Berry Phase Correction to Electron Density of States in Solids and Its Applications

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Outline

- Effective dynamics of Bloch electrons
  - Berry-phase modified equation of motion
  - Non-uniform phase space
- Physical effects
  - Fermi sea volume & Streda formula
  - Orbital magnetization
  - Linear magnetoresistance
- Non-commutative quantum mechanics

Semiclassical dynamics

Equation of motion

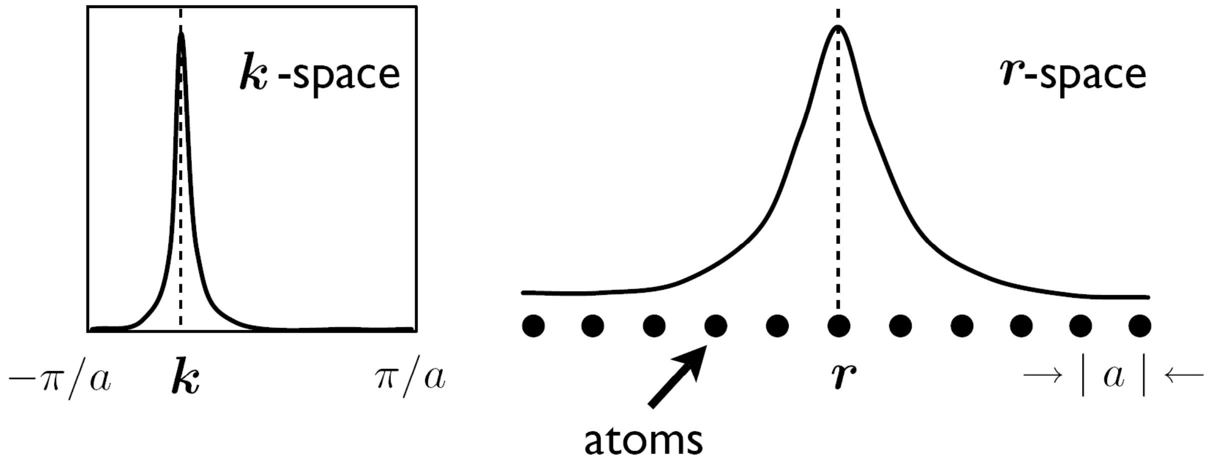
$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}}$$
$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r})$$

Density of states

$$D(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{(2\pi)^d}$$

Ashcroft & Mermin: Justifying the semiclassical model in detail is a formidable task, considerably more difficult than justifying the ordinary classical limit for free electrons.

Construction of wave packets



$$\boxed{|W(\boldsymbol{r}_c, \boldsymbol{k}_c)\rangle = \int_{\mathrm{BZ}} \mathrm{d}\boldsymbol{k}\, a(\boldsymbol{k}) e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_c - \boldsymbol{r})} |u_n(\boldsymbol{k})\rangle}$$

Phase space coordinates $\quad \boldsymbol{r}_c = \langle W|\hat{\boldsymbol{r}}|W\rangle \qquad \boldsymbol{k}_c = \langle W|\hat{\boldsymbol{k}}|W\rangle$

Lagrangian $\quad \mathcal{L} = \left\langle W \middle| i\hbar\frac{d}{dt} - \hat{H} \middle| W \right\rangle$

Effective dynamics of Bloch electrons

Equation of motion: The electron acquires an anomalous velocity

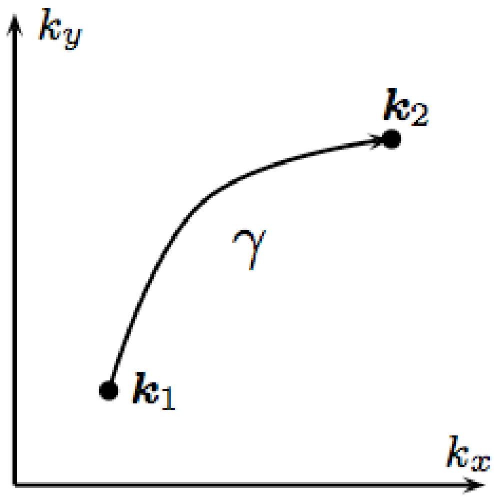
$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$
$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r})$$

