Berry Phase Effects on Charge and Spin Transport

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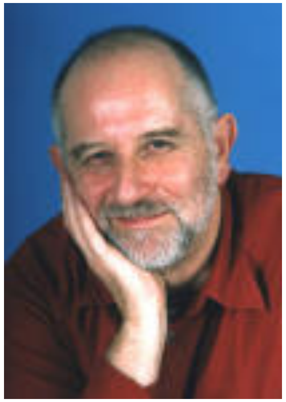
Outline

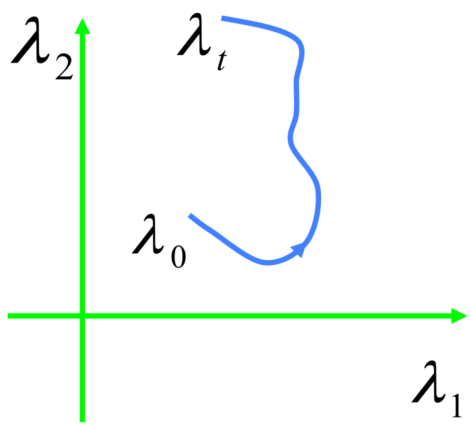
- Berry phase and its applications
- Berry curvature in space-time
  - Magnetic and electric like fields
  - e.g. Ferro-Josephson effect
- Berry curvature in momentum space
  - Anomalous velocities
  - e.g. Anomalous Hall effect
- Non-abelian generalization
  - Spin transport
  - Effective quantum theory
- Berry curvature in phase space
  - Polarization and Chern-Simons form
  - Polarization induced by magnetic field



Berry Phase

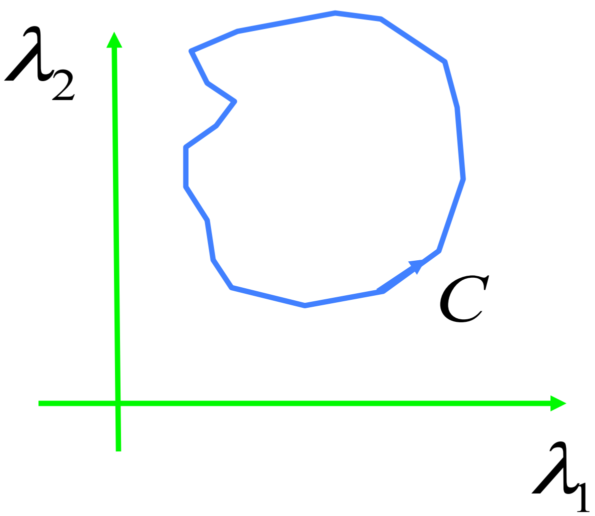
In the adiabatic limit: $$\Psi(t) = \psi_n(\lambda(t))\; e^{-i\int_0^t dt\, \varepsilon_n/\hbar}\; e^{-i\gamma_n(t)}$$

Geometric phase: $$\gamma_n = \int_{\lambda_0}^{\lambda_t} d\lambda \left\langle \psi_n \middle| i\frac{\partial}{\partial\lambda} \middle| \psi_n \right\rangle$$



Well defined for a closed path

$$\gamma_n = \oint_C d\lambda \left\langle \psi_n \middle| i \frac{\partial}{\partial \lambda} \middle| \psi_n \right\rangle$$



Stokes theorem

$$\gamma_n = \iint d\lambda_1 d\lambda_2 \, \Omega$$

Berry Curvature

$$\Omega = i \frac{\partial}{\partial \lambda_1} \left\langle \psi \middle| \frac{\partial}{\partial \lambda_2} \middle| \psi \right\rangle - i \frac{\partial}{\partial \lambda_2} \left\langle \psi \middle| \frac{\partial}{\partial \lambda_1} \middle| \psi \right\rangle$$

Analogies

Berry curvature

$$\Omega(\vec{\lambda})$$

Magnetic field

$$B(\vec{r})$$

Berry connection

$$\langle\psi| i\frac{\partial}{\partial\lambda}|\psi\rangle$$

Vector potential

$$A(\vec{r})$$

Geometric phase

$$\oint d\lambda \langle\psi| i\frac{\partial}{\partial\lambda}|\psi\rangle = \iint d^2\lambda \;\; \Omega(\vec{\lambda})$$

