The insulating state of matter: A geometrical theory

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MAQSA workshop, Rome, October 2007

Outline

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The milestone paper

W. Kohn, Phys. Rev. **133**, A171 (1964)

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

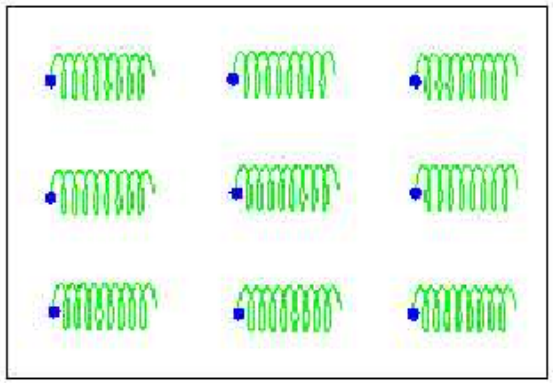
Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California

(Received 30 August 1963)

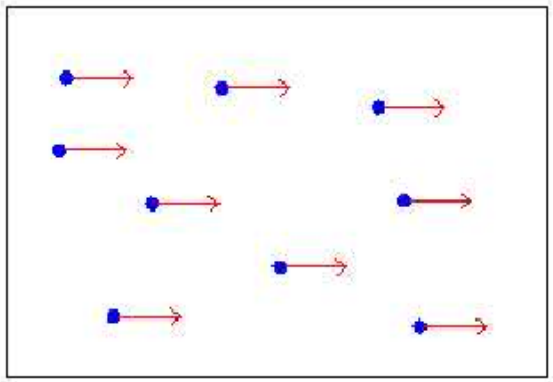
In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by Mott which, in band theory, would be metals. The essential property is this: Every low-lying wave function Φ of an insulating ring breaks up into a sum of functions, $\Phi = \sum_\alpha e^{i\alpha} \Phi_\alpha$, 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.

Theory of the insulating state before quantum mechanics



Insulator

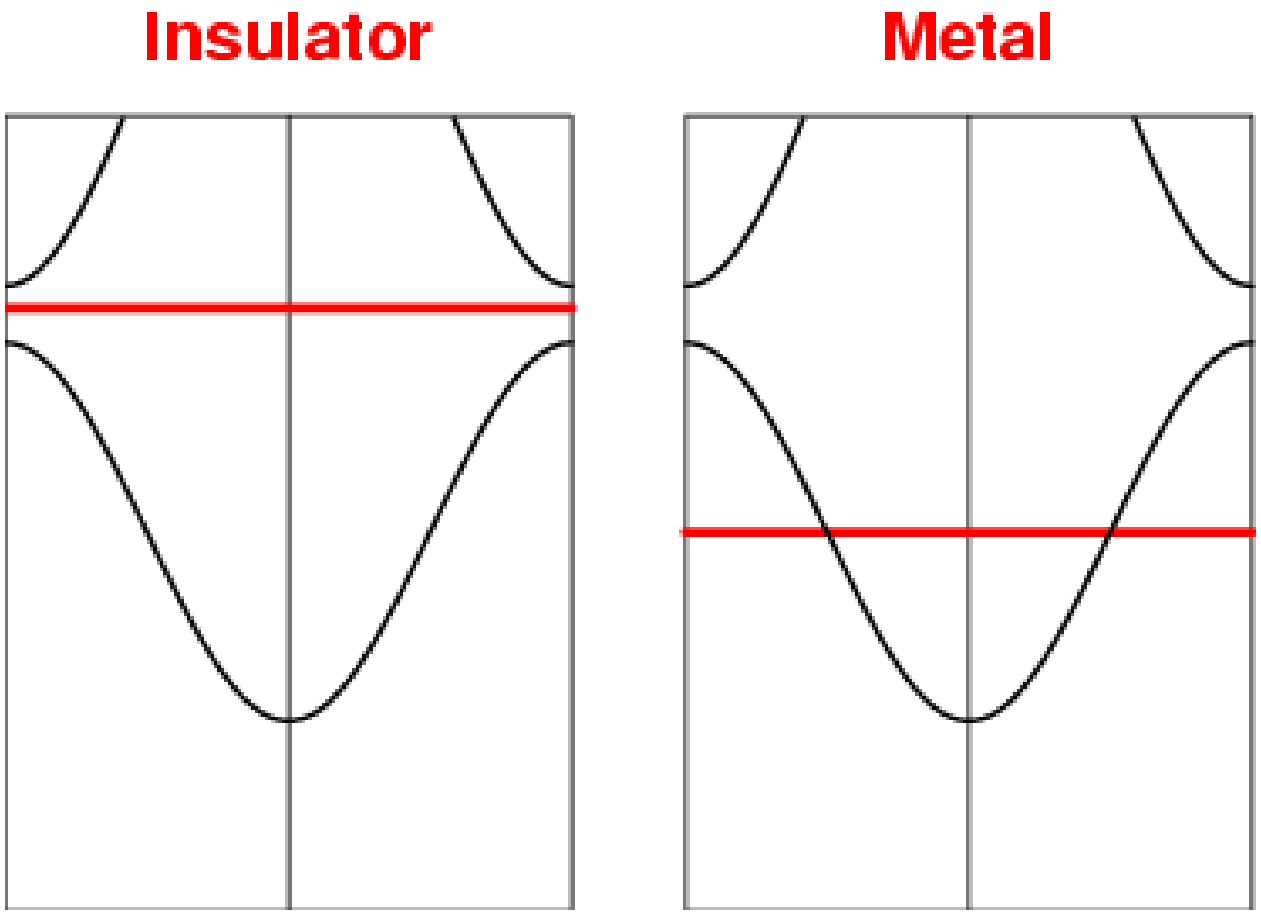
(Lorentz, 1909)



Metal

(Drude, 1900)

Theory of the insulating state: Quantum mechanics
(Bloch 1928, Wilson 1931)



Theory of the insulating state, revisited

[starting with R. Resta and S. Sorella, Phys Rev. Lett. **82**, 370 (1999)]

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- **Kohn's original message:**
  The insulating behavior reflects a certain type of organization of the electrons in the **ground state**.
- **Present formulation:**
  The "type of organization" is a **geometrical** property of the many-electron ground-state wavefunction.

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1992 onwards: The “Modern theory of polarization”

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

- **Phenomenologically:**
  - **Metal:** Has a finite dc conductivity
  - **Insulator:** Has a vanishing dc conductivity (at zero temperature!).

- **But also....**
  - **Metal:** Macroscopic electrical polarization is trivial: It is **not** a bulk effect.
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In this talk:

Focus on conductivity, **not** on polarization.

