

dc conductivity as a geometric phase B. Hetényi Bilkent University, Ankara, TURKEY

<u>What makes materials conduct or</u> <u>insulate?</u>

Classical answer: single particle localization

Localization of individual charge carriers \rightarrow free charges conduct, bound charges contribute to polarization

Quantum answer: band theory

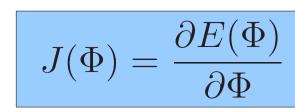
filled valence band \rightarrow insulation partially filled valence band \rightarrow conduction

<u>Current as a geometric phase</u>

We consider a Hamiltonian of a periodic (*L*) continuous system of the form:

$$H(\Phi) = \frac{1}{2m} \sum_{i=1}^{N} \left(i \frac{\partial}{\partial_{x_i}} + \Phi \right) + V(x_1, \dots, x_N)$$

The current is defined as



The current can also be written as a Berry phase (BH, *JPSJ*, 2012): $I(\Phi) = \frac{N\Phi}{i} \int_{-L}^{L} dV/W(\Phi) |\Phi| |\Psi(\Phi)|$

Interpretation (continued)

• Consider the lattice/discrete expression for D_c . Expanding the geometric phase term in ΔX and ΔK , the is term reduces to a sum of one-body positionmomentum commutators cancelling the first term. The result is zero, hence the system is insulating.

•Such an expansion is not valid when the wavefunction $|\Psi\rangle$ is an eigenstate of the current. In this case, the geometric phase term is easily shown to be zero, and the system is metallic.

There are a number of exceptions to band theory: for example, $CrO_{2.}$

Quantum answer: many-body localization

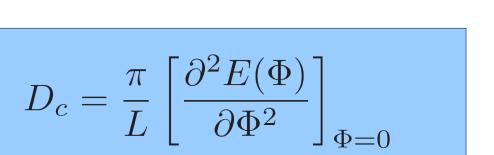
Theory of the Insulating State*

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.

W. Kohn, *Phys. Rev.* **A133** A171 (1964). Localization of the total position corresponds to insulation

Quantitative criterion: Drude weight (Kohn, 1964)



 Φ denotes an electrostatic

$$J(\Phi) = \frac{W\Psi}{m} - \frac{i}{mL} \int_0^{\infty} dX \langle \Psi(\Phi) | \partial_X | \Psi(\Phi) \rangle$$

• Lattice/discrete version (with lattice spacing ΔX): $J(\Phi) = -\frac{\langle T \rangle}{2} \Phi - \frac{i}{\Delta X} \operatorname{Im} \ln \langle \Psi(\Phi) | e^{i\Delta X \hat{K}} | \Psi(\Phi) \rangle$

$$\hat{X} = \sum_{i=1}^{N} \hat{x}_i$$

Spread in current: $\sigma_{K}^{2} = -\frac{1}{2\Delta X^{2}} \operatorname{Re} \ln \langle \Psi | e^{i\Delta X \hat{K}} | \Psi \rangle$

<u>The Drude weight as a geometric</u> <u>phase</u>

Continuous version:

 $\frac{LD_c}{\pi} = \frac{N}{m} - \frac{1}{2\pi} \int_{-\pi/L}^{\pi/L} dK \int_0^L dX [\langle \partial_K \Psi | \partial_X \Psi \rangle - \langle \partial_X \Psi | \partial_K \Psi \rangle]$

Connection to localization

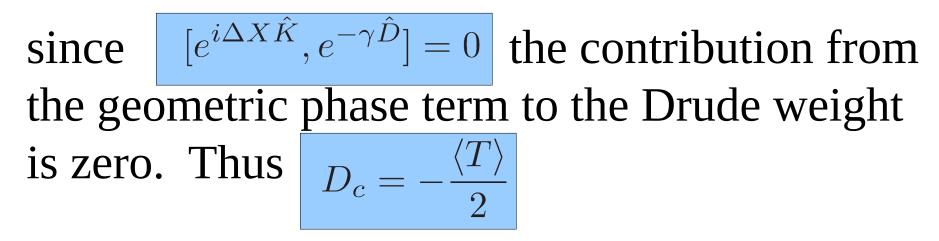
• If $|\Psi>$ is an eigenstate of the current it holds that $e^{i\Delta K\hat{X}}|\Psi(K)\rangle = |\Psi(K + \Delta K)\rangle$

and
$$\sigma_X^2 = -\frac{L^2}{2\pi^2} \operatorname{Re} \ln \langle \Psi | e^{i2\pi \hat{X}/L} | \Psi \rangle = \infty$$

• If $|\Psi>$ is a continuous function in momentum space, then the spread is finite.