$\boldsymbol{\Omega}_n(\boldsymbol{k})$ Berry curvature - reciprocal space magnetic field. It is nonzero in systems

- Broken time-reversal symmetry: magnetic materials
- Broken space inversion symmetry: surface, interface, nanotubes…

Chang & Niu, PRL 1995, PRB 1996, Sundaram & Niu PRB 1999

Berry phase and k-space magnetic field



$$\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r})$$

$$\hat{H}(\boldsymbol{k}) u_{n\boldsymbol{k}} = \varepsilon_n(\boldsymbol{k}) u_{n\boldsymbol{k}}$$

$$\hat{H}(\boldsymbol{k}) = \frac{\hbar^2(-i\boldsymbol{\nabla} + \boldsymbol{k})^2}{2m} + V(\boldsymbol{r})$$

Berry phase $$\phi_B = \oint_\gamma \boldsymbol{\mathcal{A}}(\boldsymbol{k}) \cdot \mathrm{d}\boldsymbol{k}$$

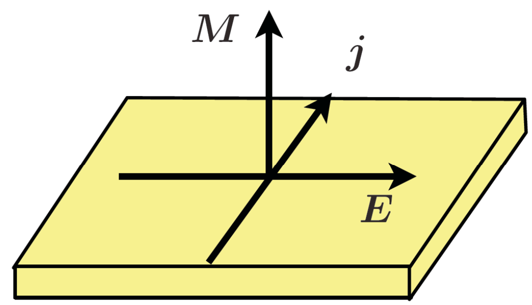
k-space gauge field $$\boldsymbol{\mathcal{A}}_n(\boldsymbol{k}) = i\langle u_{n\boldsymbol{k}} | \boldsymbol{\nabla}_{\boldsymbol{k}} u_{n\boldsymbol{k}} \rangle$$

Berry curvature $$\boldsymbol{\Omega}_n = \boldsymbol{\nabla}_k \times \boldsymbol{\mathcal{A}}_n(\boldsymbol{k}) = \boldsymbol{\nabla}_k \times \langle u_n(\boldsymbol{k}) | i\boldsymbol{\nabla}_{\boldsymbol{k}} | u_n(\boldsymbol{k}) \rangle$$

The intrinsic anomalous Hall effect

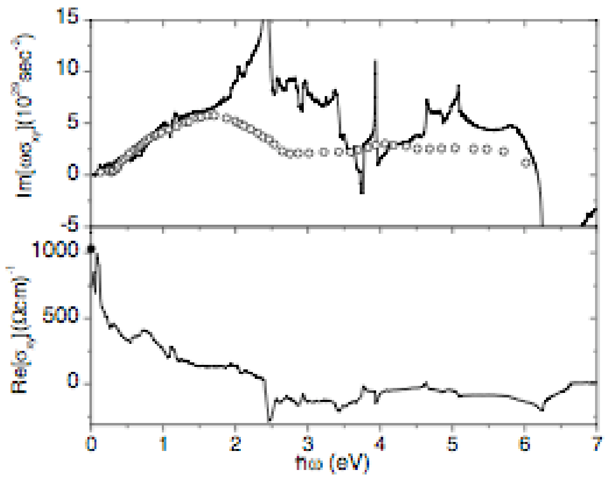
Hall effect in ferromagnets

$$\rho_{xy} = R_0 B + (4\pi M) R_s$$



Intrinsic contribution

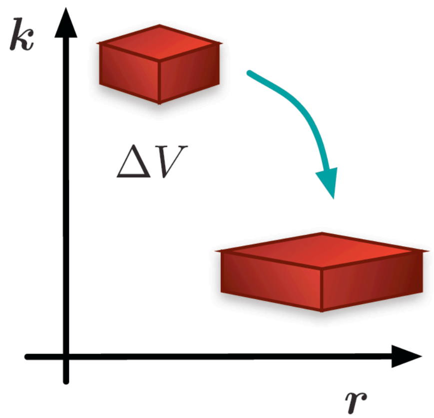
$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} + e\boldsymbol{E}\times\boldsymbol{\Omega}(\boldsymbol{k})$$



$$\boldsymbol{j}_{AH} = -\frac{e^2}{\hbar}\boldsymbol{E}\times\int\frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{\Omega}(\boldsymbol{k})$$