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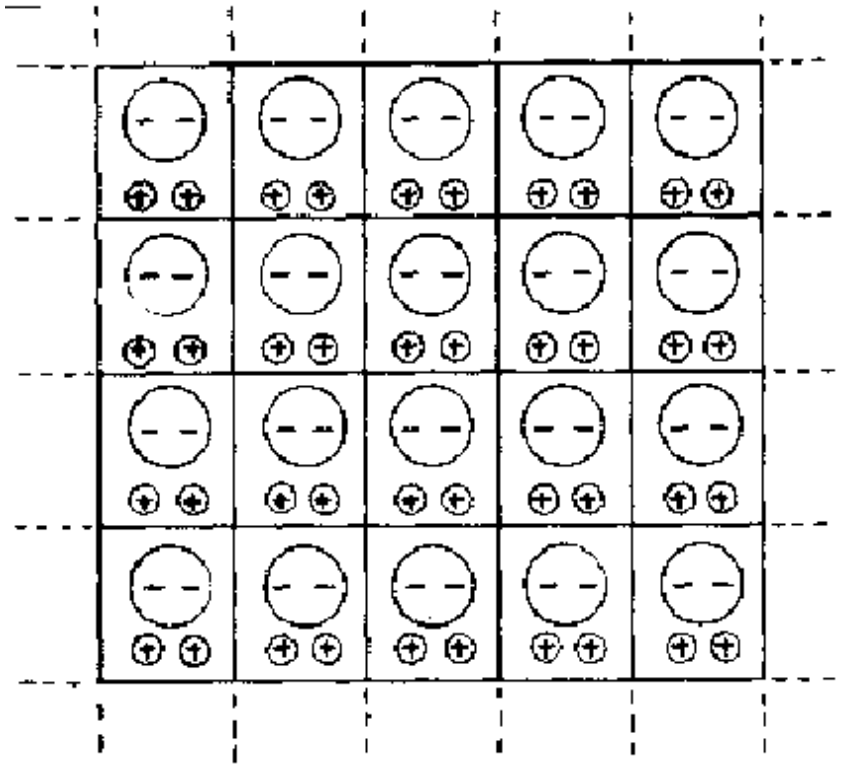

Fig. 11–8. A complex crystal lattice can have a permanent intrinsic polarization P.

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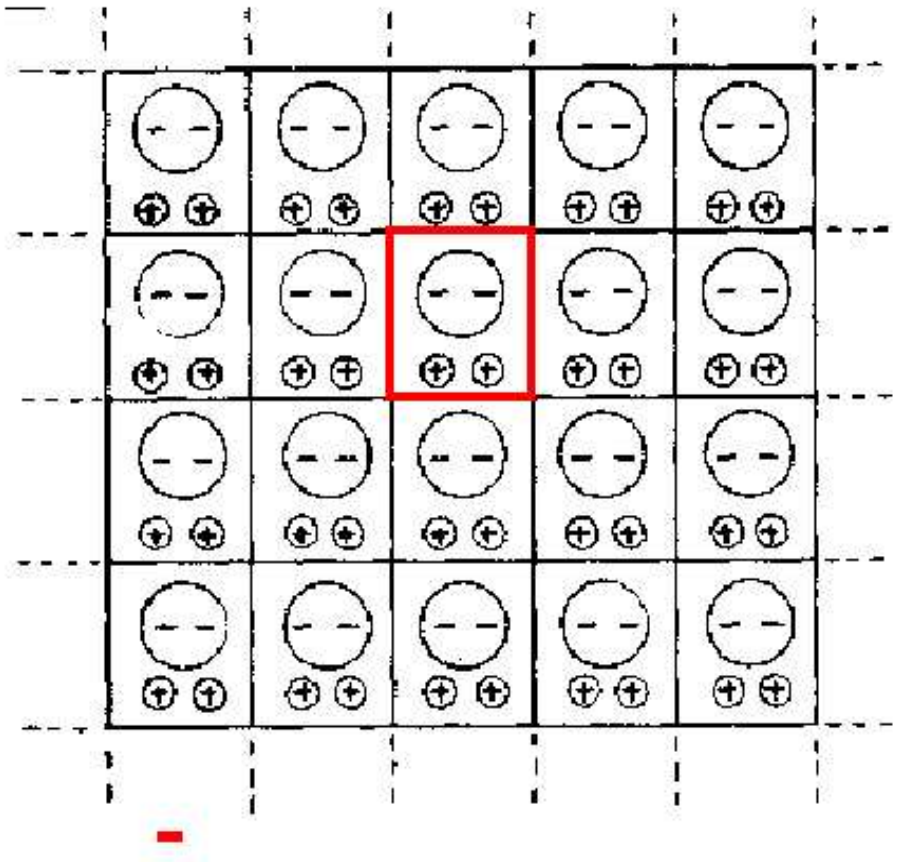

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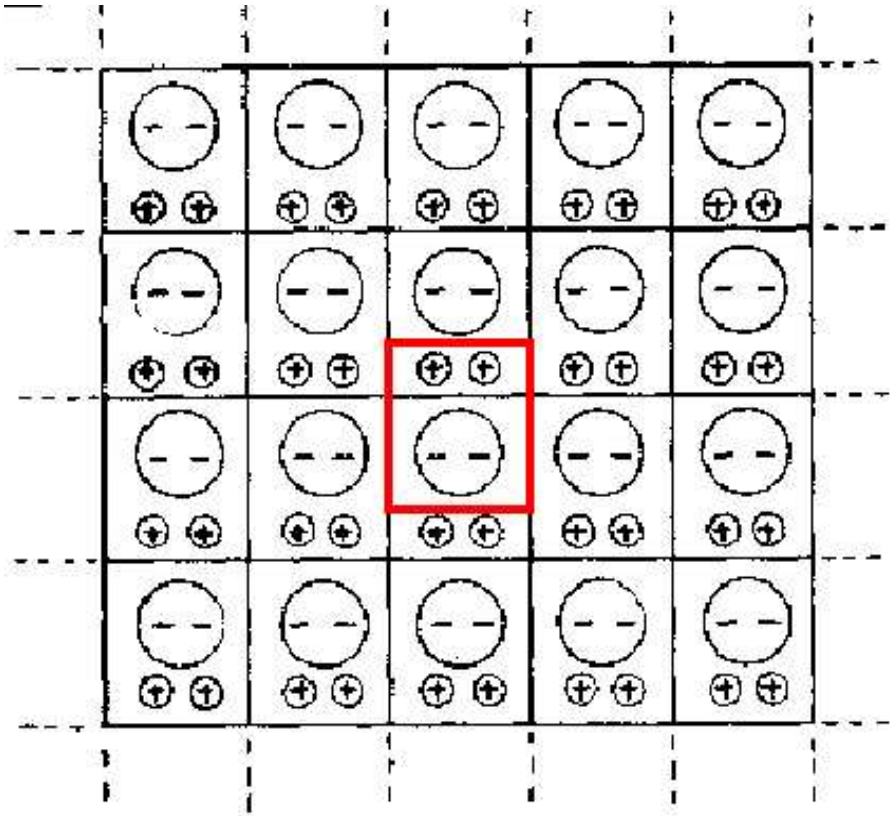

