Theory of the insulating state: Part 1

Raffaele Resta

Trieste, 2020

Outline

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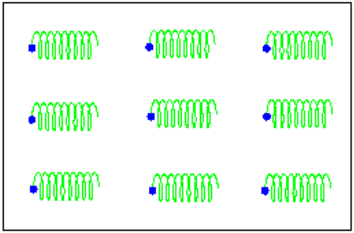
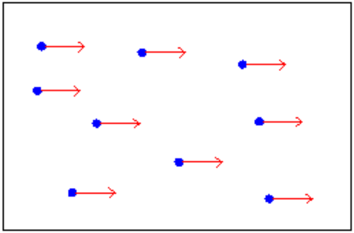
Before quantum mechanics
(Discovery of the electron: J.J. Thomson 1897)

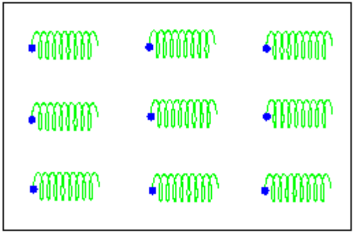


Insulator (Lorentz, 1906)

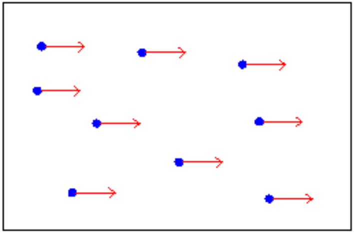


Metals (Drude, 1900)

Under the action of a field

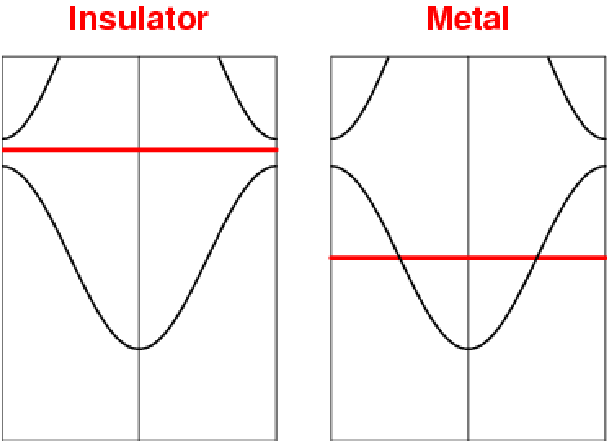


Electrons do not flow freely
(they polarize instead)



Electrons flow freely
(hindered by scattering)

Soon after quantum mechanics
(Bloch 1928, Wilson 1931)



Outline

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)

The Nobel Prize in Physics 1977

"for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"

		
Philip Warren Anderson	Sir Nevill Francis Mott	John Hasbrouck van Vleck
1/3 of the prize	1/3 of the prize	1/3 of the prize
USA	United Kingdom	USA
Bell Telephone Laboratories Murray Hill, NJ, USA	University of Cambridge Cambridge, United Kingdom	Harvard University Cambridge, MA, USA
b. 1923	b. 1905 d. 1996	b. 1899 d. 1980

Outline

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, $\Phi = \sum_{-\infty}^{\infty} \Phi_M$, 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.

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

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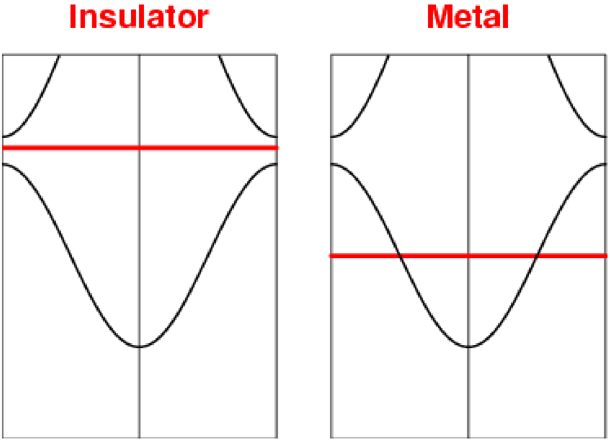
- **Kohn's revolutionary message (1):**
  The insulating behavior reflects a certain type of organization of the electrons in their **ground state**.

