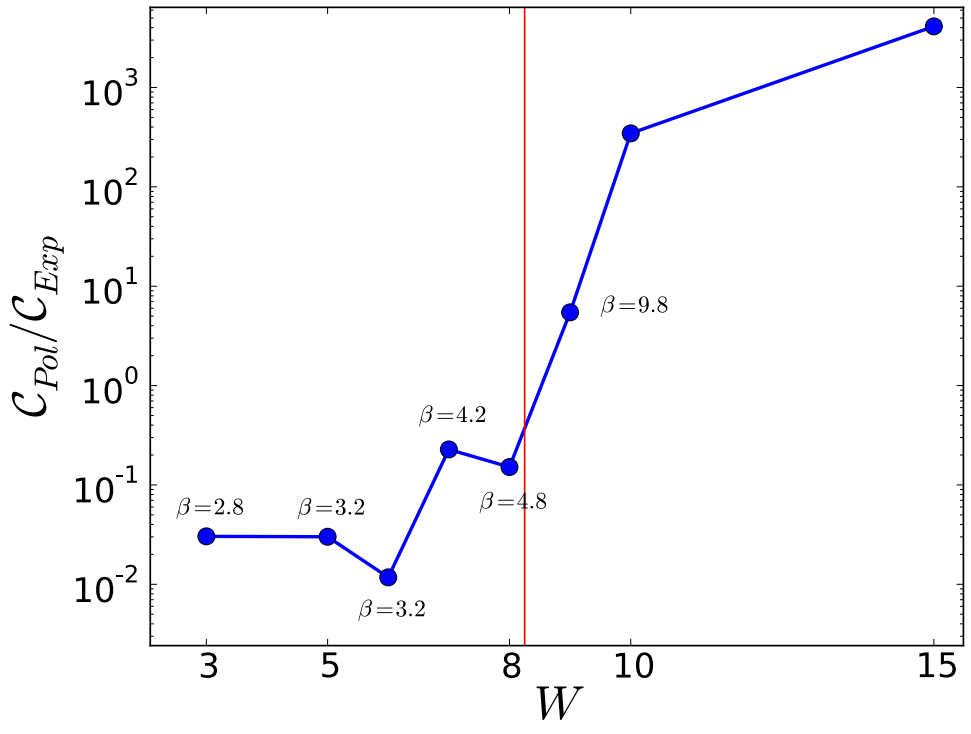
Anderson transition as a ground-state property

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**

Summary

- Phenomenology:
  - Insulators differs from conductors in their dc conductivity;
  - But also: insulators and metals polarize in a different way.
- Theory:
  - Textbook viewpoint: Insulators and metals have a qualitatively different **excitation spectrum** (gapped/gapless)
  - Modern viewpoint (inspired by **Kohn**): Even before any probe is applied to the system, the **ground-state** organization of the electrons is different in insulators and metals.
- I have shown a couple of ways for sampling such organization:
  - Resta-Sorella within PBCs
  - The quantum metric within OBCs

Outline

Noninteracting electrons, OBCs

- All ground-state properties obtain from the projector:

$$\langle \mathbf{r}| \mathcal{P} |\mathbf{r}'\rangle = \sum_{\epsilon_j \leq \mu} \langle \mathbf{r}|\varphi_j\rangle\langle\varphi_j|\mathbf{r}'\rangle$$

- Metric (quantum fluctuation of the dipole):

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

- A real symmetric tensor, even in **absence** of TR symmetry.

Anomalous Hall conductivity (AHC)

- Nonzero only when TR symmetry is absent
- Quantized in insulators, nonquantized in metals
- AHC is a Chern number in 2d: Haldane's Nobel prize (part of)
- AHC is topological in insulators;
  AHC has a geometrical contribution in metals
- QAHE materials synthesized recently
- Geometrical & topological quantities dealt with in **k**-space, adopting PBCs

- PBCs and **k** vectors are a (very useful) creation of our mind: they do not exist in nature. AHC should be accessible even:
  - Inside finite samples (e.g. bounded crystallites)
  - In noncrystalline samples
  - In macroscopically inhomogeneous samples
    (e.g. heterojunctions)

Geometry & topology in **r**-space

- **Insulators**:

  R. Bianco and R. Resta,
  Mapping topological order in coordinate space,
  Phys. Rev. B **84**, 241106(R) (2011)

- **Metals**:

  A. Marrazzo and R. Resta,
  Locality of the anomalous Hall conductivity,
  Phys. Rev. B **95**, 121114(R) (2017)

AHC as a local quantity

$$\tilde{g}_{\alpha\beta} = -\frac{1}{N}\int_{\text{sample}} d\mathbf{r}\, \mathcal{F}_{\alpha\beta}(\mathbf{r}), \qquad \mathcal{F}_{\alpha\beta}(\mathbf{r}) = \langle \mathbf{r}|\, \mathcal{P}\,[r_\alpha, \mathcal{P}]\,[r_\beta, \mathcal{P}]\,|\mathbf{r}\rangle$$

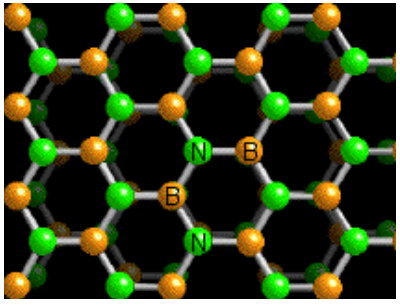
- Next we integrate $\mathcal{F}_{\alpha\beta}(\mathbf{r})$ over an **inner region** of the sample, **not** over the whole sample
- For a crystallite:

$$\frac{1}{N}\int_{\text{sample}} d\mathbf{r}\, \mathcal{F}_{\alpha\beta}(\mathbf{r}) \to \frac{1}{N_c}\int_{\text{cell}} d\mathbf{r}\, \mathcal{F}_{\alpha\beta}(\mathbf{r})$$

- In absence of TR symmetry such integral is endowed with an **antisymmetric imaginary** part

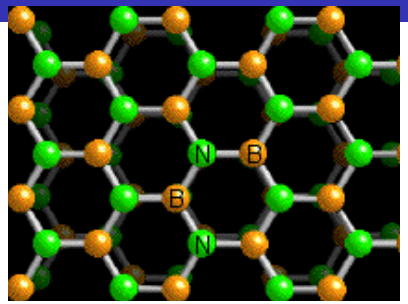
$$\sigma^{(-)}_{\alpha\beta} = -\frac{2e^2}{\hbar V_{\text{cell}}}\int_{\text{cell}} d\mathbf{r}\ \text{Im}\ \mathcal{F}_{\alpha\beta}(\mathbf{r})$$

The “Haldanium” paradigm (F.D.M. Haldane, 1988)



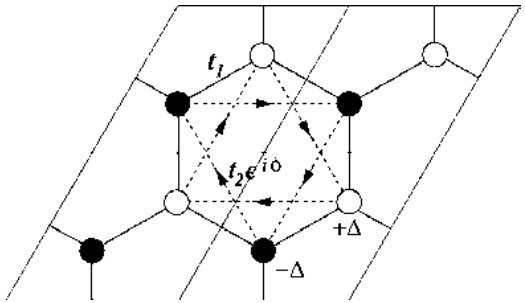
+ **staggered** B field

The "Haldanium" paradigm (F.D.M. Haldane, 1988)



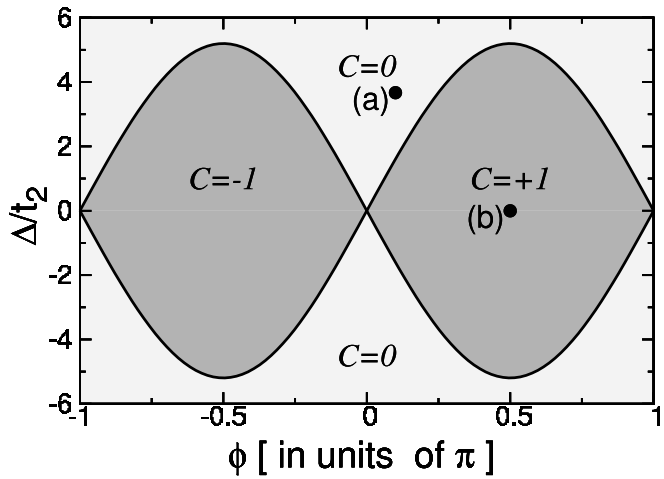
$+$ **staggered** B field

- A two-band model (T-broken)
- Tight-binding parameters:
  - 1st-neighbor hopping t_1
  - staggered onsite $\pm\Delta$
  - complex 2nd-neighbor $t_2 e^{i\phi}$
- In the topological phase: **QAHE**