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- Macroscopic polarization has **nothing to do** with the periodic charge of a polarized dielectric (contrary to common statements in most textbooks).
- Polarization can be expressed as a **geometric phase** (Berry phase) of the electronic wavefunction.
- Nowadays, the Berry phase is computed as a standard option within all the electronic-structure codes on the market.
- This gives an idea of how, when, and why geometrical concepts entered electronic-structure theory in condensed matter.

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Outline

Bures distance

D. Bures, Trans. Am. Math. Soc. **135**, 199 (1969)

- A parametric quantum Hamiltonian:
  $H(\mathbf{k})|\Psi(\mathbf{k})\rangle = E(\mathbf{k})|\Psi(\mathbf{k})\rangle$
- Nondegenerate ground state $|\Psi_0(\mathbf{k})\rangle$;
- Arbitrary phase factor $e^{i\theta(\mathbf{k})}$: **"gauge"** freedom.
- Distance between quantum states
  $D_{12}^2 = \inf_{\theta_1\theta_2} \|\psi_0(\mathbf{k}_1)e^{i\theta_1} - \psi_0(\mathbf{k}_2)e^{i\theta_2}\|$
  $D_{12}^2 = 2 - 2|\langle\psi_0(\mathbf{k}_1)|\psi_0(\mathbf{k}_2)\rangle|^2$
- Manifestly gauge invariant.
- Projectors:
  $P(\mathbf{k}) = |\Psi_0(\mathbf{k})\rangle\langle\Psi_0(\mathbf{k})|\,, \quad Q(\mathbf{k}) = 1 - P(\mathbf{k})$
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Quantum metric & curvature

J. P. Provost and G. Vallee, Commun. Math Phys. **76**, 289 (1980)

$$D^2_{\mathbf{k},\mathbf{k}+d\mathbf{k}} = \sum_{\alpha,\beta=1}^{d} g_{\alpha\beta}(\mathbf{k}) dk_\alpha dk_\beta$$

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Fubini-Study metric

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J. P. Provost and G. Vallee, Commun. Math Phys. **76**, 289 (1980)

$$D^2_{\mathbf{k},\mathbf{k}+d\mathbf{k}} = \sum_{\alpha,\beta=1}^{d} g_{\alpha\beta}(\mathbf{k}) dk_\alpha dk_\beta$$

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Outline

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Many-electron Hamiltonian in $3d$

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

- $\mathbf{A}$ is a vector potential of magnetic origin.
- $\hat{V}$ includes one-body and two-body terms.
- The wavefunctions $|\Psi(\mathbf{k})\rangle$ obey periodic (toroidal) boundary conditions over a cubic box of side L (over each electron coordinate **independently**).
- $\mathbf{k}$ is a $3d$ parameter (dimensions: inverse length) usually called "flux", or "twist".
  - **Here:** Twisted Hamiltonian, fixed boundary conditions;
  - **Alternatively:** Fixed Hamiltonian, twisted boundary conditions.

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(a.k.a. first cumulant moment of the electron distribution)

- Eventually, we are interested in the "thermodynamic limit":
  $N \to \infty, \quad L \to \infty, \quad N/L^3 = \text{constant}.$

- $\langle \partial_\alpha \Psi_0(\mathbf{k}) | Q(\mathbf{k}) | \partial_\beta \Psi_0(\mathbf{k}) \rangle$ is **extensive**
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- We focus on $\mathbf{k} = 0$, and we define the **intensive** quantity:

  $$\langle r_\alpha r_\beta \rangle_c = \langle \partial_\alpha \Psi_0(0) | Q(0) | \partial_\beta \Psi_0(0) \rangle / N$$

  - Both real and imaginart parts.
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- Metric per electron at $\mathbf{k} = 0$ (real part);
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- "Geometric" response of the system to an infinitesimal "twist" of the many-body Hamiltonian.

Main message of the present talk

- Re $\langle r_\alpha r_\beta \rangle_c$ discriminates between insulators and metals.
- It is **the** ground-state property which vindicates Kohn's (1964) viewpoint.

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Sum over states again

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

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From now on, $\mathbf{k} = 0$ **implicit**.

$$\langle r_\alpha r_\beta\rangle_c = \frac{1}{N}\langle\partial_\alpha\Psi|Q|\partial_\beta\Psi_0\rangle = \frac{\hbar^2}{N}{\sum_{n\neq 0}}'\frac{\langle\Psi_0|\,\partial_\alpha\hat{H}\,|\Psi_n\rangle\langle\Psi_n|\,\partial_\beta\hat{H}\,|\Psi_0\rangle}{(E_0-E_n)^2}$$

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Conductivity tensor

Kubo formula:

$$\sigma_{\alpha\beta}(\omega) = \frac{ie^2}{\hbar L^3} \lim_{\eta\to 0^+} \sum_{n\neq 0}{}' \frac{1}{\omega_{0n}} \left(\frac{\langle\Psi_0|\hat{v}_\alpha|\Psi_n\rangle\langle\Psi_n|\hat{v}_\beta|\Psi_0\rangle}{\omega - \omega_{0n} + i\eta} - \frac{\langle\Psi_0|\hat{v}_\beta|\Psi_n\rangle\langle\Psi_n|\hat{v}_\alpha|\Psi_0\rangle}{\omega + \omega_{0n} + i\eta} \right)$$

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Outline

Localization tensor (real part) & longitudinal conductivity

I. Souza, T. Wilkens, and R. M. Martin, Phys. Rev. B **62**, 1666 (2000)

$$\begin{aligned}
\text{Re}\,\langle r_\alpha r_\beta\rangle_c &= \frac{1}{N}\text{Re}\,\langle\partial_\alpha\Psi|Q|\partial_\beta\Psi_0\rangle = \frac{1}{N}g_{\alpha\beta}(\mathbf{k}=0) \\
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  e.g. $\sigma_{11}(\omega) \equiv 0$ for $\hbar\omega \leq E_{\text{gap}}$ in "normal" insulators .
  The real part of the localization tensor **is finite**.