Aharonov-Bohm phase

$$\oint dr\; A(\vec{r}) = \iint d^2r\; B(\vec{r})$$

Chern number

$$\oiint d^2\lambda \;\; \Omega(\vec{\lambda}) = \text{integer}$$

Dirac monopole

$$\oiint d^2r \;\; B(\vec{r}) = \text{integer}\; h/e$$

Applications

- Berry phase

    interference,

    energy levels,

    polarization in crystals

- Berry curvature

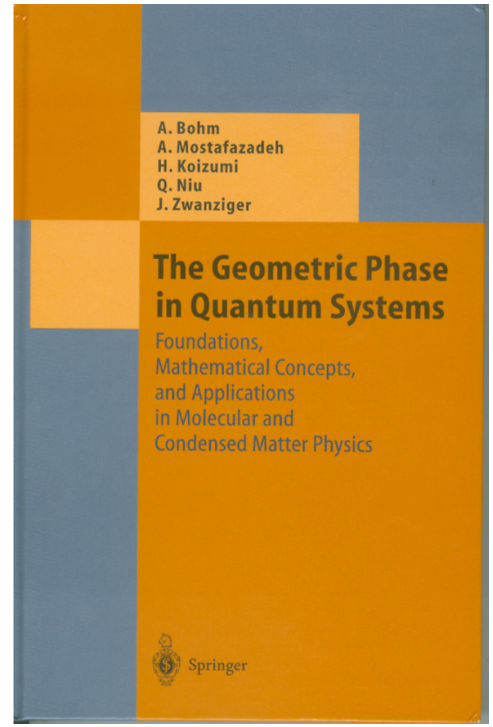
    spin dynamics,

    electron dynamics in Bloch bands

- Chern number

    quantum Hall effect,

    quantum charge pump



``Berry Phase Effects on Electronic Properties'',
by D. Xiao, M.C. Chang, Q. Niu,
Review of Modern Physics

Electron dynamics in phase space

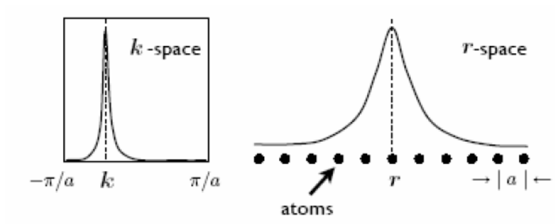
(Suderam and Niu 1999)

- Crystal under slowly varying perturbations

$$H[\boldsymbol{r}, \boldsymbol{p}; \beta_1(\boldsymbol{r}, t), \ldots \beta_g(\boldsymbol{r}, t)]$$

b can be gauge potentials of electromagnetic fields

- Local approximation and wave packet in a Bloch band



- Semiclassical dynamics of center of mass (charge)

$$\dot{\boldsymbol{r}}_c = \frac{\partial \varepsilon}{\partial \boldsymbol{q}_c} - (\overleftrightarrow{\Omega}_{\boldsymbol{qr}} \cdot \dot{\boldsymbol{r}}_c + \overleftrightarrow{\Omega}_{\boldsymbol{qq}} \cdot \dot{\boldsymbol{q}}_c) - \boldsymbol{\Omega}_{\boldsymbol{q}t} \ ,$$

$$\dot{\boldsymbol{q}}_c = -\frac{\partial \varepsilon}{\partial \boldsymbol{r}_c} + (\overleftrightarrow{\Omega}_{\boldsymbol{rr}} \cdot \dot{\boldsymbol{r}}_c + \overleftrightarrow{\Omega}_{\boldsymbol{xq}} \cdot \dot{\boldsymbol{q}}_c) + \boldsymbol{\Omega}_{\boldsymbol{r}t}$$

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Adiabatic pumping

$$\dot{\mathbf{r}} = \frac{\partial \mathcal{E}}{\hbar \partial \mathbf{k}} - (\Omega_{\mathbf{kr}} \cdot \dot{\mathbf{r}} + \Omega_{\mathbf{kk}} \cdot \dot{\mathbf{k}}) + \boldsymbol{\Omega}_{\mathbf{k}t}$$

$$\dot{\mathbf{k}} = -\frac{\partial \mathcal{E}}{\hbar \partial \mathbf{r}} + (\Omega_{\mathbf{rr}} \cdot \dot{\mathbf{r}} + \Omega_{\mathbf{rk}} \cdot \dot{\mathbf{k}}) + \boldsymbol{\Omega}_{\mathbf{r}t}$$