Property of the ground state or of the excitations?



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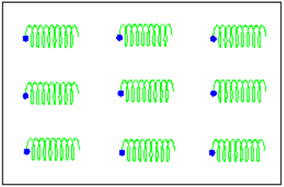
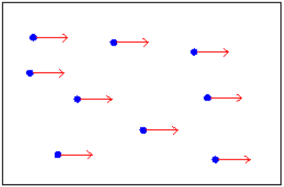
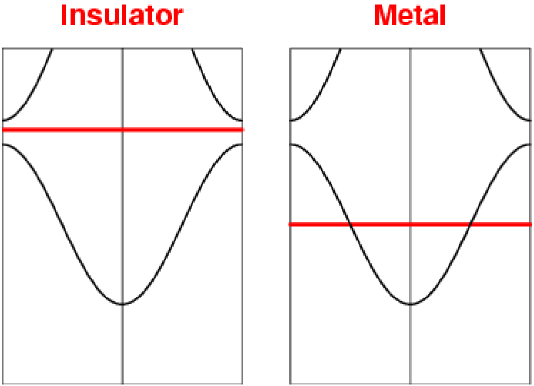
- **Kohn's revolutionary message (2):**
  Insulating characteristics are a strict consequence of **electronic localization** (in an appropriate sense) and do not require an energy gap.

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





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



What Kohn did not provide:

A “marker” for the insulating/metallic state of matter

Outline

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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 **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 positive & negative charge:**

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

Center of charge

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- **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

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

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

Single-point Berry phase

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

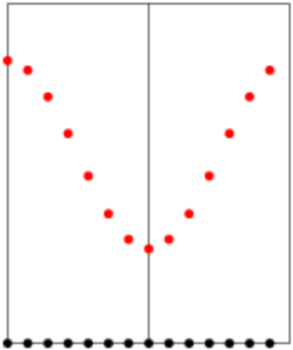
$$P_x = \frac{e}{2\pi} \text{Im ln } \langle \Psi_0 | \mathrm{e}^{i\frac{2\pi}{L}\left(\sum_\ell Z_\ell X_\ell - 2\sum_j x_j\right)} | \Psi_0 \rangle = e\frac{\gamma}{2\pi}$$

- γ is a Berry phase in disguise
- How can one prove that the formula **really** yields polarization?

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:

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

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**.

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

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

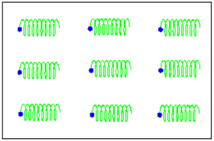
$$\gamma = i \int_{\mathrm{BZ}} dk \, \langle \psi_k | \frac{d}{dk} \psi_k \rangle = \lim_{N \to \infty} \operatorname{Im} \ln \prod_{j=1}^{M} S(q_j, q_{j-1}) = \lim_{N \to \infty} \operatorname{Im} \ln \mathfrak{z}_N$$

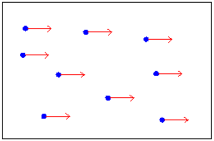
Outline

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

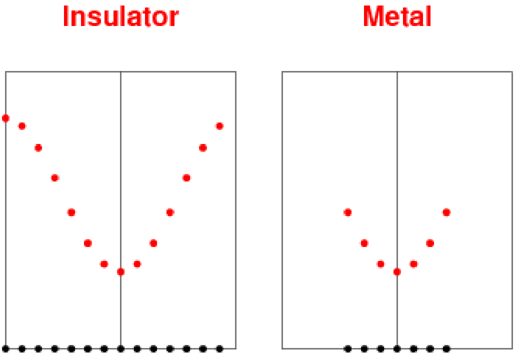
RS localization length

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

- 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

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

- **Zero determinant** in the metallic case!
- In a band metal $\lambda^2 = \infty$ **even at finite N**
- What is the meaning of λ^2 for a band insulator?