Localization tensor (real part) & longitudinal conductivity

I. Souza, T. Wilkens, and R. M. Martin, Phys. Rev. B **62**, 1666 (2000)

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\text{Re}\,\langle r_\alpha r_\beta\rangle_c &= \frac{1}{N}\text{Re}\,\langle\partial_\alpha\Psi|Q|\partial_\beta\Psi_0\rangle = \frac{1}{N}g_{\alpha\beta}(\mathbf{k}=0) \\
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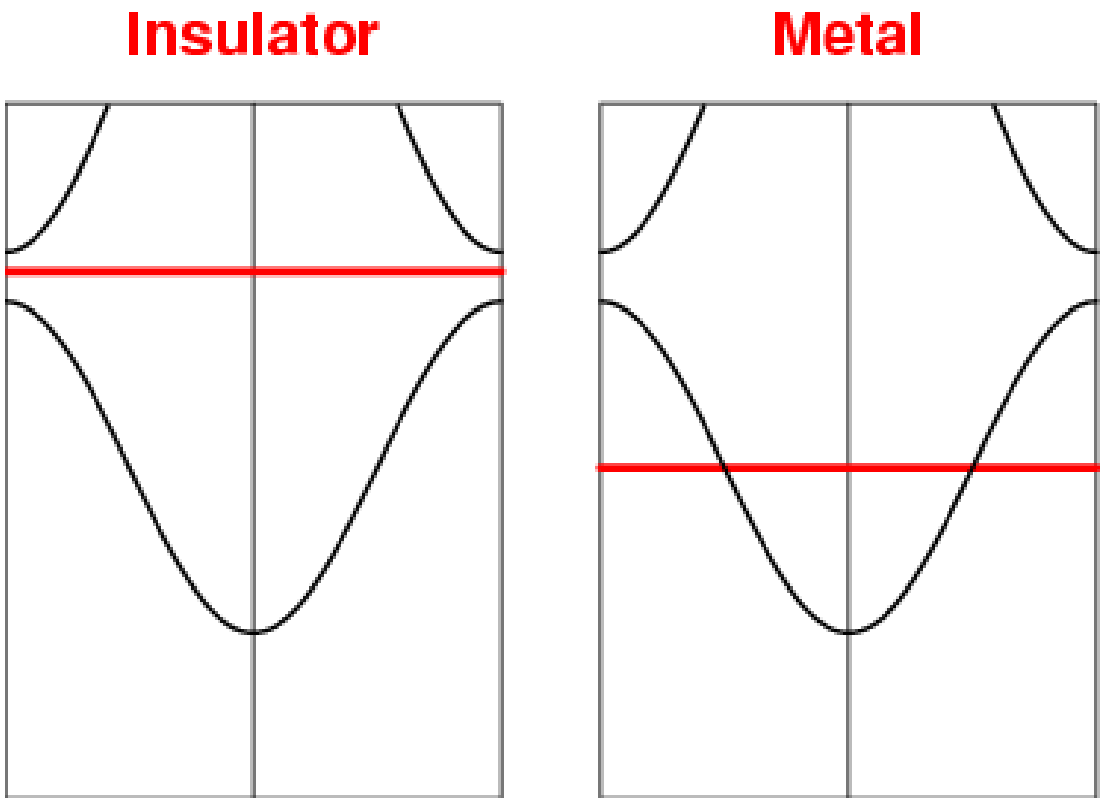
Outline

Special case:
Crystalline system of independent electrons
(e.g. Hartree-Fock or Kohn-Sham)

For presentation purpose: electrons in 1d.



Crystalline system of independent electrons

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

- $|\Psi_0\rangle$ is an N–particle Slater determinant of Bloch orbitals.
- **Caveat:**
  The many-body "flux" k and the Bloch vector q are **different** quantities (k equals **zero** in $|\Psi_0\rangle$).
- Periodic (toroidal) boundary conditions imposed over $L = Ma$: M allowed Bloch vectors in the reciprocal cell.
- $|\Psi_0\rangle$ 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 $|\Psi_0\rangle$.

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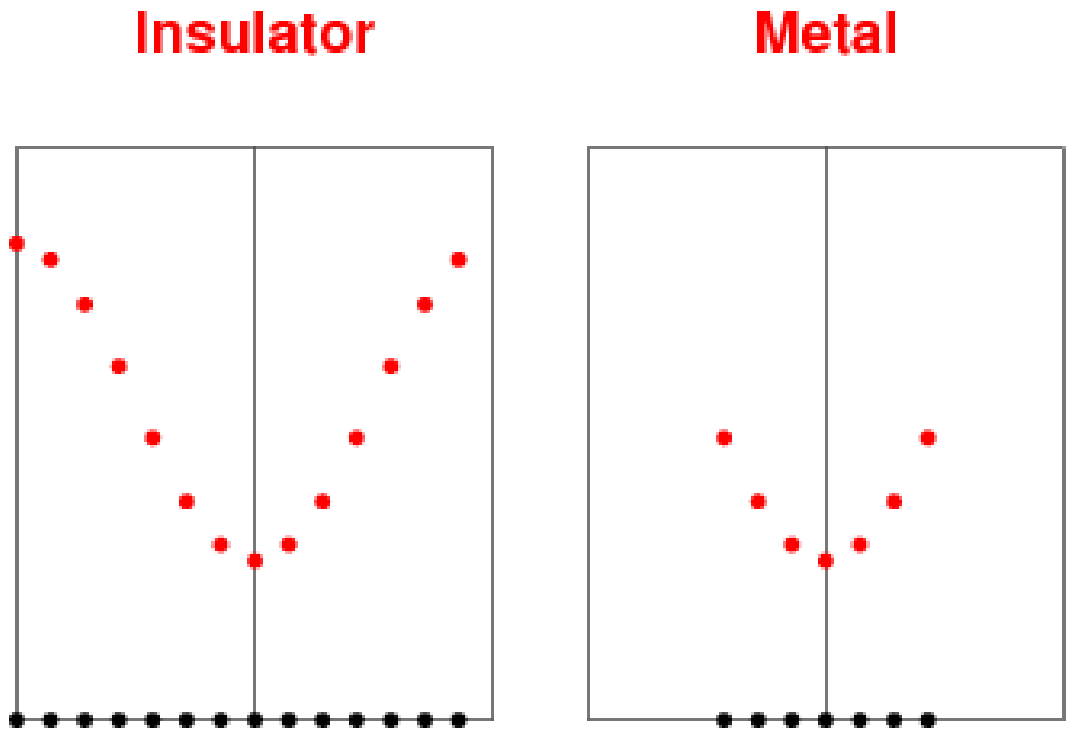