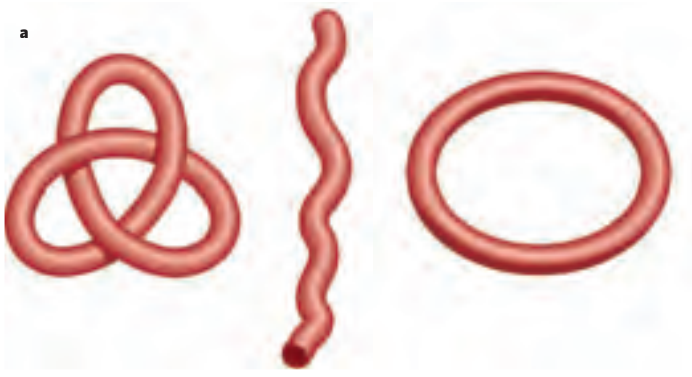


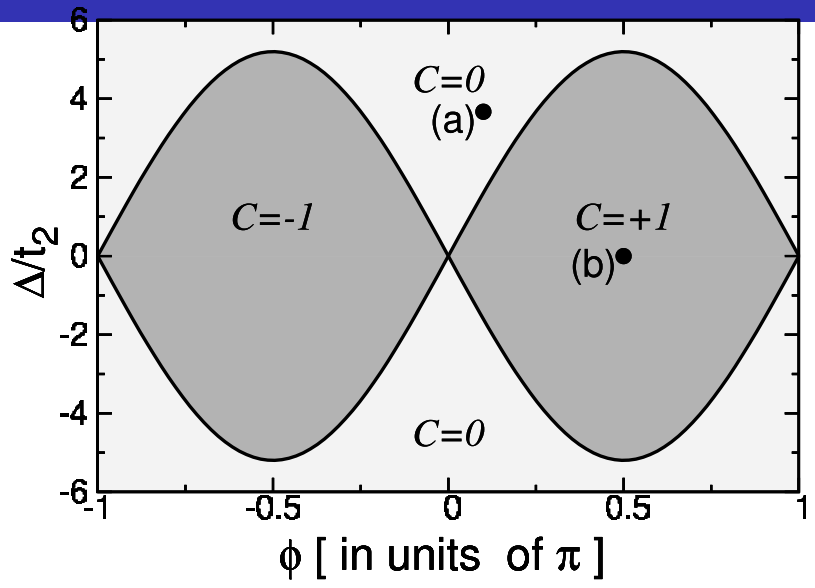
Normal insulator, topological insulator, metal