Karplus & Luttinger PR (1954); Onoda & Nagaosa, JPSJ (2001); Jungwirth, *et al*, PRL (2002); Fang, *et al*, Science (2003); Yao, *et al*, PRL (2004); Zeng, *et al*, PRL (2006)

Evolution of the phase-space volume



Volume element $\Delta V = \Delta \boldsymbol{r} \Delta \boldsymbol{k}$

Conservation of phase space volume

$$\frac{1}{\Delta V}\frac{d\Delta V}{dt} = \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \boldsymbol{\nabla}_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}} = 0$$

With the Berry curvature field $\frac{1}{\Delta V}\frac{d\Delta V}{dt} \neq 0$

$$\boxed{\Delta V = \frac{\Delta V_0}{1 + (e/\hbar)\boldsymbol{B}(\boldsymbol{r}) \cdot \boldsymbol{\Omega}(\boldsymbol{k})}}$$

Non-uniform phase space

Phase space volume of a quantum state

$$(2\pi)^d \quad \Rightarrow \quad \frac{(2\pi)^d}{1+(e/\hbar)\boldsymbol{B}\cdot\boldsymbol{\Omega}}$$

Statistical physics - Phase-space measure

$$D(\boldsymbol{r},\boldsymbol{k}) = \frac{1}{(2\pi)^d} \quad \Rightarrow \quad D(\boldsymbol{r},\boldsymbol{k}) = \frac{1}{(2\pi)^d}(1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})$$

Physical quantity

$$\langle\mathcal{O}\rangle = \int d\boldsymbol{r}d\boldsymbol{k}\, D(\boldsymbol{r},\boldsymbol{k})\mathcal{O}(\boldsymbol{r},\boldsymbol{k})f(\boldsymbol{r},\boldsymbol{k})$$

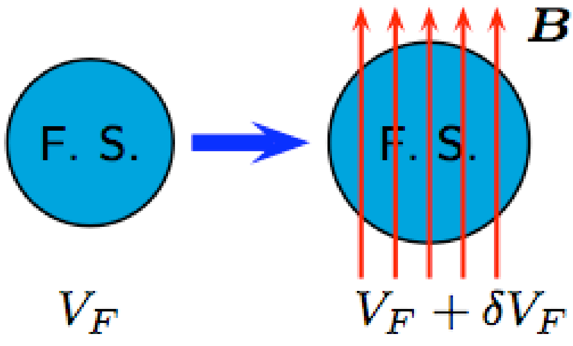
$f(\boldsymbol{r},\boldsymbol{k})$ - Distribution function

Fermi volume and Streda formula

Fermi sea volume

$$n = \int_{V_F+\delta V_F} \frac{d\boldsymbol{k}}{(2\pi)^d}\left(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}\right)$$

$$\delta V_F = -\frac{e}{\hbar}\int_{V_F} \frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{B}\cdot\boldsymbol{\Omega}$$



Streda formula

$$\sigma_{xy} = -e\left(\frac{\partial n}{\partial B}\right)_\mu = -\frac{e^2}{\hbar}\int \frac{d\boldsymbol{k}}{(2\pi)^d}\Omega_z(\boldsymbol{k})$$

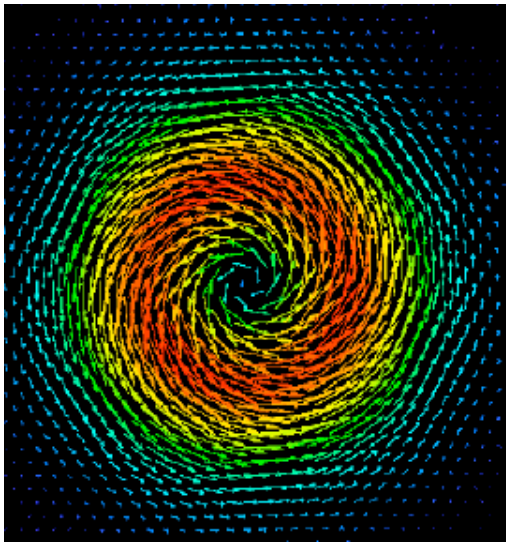
$$= -\frac{e^2}{\hbar}\int_{BZ} \frac{d\boldsymbol{k}}{(2\pi)^2} i\left[\left\langle \frac{\partial u}{\partial k_x}\middle|\frac{\partial u}{\partial k_y}\right\rangle - \left\langle \frac{\partial u}{\partial k_y}\middle|\frac{\partial u}{\partial k_x}\right\rangle\right]$$