due to time dependence in the Hamiltonian, lead to pumping effects

charge pumping in a 1D band insulator

$$Q = \int_0^T dt\ j_x = e \int_0^T dt \int_{\mathrm{BZ}} \frac{dk_x}{2\pi}\ \Omega_{k_x t} = e\ Z$$

integral of curvature over a closed surface must be quantized

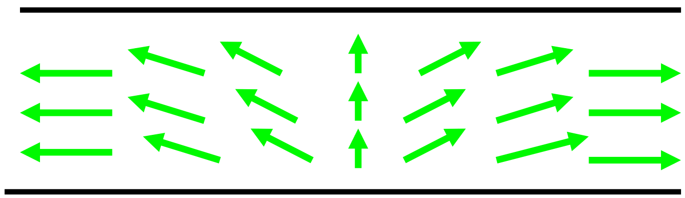
pumps an emf

$$\mathcal{E} = -\frac{\hbar}{e} \int_l d\mathbf{r} \cdot \boldsymbol{\Omega}_{\mathbf{r}t}$$

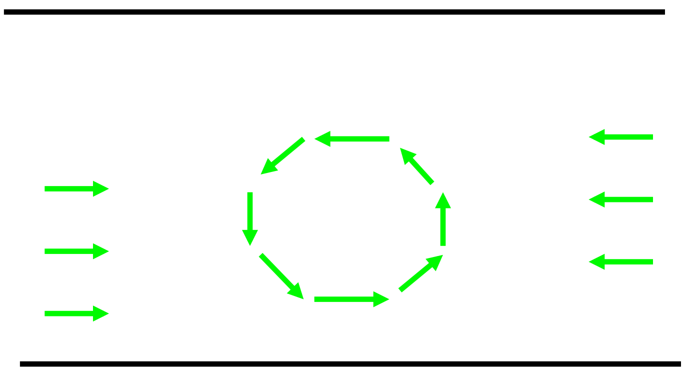
Is there a similar quantization relation?

Thouless, *PRB (1983)*

Texture in Ferromagnets



Transverse domainwall



Vortex domainwall

The domainwall can also be made to move.

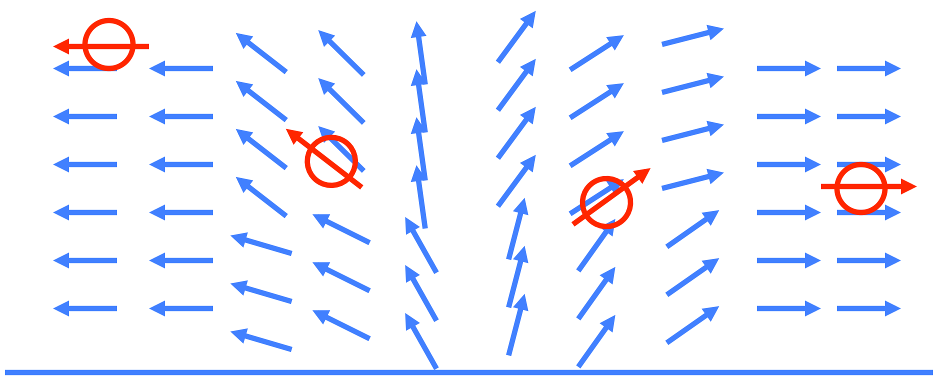
Interplay Between Electric Current and Domain Wall Dynamics

- **Electrical resistance of domain wall**
  - J. F. Gregg et. al., PRL **77**, 1580 (1996)
  - U. Ebels et. al., PRL **84**, 983 (2000)
- **Electric current can drive domain wall motion.**
  - A. Yamaguchi et. al. PRL 92, 077205 (2004)
  - G. S. D. Beach et. al. PRL 97, 057203 (2006)
  - M. Hayashi et. al. PRL 96, 197207 (2006)
- **Domain wall motion drives electrons**
  - L. Berger, PRB 33, 1572 (1986)
  - S. E. Barnes et. al., APL 89, 122507 (2006); PRL 98, 246601 (2007)
  - R. A. Duine, PRB 77, 014409 (2008)
  - W. M. Saslow, PRB 76, 184434 (2007)