- Phase diagram at half filling
- Metallic at any other filling



Topological order



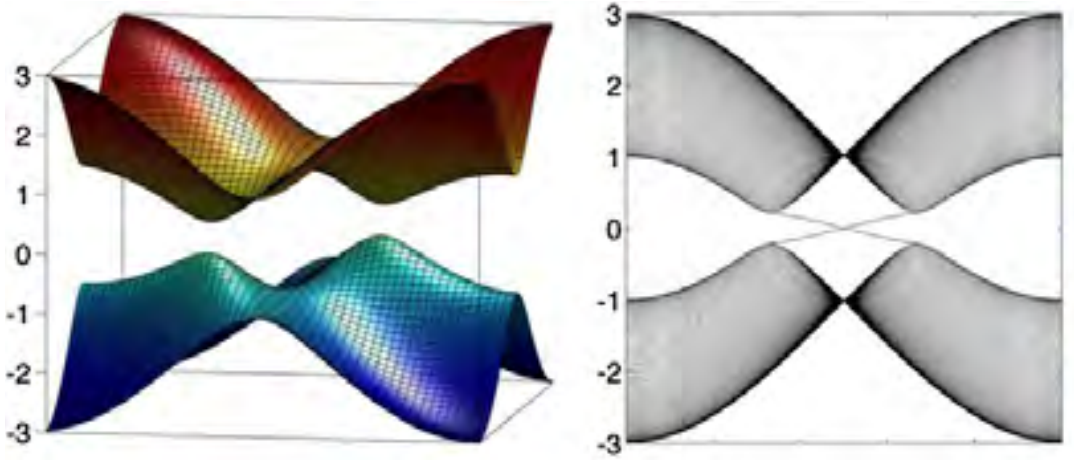


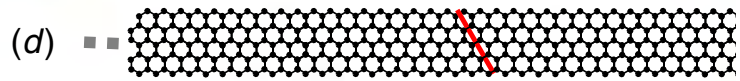
- Ground state wavefunctions differently "knotted" in **k** space
- Topological order very robust
- C_1 switched only via a metallic state: "cutting the knot"
- Displays quantum **anomalous** Hall effect:

$$\sigma_{xy}^{(-)} = -\frac{e^2}{h} C_1$$

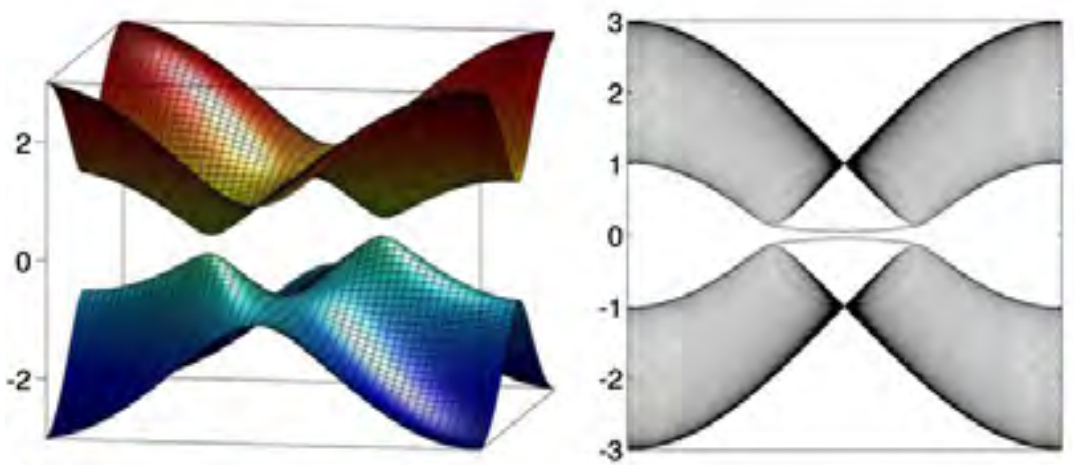
Bulk-boundary correspondence

$C_1 \neq 0$



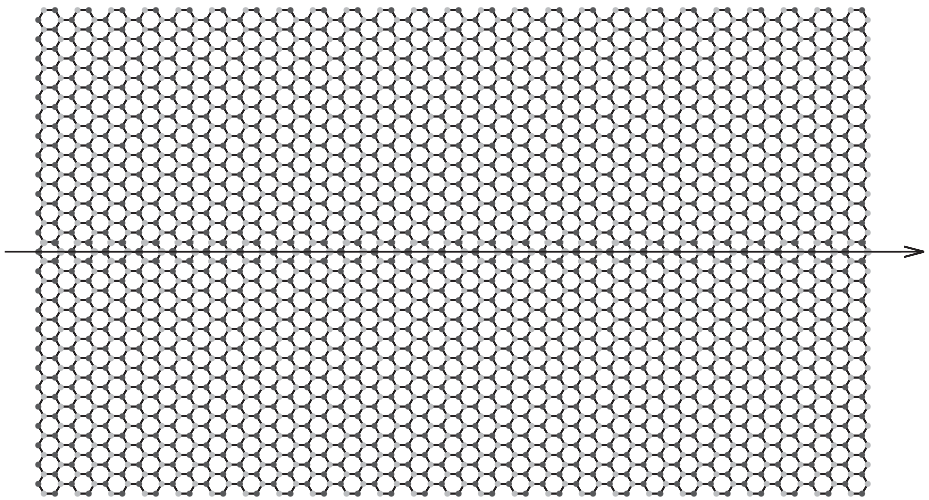


$C_1 = 0$



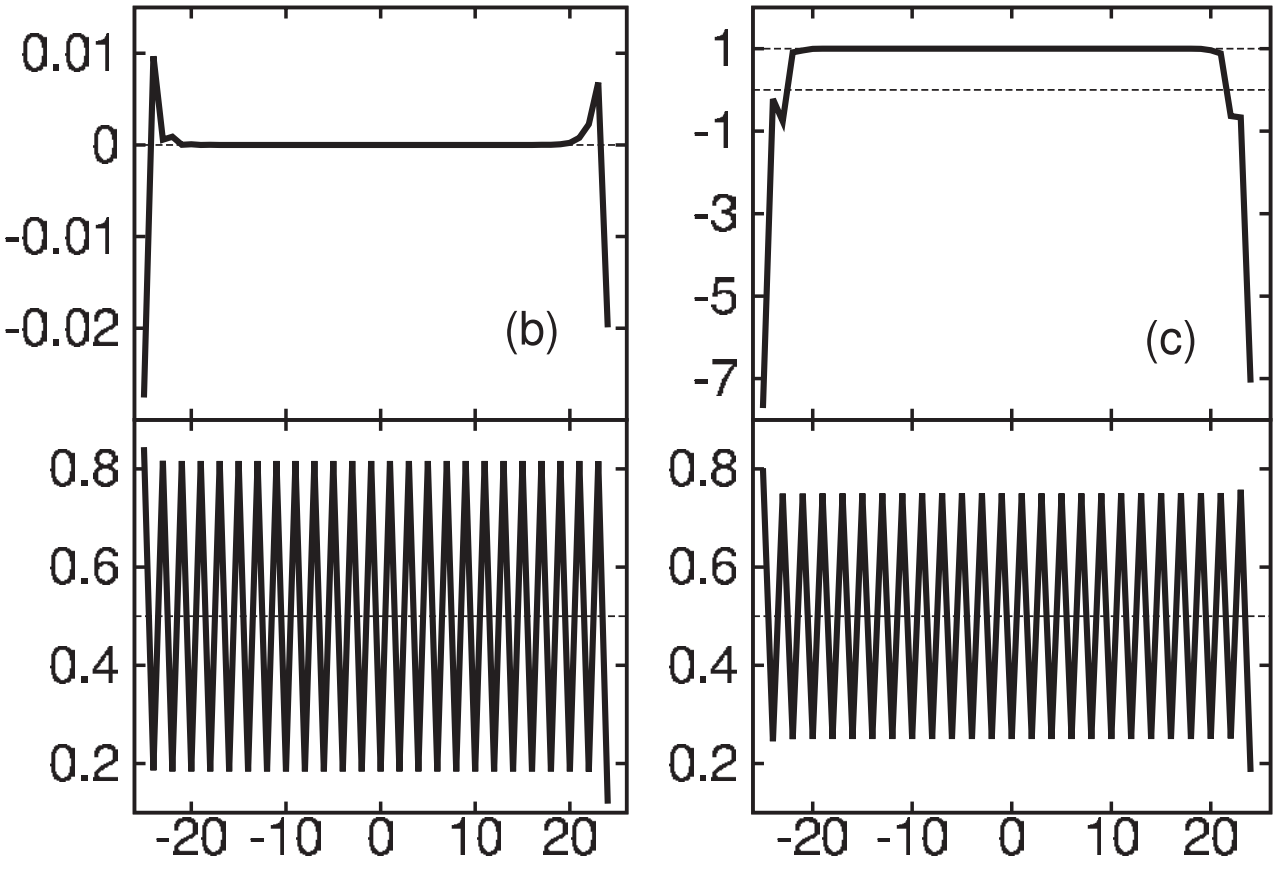
bulk ribbon

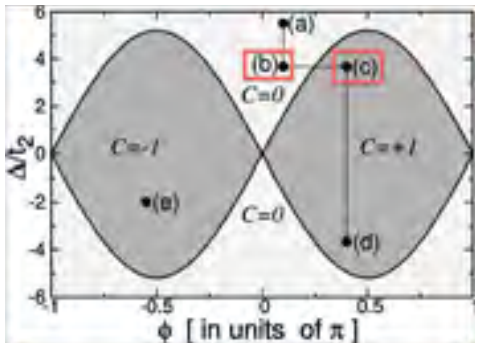
A “macroscopic” flake of Haldanium (OBC)