$L = Ma$, $M = 14$ in this drawing:

14 Bloch vectors in the Brillouin zone.

14 occupied orbitals in the insulating state,

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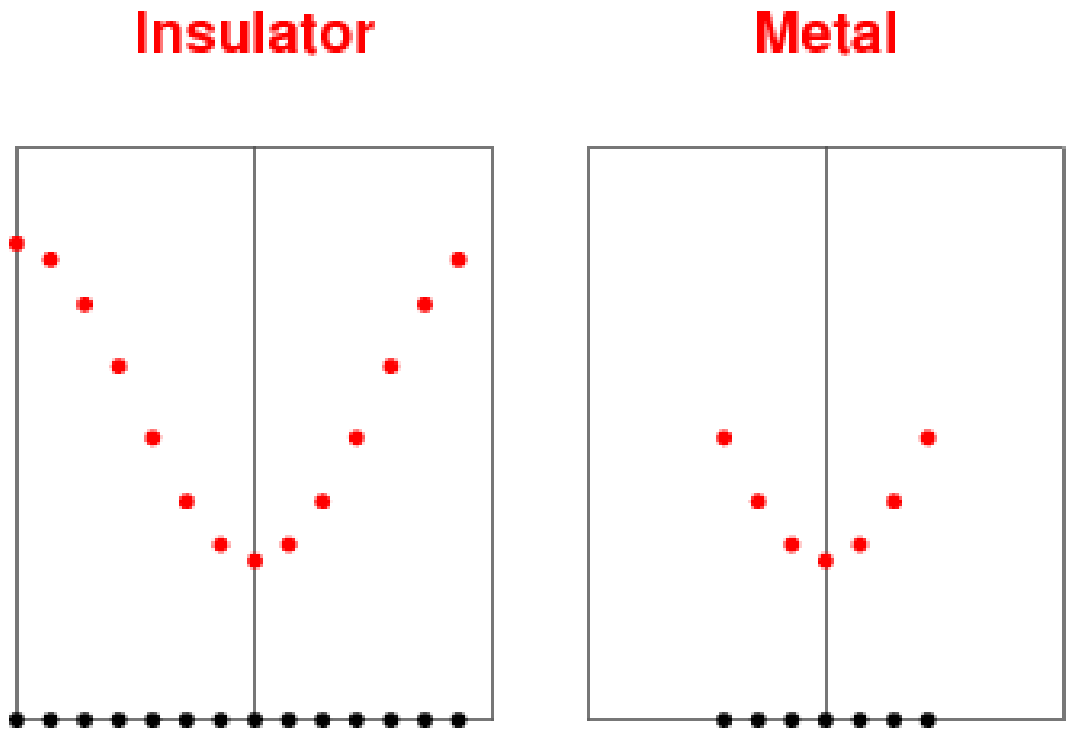

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Crystalline system of independent electrons
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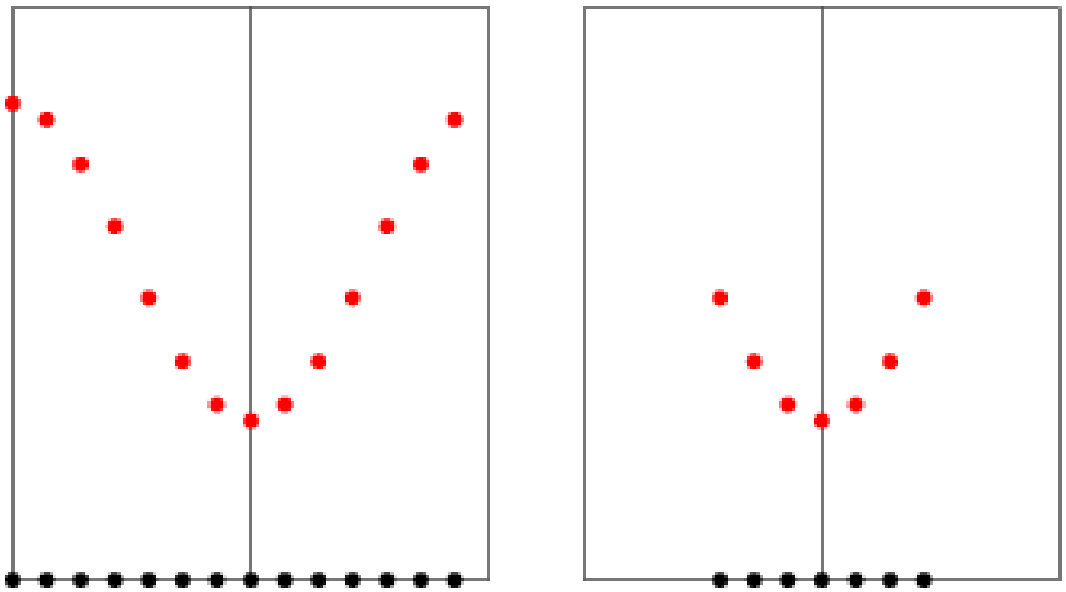

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In the thermodynamic limit ($M \to \infty$ limit):

- $\langle x^2 \rangle_c$ **converges** to a finite value in the insulating case;
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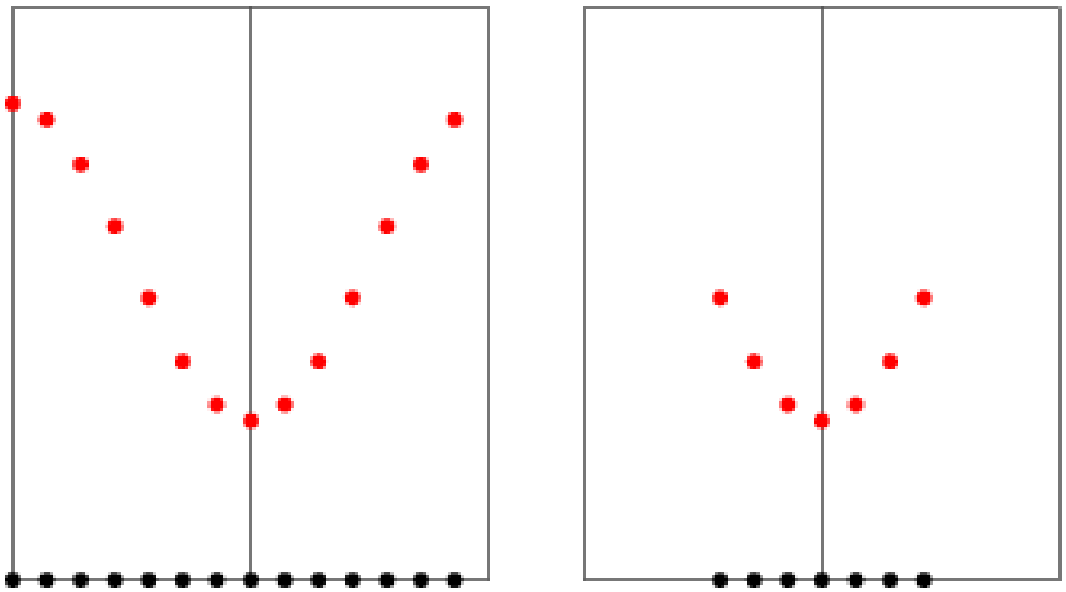