Thouless *et al*, PRL (1982)

Orbital magnetization

Formal definition

$$\boldsymbol{M} = -\frac{e}{2}\langle \boldsymbol{r} \times \boldsymbol{v} \rangle$$



A rotating wave packet

$$\begin{aligned} \boldsymbol{m}(\boldsymbol{k}) &= -\frac{e}{2}\langle W|(\hat{\boldsymbol{r}} - \boldsymbol{r}_c) \times \boldsymbol{v}|W\rangle \\ &= -i\frac{e}{2\hbar}\langle \boldsymbol{\nabla}_{\boldsymbol{k}} u| \times (\hat{H} - \varepsilon_{\boldsymbol{k}})|\boldsymbol{\nabla}_{\boldsymbol{k}} u\rangle \end{aligned}$$

Correction to electron energy

$$\tilde{\varepsilon} = \varepsilon(\boldsymbol{k}) - \boldsymbol{m}(\boldsymbol{k}) \cdot \boldsymbol{B}$$

Does this mean the magnetization is

$$\boldsymbol{M} = \int \frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{m}(\boldsymbol{k}) \qquad ?$$

Thermodynamic derivation

Thermodynamic definition

$$\boldsymbol{M} = -\left(\frac{\partial F}{\partial \boldsymbol{B}}\right)_{\mu,T}$$

Free energy

$$F = -\frac{1}{\beta}\sum_{\boldsymbol{k}} \log(1 + e^{-\beta(\tilde{\varepsilon}-\mu)})$$
$$= -\frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^d}(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})(1 + e^{-\beta(\varepsilon - \boldsymbol{B}\cdot\boldsymbol{m}(\boldsymbol{k})-\mu)})$$

Orbital magnetization

$$\boldsymbol{M}(\boldsymbol{r}) = \int \frac{d\boldsymbol{k}}{(2\pi)^d} f(\boldsymbol{r},\boldsymbol{k})\boldsymbol{m}(\boldsymbol{k})$$
$$+ \frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})\log(1 + e^{-\beta(\varepsilon-\mu)})$$

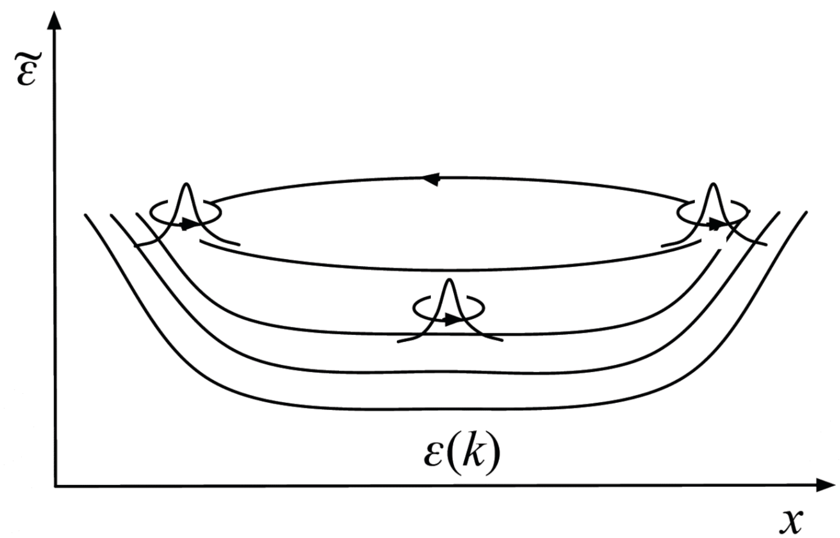
T=0 formula also obtained by Thonhauser *et al.* PRL (2005)

Contribution to the magnetization

- Self-rotation: $\boldsymbol{m}(\boldsymbol{k})$
- Center-of-mass motion: $\boldsymbol{\Omega}(\boldsymbol{k})$