Sample of 2550 sites, line with 50 sites

Crystalline Haldanium (normal & Chern)

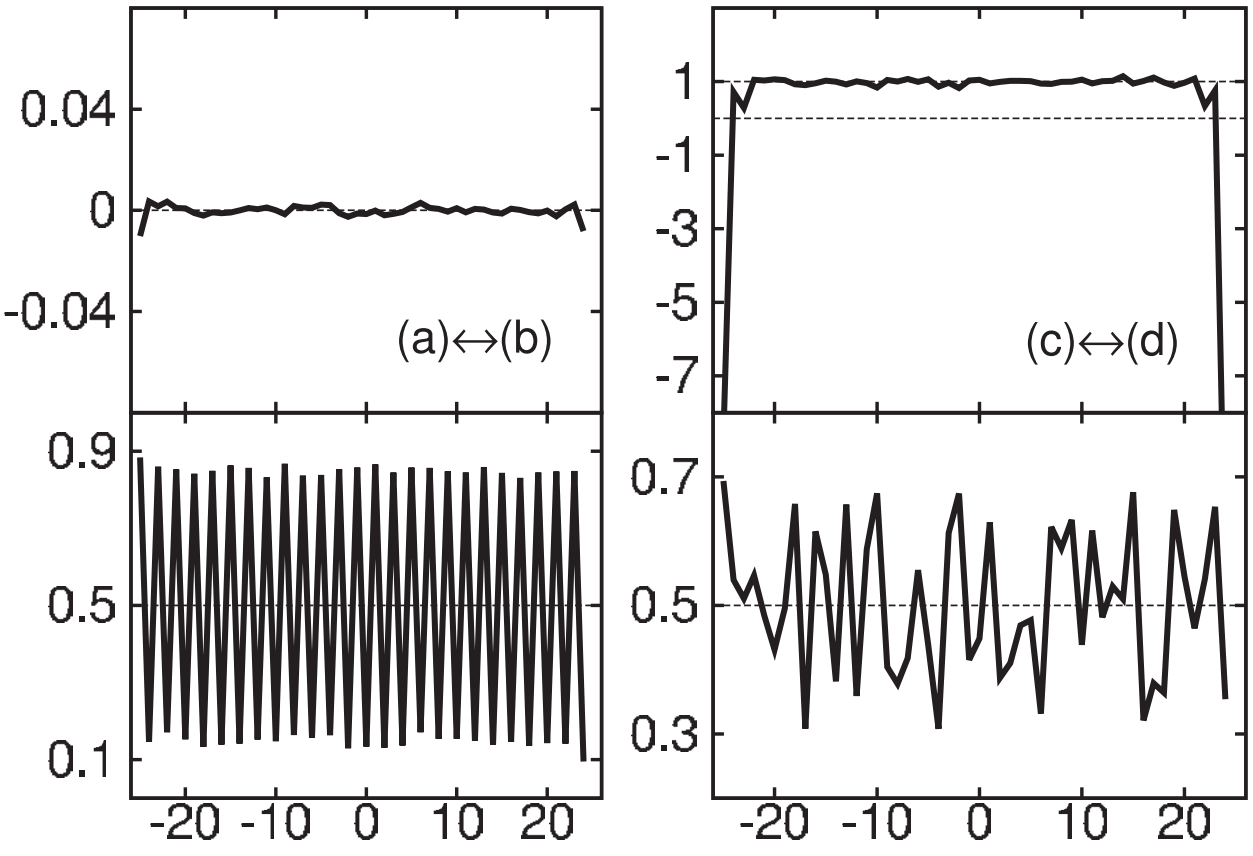


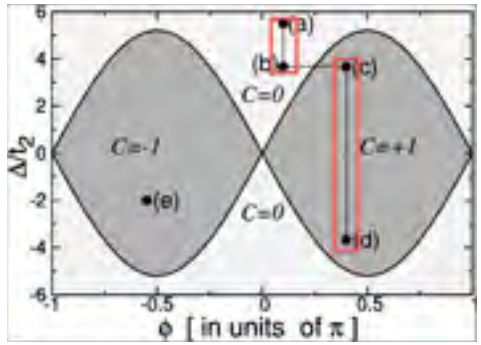


Topological marker (top); site occupancy (bottom)

Notice: trace per unit area vs. trace over the whole flake!