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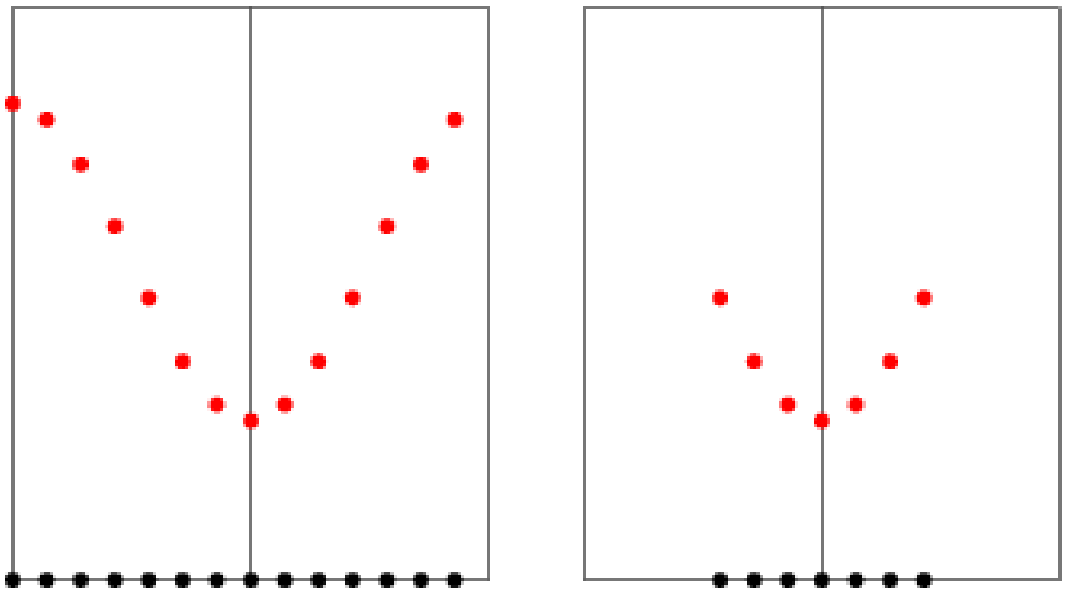

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Semantics: Why “localization tensor”?
(or even: why “second cumulant moment of the electron distribution”?)

Here: Only independent-electron explanation.

- So far, we have written $|\Psi_0\rangle$ an N-particle Slater determinant of Bloch orbitals.
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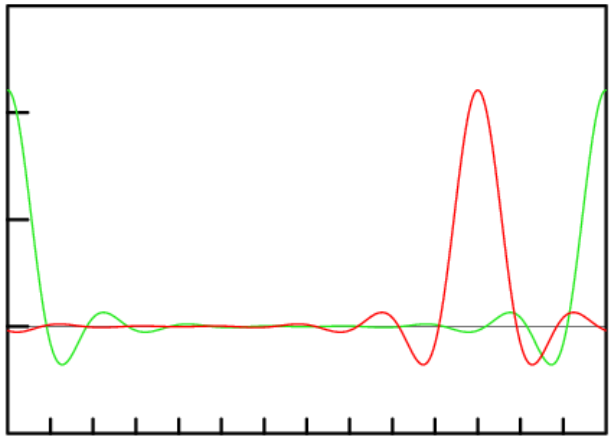

- In this drawing, again $L = Ma$, with $M = 14$:
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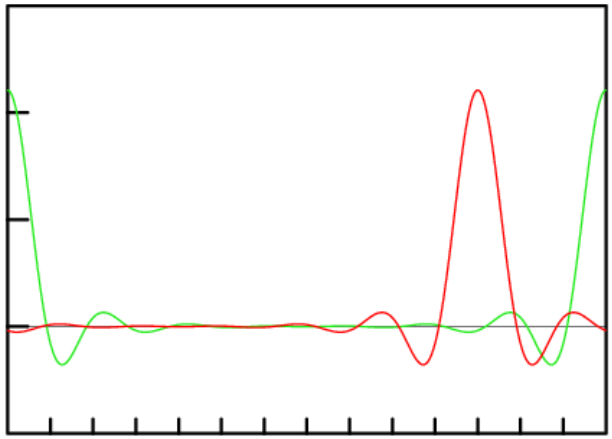

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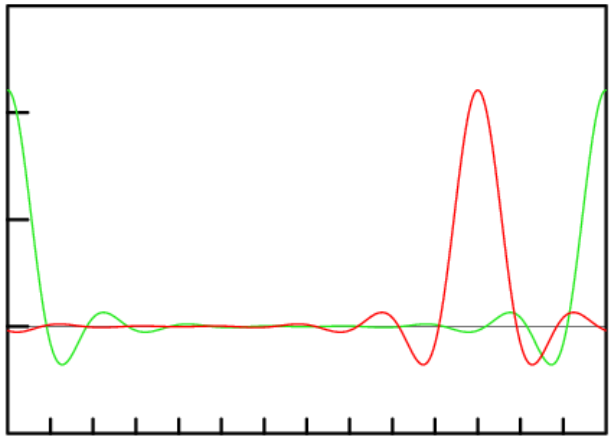

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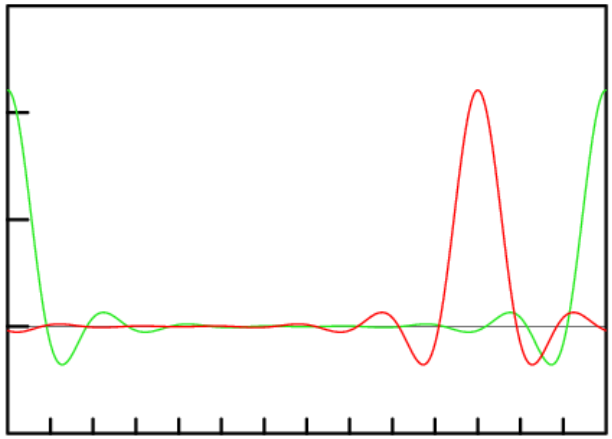