Anomalous velocity
at boundary

$$\boldsymbol{v} = \frac{1}{\hbar}\boldsymbol{\nabla} V \times \boldsymbol{\Omega}(\boldsymbol{k})$$



$$M_z = \int_{V_F} \frac{d\boldsymbol{k}}{(2\pi)^d}\left[\boldsymbol{m}(\boldsymbol{k}) + \frac{e}{\hbar}\boldsymbol{\Omega}(\mu - \varepsilon_{\boldsymbol{k}})\right]$$

Linear magnetoresistance

Density of states at Fermi surface

$$\rho(\mu, B) = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \Big(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}\Big)\delta(\varepsilon(\boldsymbol{k}) - \boldsymbol{B}\cdot\boldsymbol{m}(\boldsymbol{k}) - \mu)$$

Linear magnetoresistance

$$\sigma_{xx} = e^2\rho(\mu, B)v_F^2(\mu, B)\tau(\mu, B)$$

$$v_F(\mu, B) = \frac{v_F^0(\mu) - \boldsymbol{B}\cdot[\partial\boldsymbol{m}(k_F)/\partial k_F]}{1 + (e/\hbar)\boldsymbol{B}\cdot\boldsymbol{\Omega}}$$

$$\frac{1}{\tau} = \int \frac{d\boldsymbol{k}'}{(2\pi)^d} \Big(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}\Big) W_{\boldsymbol{k}\boldsymbol{k}'}\Big(1 - \frac{\boldsymbol{k}\cdot\boldsymbol{k}'}{k^2}\Big)$$

Non-commutative quantum mechanics

Commutators

$$[\hat{x}, \hat{k}_x] = [\hat{y}, \hat{k}_y] = i\frac{1}{1+(e/\hbar)B\Omega}$$

$$[\hat{x}, \hat{y}] = i\frac{\Omega}{1+(e/\hbar)B\Omega}\,, \qquad [\hat{k}_x, \hat{k}_y] = -i\frac{(e/\hbar)B}{1+(e/\hbar)B\Omega}$$

Density of states enters the commutators

Uncertain volume in phase space

$$\min(\Delta\boldsymbol{r}\Delta\boldsymbol{k}) \propto \det|\mathrm{commut.}|^{-1/2} = (1+\frac{e}{\hbar}B\Omega)^{-1}$$

The origin of the non-commutativity

Peierls substitution

$$\boldsymbol{k} = \boldsymbol{q} + \frac{e}{\hbar}\boldsymbol{A}(\boldsymbol{r})$$

$$\boldsymbol{r} = \boldsymbol{R} + \boldsymbol{\mathcal{A}}(\boldsymbol{k})$$

$$[k_x, k_y] = -i\frac{eB}{\hbar}$$

$$[\hat{x}, \hat{y}] = i\Omega$$

Projection to a single band

$$\mathcal{P}_n \equiv \sum_{\boldsymbol{k}} |\psi_{n\boldsymbol{k}}\rangle\langle\psi_{n\boldsymbol{k}}|$$

$$[\mathcal{P}_n x \mathcal{P}_n, \mathcal{P}_n y \mathcal{P}_n] = i\Omega$$

General formula in the phase space

Phase space coordinates $\xi = (\boldsymbol{r}, \boldsymbol{k})$

Lagrangian $L = \frac{1}{2}\dot{\xi}^a J_{ab} \xi^b - \varepsilon(\boldsymbol{\xi}) + \dot{\xi}^a \mathcal{A}_a(\boldsymbol{\xi})$ $\quad \mathbf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Gauge field $\mathcal{A}_a(\boldsymbol{\xi}) \equiv i\langle u(\boldsymbol{\xi}) | \nabla_a u(\boldsymbol{\xi})\rangle$

Equation of motion $(\boldsymbol{\Omega} - \mathbf{J})_{ab}\dot{\xi}^b = \partial_a \varepsilon(\boldsymbol{\xi})$

Berry curvature $\Omega_{ab} = \partial_a \mathcal{A}_b - \partial_b \mathcal{A}_a$

Commutator $[\hat{\xi}^a, \hat{\xi}^b] = iM_{ab}$ $\quad \mathbf{M} = (\boldsymbol{\Omega} - \mathbf{J})^{-1}$

Summary

- In the presence of both the magnetic field and Berry curvature, the phase space becomes nonuniform
- Rich physical effects: Fermi sea volume, Streda formula, orbital magnetization, linear magnetoresistance…
- Non-commutative quantum mechanics