dc conductivity as a geometric phase

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What makes materials conduct or insulate?

- **<u>Classical answer: single particle localization</u>**

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

- **<u>Quantum answer: band theory</u>**

filled valence band → insulation

partially filled valence band → conduction

There are a number of exceptions to band theory: for example, CrO_2.

- **<u>Quantum answer: many-body localization</u>**

Theory of the Insulating State*

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(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

- **<u>Quantitative criterion:</u>** Drude weight (Kohn, 1964)

$$D_c = \frac{\pi}{L}\left[\frac{\partial^2 E(\Phi)}{\partial \Phi^2}\right]_{\Phi=0}$$

Φ denotes an electrostatic perturbation

<u>Question: can we demonstrate the equivalence between the Drude weight and localization?</u>

<u>Difficulty: the total position operator in crystalline systems is ill-defined</u>

The modern theory of polarization

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

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

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

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

- Spread in total position, criterion for localization: $\sigma^2 = -\frac{L^2}{2\pi^2}\mathrm{Re}\ln\langle\Psi|e^{i2\pi X/L}|\Psi\rangle$

<u>Question: can we demonstrate equivalence between D_c and σ_X^2?</u>

Current as a geometric phase

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

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

- The current is defined as

$$J(\Phi) = \frac{\partial E(\Phi)}{\partial \Phi}$$

- The current can also be written as a Berry phase (BH, *JPSJ*, 2012):

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

- Lattice/discrete version (with lattice spacing ΔX):

$$J(\Phi) = -\frac{\langle T\rangle}{2}\Phi - \frac{i}{\Delta X}\mathrm{Im}\ln\langle\Psi(\Phi)|e^{i\Delta X\hat{K}}|\Psi(\Phi)\rangle$$

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

- Spread in current:

$$\sigma_K^2 = -\frac{1}{2\Delta X^2}\mathrm{Re}\ln\langle\Psi|e^{i\Delta X\hat{K}}|\Psi\rangle$$

The Drude weight as a geometric phase

- Continuous version:

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

- Lattice/discrete version:

$$\frac{LD_c}{\pi} = -\frac{\langle T\rangle}{2} - \frac{1}{\Delta K\Delta X}\mathrm{Im}\ln\frac{\langle\Psi|e^{i\Delta K\hat{X}}e^{i\Delta X\hat{K}}|\Psi\rangle}{\langle\Psi|e^{i\Delta X\hat{K}}|\Psi\rangle} - \frac{1}{\Delta K\Delta X}\mathrm{Im}\ln\frac{\langle\Psi|e^{i\Delta X\hat{K}}e^{-i\Delta K\hat{X}}|\Psi\rangle}{\langle\Psi|e^{i\Delta X\hat{K}}|\Psi\rangle}$$

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</u>

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

(Hall conductance, TKNN, *PRL*, 1982)

- <u>Metallic and insulating states are topologically distinct.</u>

Interpretation (continued)

- <u>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 position-momentum commutators cancelling the first term. The result is zero, hence the system is insulating.</u>

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

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

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

Examples

- **Fermi sea, BCS,** trivial to verify (eigenstates of the total current).
- **Gutzwiller wavefunction** (metallic)

$$|\Psi_G(\gamma)\rangle = e^{-\Gamma\hat{D}}|FS\rangle$$

since $[e^{i\Delta X\hat{K}}, e^{-\gamma\hat{D}}] = 0$ the contribution from the geometric phase term to the Drude weight is zero. Thus $D_c = -\frac{\langle T\rangle}{2}$

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

U	σ_K	-<T>/2	σ_X	D_cL/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 many-body space was explicitly demonstrated and refined: a wavefunction which is an eigenstate of the total current gives rise to a finite Drude weight and diverging localization.

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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).