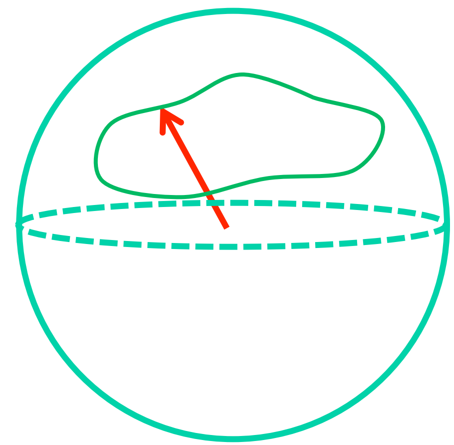
Berry curvature field

s-d coupling

$$H = H_0[\mathbf{q} + (e/\hbar)\mathbf{A}(\mathbf{r},t)] - J\mathbf{n}(\mathbf{r},t)\cdot\boldsymbol{\sigma} - \mathbf{h}\cdot\boldsymbol{\sigma}$$



Berry phase



- **Effective magnetic field on conduction electrons**

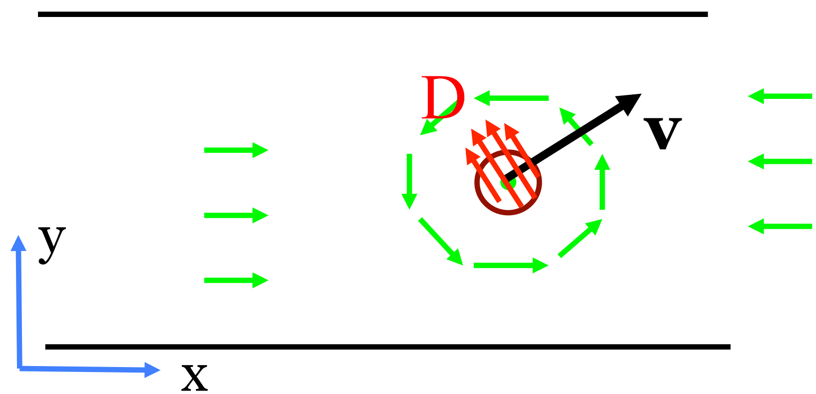
$$\mathbf{C}(\mathbf{r},t) \equiv \frac{1}{2}\sin\theta\,(\nabla\theta\times\nabla\phi)$$

Effective Force Field

- **If domain wall moves**

$$\mathbf{D}(\mathbf{r},t) \equiv \frac{1}{2}\sin\theta\left(\frac{\partial\phi}{\partial t}\nabla\theta - \frac{\partial\theta}{\partial t}\nabla\phi\right)$$

G. E. Volovik, J. Phys. C 20, L83 (1987)



- **Effective magnetic and electric forces**

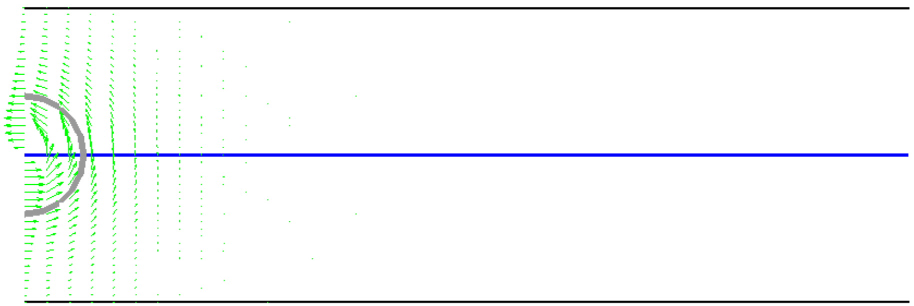
$$\dot{\mathbf{r}} = \frac{\partial \mathcal{E}_0}{\hbar\partial\mathbf{k}},$$

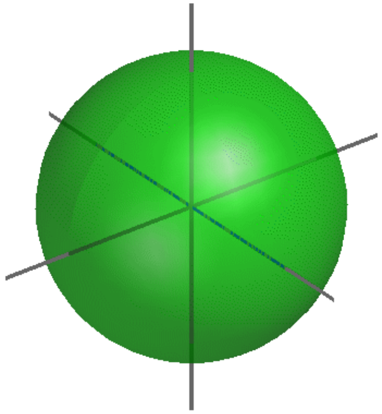
$$\dot{\mathbf{k}} = \frac{\partial K}{\hbar\partial\mathbf{r}} - \frac{e}{\hbar}\dot{\mathbf{r}}\times\mathbf{B} - \dot{\mathbf{r}}\times\mathbf{C} - \mathbf{D}$$

- **Longitudinal voltage due to transverse motion of vortex**
  ferro-Josephson effect

$$\boxed{V_x = \pi\frac{\hbar}{e}\frac{v_y}{w}} \rightarrow \bar{V}_x = \frac{\hbar}{e}2\pi f_y$$