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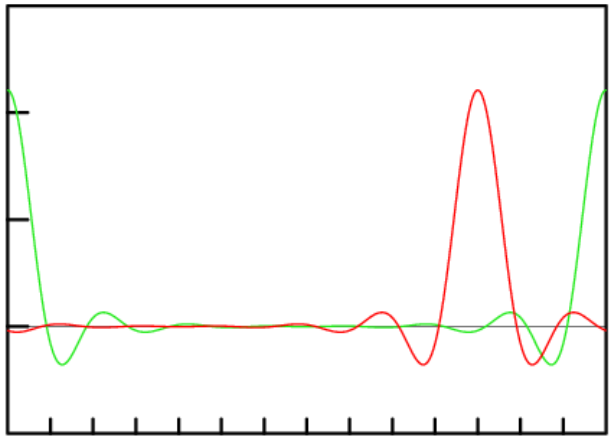

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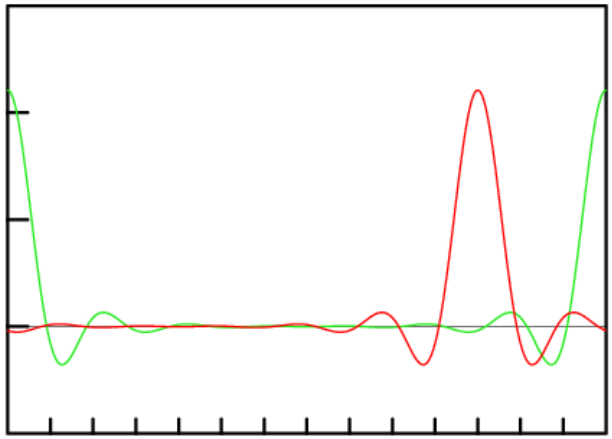

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In insulators:

- $\sigma_{11}(\omega) \to 0$ for $\omega \to 0$ fast enough to make the integral converge.
- The **real part** of the localization tensor **is finite**.
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Localization tensor (real part) & longitudinal conductivity

I. Souza, T. Wilkens, and R. M. Martin, Phys. Rev. B **62**, 1666 (2000)

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R. Resta, Phys. Rev. Lett. **95**, 196805 (2005)

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The quantum Hall effect
(both integer and fractional)

VOLUME 45, NUMBER 6 PHYSICAL REVIEW LETTERS 11 AUGUST 1980

New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance

K. v. Klitzing,
Max-Planck-Institut für Festkörperforschung, D-8000 Stuttgart, Federal Republic of Germany, and Technische Universität Wien, A-1040 Vienna, Austria

and

G. Dorda
Forschungslaboratorium der Siemens AG, D-8000 München, Federal Republic of Germany

and

M. Pepper
Cavendish Laboratory, Cambridge CB3 0HE, United Kingdom
(Received 30 May 1980)

Measurements of the Hall voltage of a two-dimensional electron gas, realized in a silicon metal-oxide-semiconductor field-effect transistor, show that the Hall resistance in particular, experimentally well-defined surface carrier concentrations has fixed values which depend only on the fine-structure constant and speed of light, and is insensitive to the geometry of the device. Preliminary data are reported.

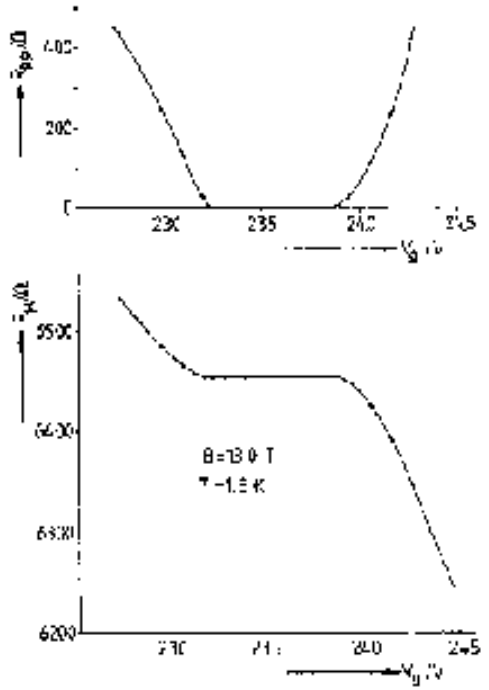

FIG. 2. Hall resistance R_{21} and resistance R_{xx} between the potential probes as a function of gate voltage V_g in a region of gate voltage corresponding to a fully occupied lowest Landau level. The plateau in R_{21} has a value of 25813.0 ± 0.5 Ω. The geometry of the device was $L = 400$ μm, $W = 50$ μm, and $L_{pp} = 130$ μm. $B = 18$ T.

$$\rho_{11} = \frac{\sigma_{11}}{\sigma_{11}^2+\sigma_{12}^2} \qquad \rho_{12} = -\frac{\sigma_{12}}{\sigma_{11}^2+\sigma_{12}^2}$$

In the QH regime σ_{12} is quantized **and** $\sigma_{11} = 0$:

$\longrightarrow$ The system is **insulating**

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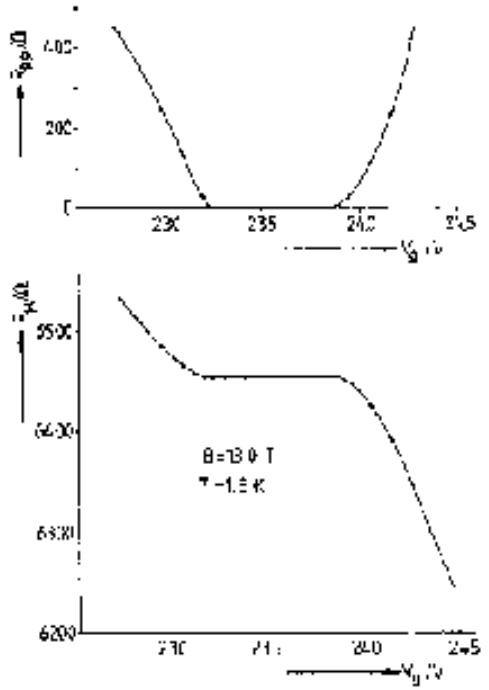

FIG. 2. Hall resistance R_H and resistivity ρ_{xx} between the potential probes as a function of gate voltage V_g in a region of gate voltage corresponding to a fully occupied lowest orbital Landau level. The plateau in R_H has a value of 6453.5 ± 0.3 Ω. The geometry of the device was $L = 130$ μm, $W = 50$ μm, and $L_{pp} = 130$ μm, $B = 18$ T.