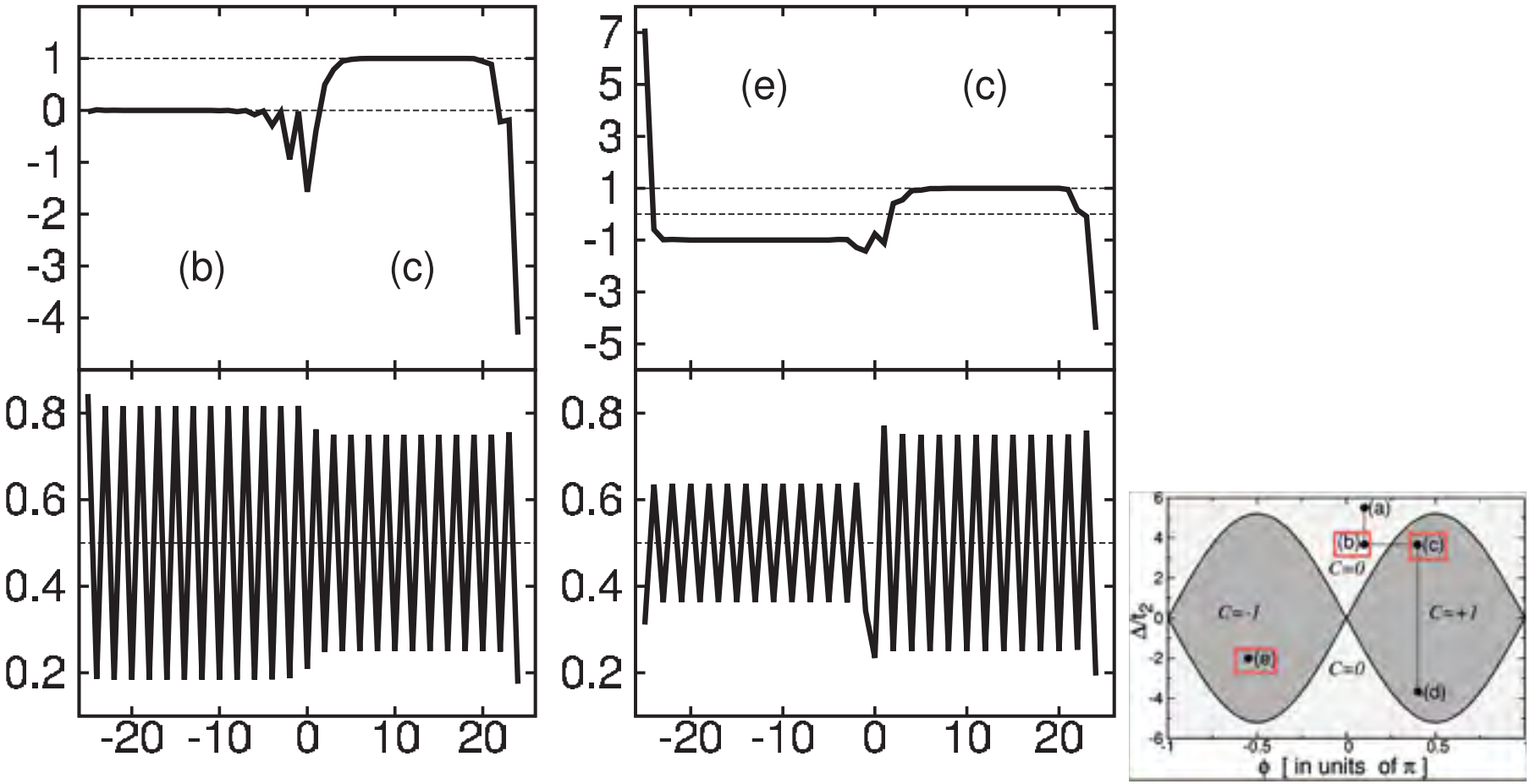
Haldanium alloy (normal & Chern)





Topological marker (top); site occupancy (bottom)

Haldanium heterojunctions



Topological marker (top); site occupancy (bottom)