<u>Examples</u>

Fermi sea, BCS, trivial to verify (eigenstates of the total current).
Gutzwiller wavefunction (metallic) $|\Psi_G(\gamma)\rangle = e^{-\Gamma \hat{D}}|FS\rangle$



perturbation

Question: can we demonstrate the equivalence between the Drude weight and localization?

Difficulty: the total position operator in crystalline systems is ill-defined

<u>The modern theory of polarization</u>

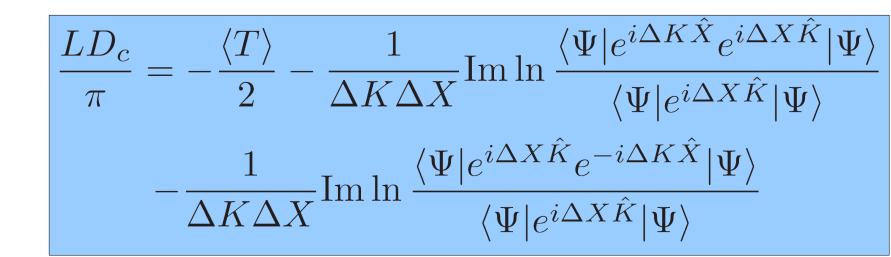
Polarization in crystalline systems can be expressed in terms of a Berry phase (King-Smith and Vanderbilt, *PRB*, 1993 and Resta, *RMP* 1994).

$$P = \frac{ie}{2\pi} \int dK \langle \Psi(K) | \partial_K | \Psi(K) \rangle$$

Discretized expression (Resta, *PRL*, 1998, Resta and Sorella, *PRL*, 1999):

 $P = \frac{eL}{2\pi} \operatorname{Im} \ln \langle \Psi | e^{i2\pi \hat{X}/L} | \Psi \rangle \qquad \hat{X} = \sum_{i=1}^{N} \hat{x}_i$

Lattice/discrete version:



<u>Interpretation</u>

The Drude weight is given by a single body term and a geometric phase term, similar to the Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) invariant used in the theory of the quantum Hall effect

 $\sigma_{\rm H} = \frac{ie^2}{2\pi h} \sum \int d^2k \int d^2r \left(\frac{\partial u^*}{\partial k_1} \frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2} \frac{\partial u}{\partial k_1} \right)$ $= \frac{ie^2}{4\pi h} \sum \oint dk_j \int d^2r \left(u^* \frac{\partial u}{\partial k_j} - \frac{\partial u^*}{\partial k_j} u \right), \quad (5)$

(Hall conductance, TKNN, PRL, 1982)

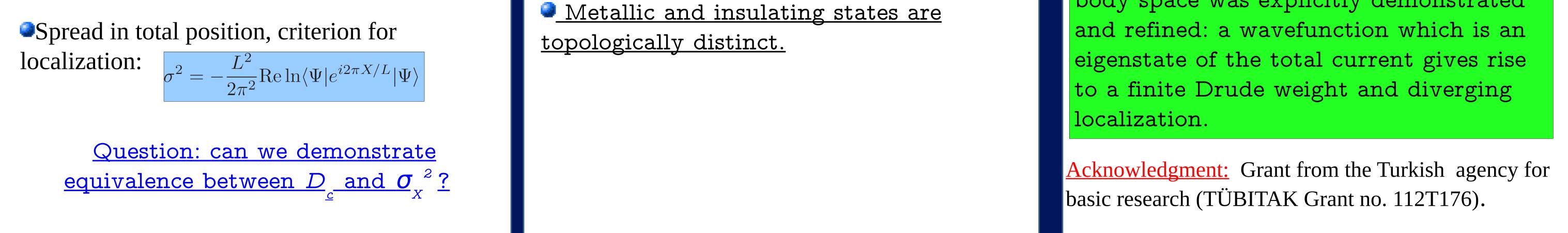
Anderson localization in 1D (tight-binding + random potential (strength U)):

| U | σ _κ | - <t>/2</t> | σχ | D _c L/π |
|-----|----------------|-------------|---------|--------------------|
| 0.0 | 0.0 | 327.95 | - | 327.95 |
| 1.0 | 5.8(2) | 0.01154(4) | 38.4(4) | 297(7) |
| 2.0 | 9.8(2) | 0.0087(1) | 17.8(9) | 233(3) |
| 3.0 | 12.8(2) | 0.0066(2) | 11.7(5) | 175(5) |

Conclusions

The Drude weight, the quantity which distinguishes conductors from insulators, was expressed in terms of a geometric phase, similar to the TKNN invariant.
 The metallic and insulating phases are topologically distinct.

The tenet of Kohn, that insulation corresponds to localization in the manybody space was explicitly demonstrated



References: [1] B. Hetényi, *Phys. Rev. B* 87 235123 (2013), [2] *J. Phys. Soc. Japan* 81 124711 (2012), [3] *J. Phys. Soc. Japan* 81 023701 (2012).