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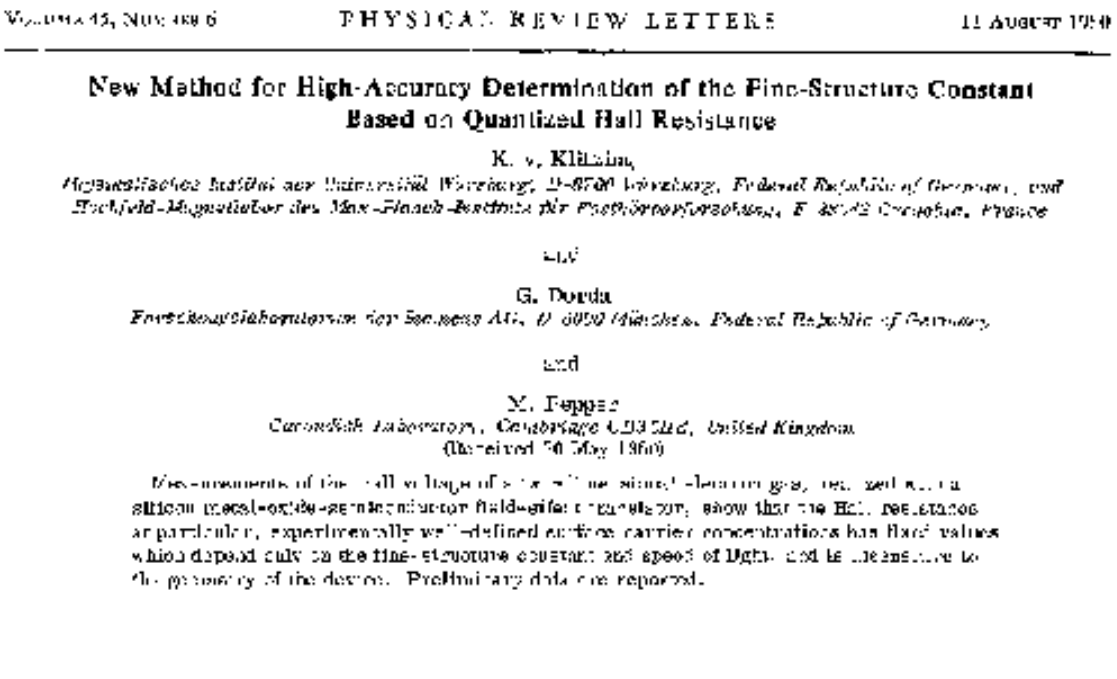

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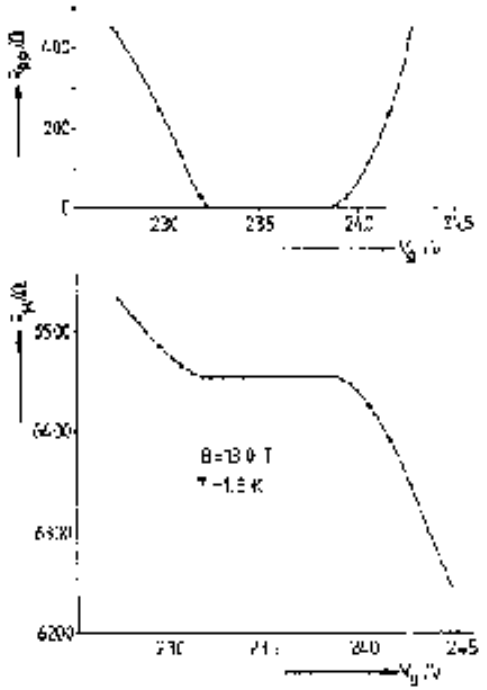

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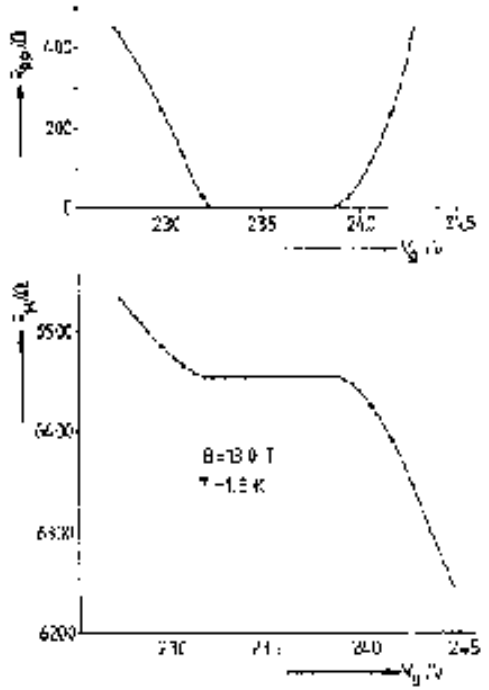

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Chern numbers & the quantum Hall effect, $2d$

Q. Niu, D. J. Thouless, and Y. S. Wu, Phys. Rev. B **31**, 3372 (1985)

- C_1 is the integral of the curvature over the "flux", or "twist".
- NTW proved that the quantized Hall conductivity is:
  .Re $\sigma_{12}(0) = -\frac{e^2}{h} C_1 = -\frac{e^2}{2\pi\hbar} C_1$

- Within our toroidal boundary conditions over a square of side L, the "twist" $\mathbf{k} \in [0, \frac{2\pi}{L}) \times [0, \frac{2\pi}{L})$:

$$C_1 = \frac{1}{2\pi} \int_0^{2\pi/L} dk_1 \int_0^{2\pi/L} dk_2 \; \Omega_{12}(\mathbf{k})$$

- In the limit of a large system

$$C_1 \to \frac{2\pi}{L^2} \Omega_{12}(0)$$

(the integration domain "shrinks" to single point).

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  .Re $\sigma_{12}(0) = -\frac{e^2}{h} C_1 = -\frac{e^2}{2\pi\hbar} C_1$
- Within our toroidal boundary conditions over a square of side L, the "twist" $\mathbf{k} \in [0, \frac{2\pi}{L}) \times [0, \frac{2\pi}{L})$:

$$C_1 = \frac{1}{2\pi} \int_0^{2\pi/L} dk_1 \int_0^{2\pi/L} dk_2 \; \Omega_{12}(\mathbf{k})$$

- In the limit of a large system

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