Topology of the vortex motion





Experimental measurement

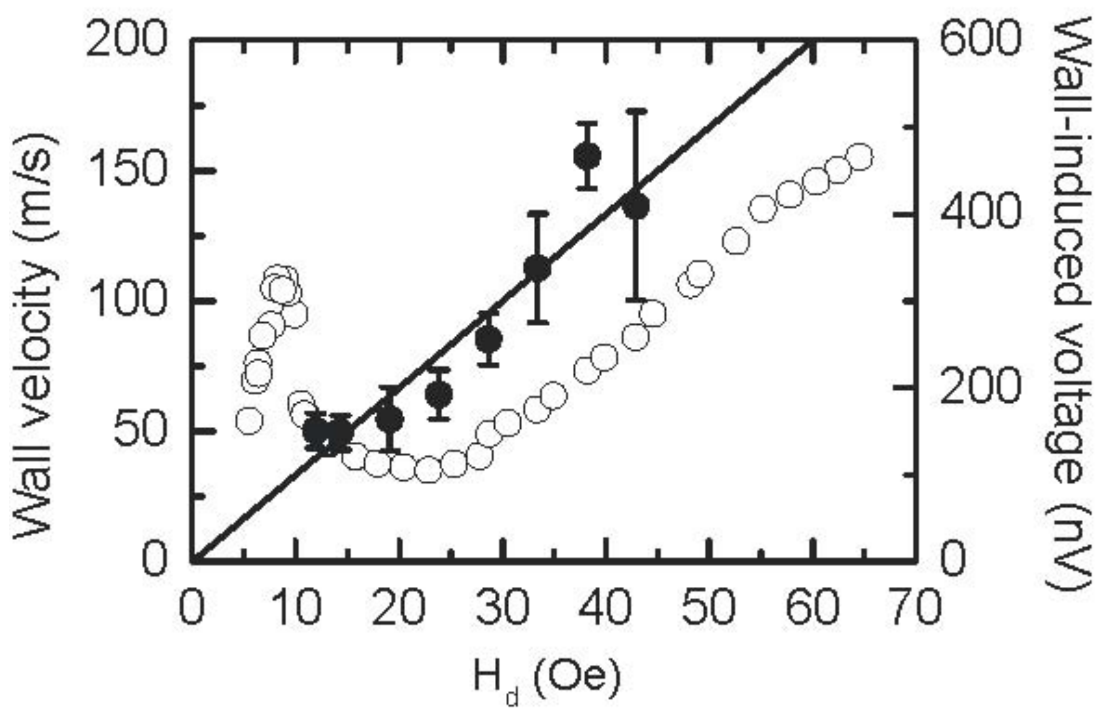
G.S.D. Beach, M. Tsoi, and J. L. Erskine

- **The frequency of transverse motion**

M. Hayashi, et al. Nature Physics (2007)
J.-Y. Lee, et al. cond-mat/07062542 (2007)

$$2\pi f_y = \gamma H$$

$$\boxed{\bar{V}_x = \frac{\hbar}{e}\gamma H}$$



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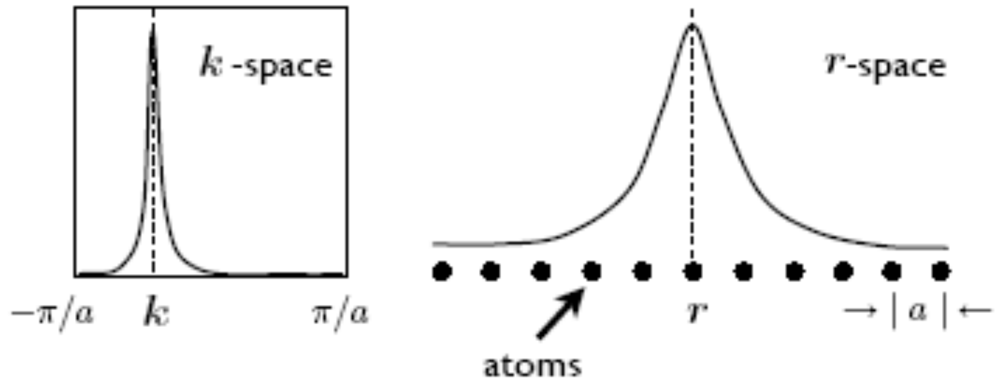
Semiclassical Equations of Motion

Wave-packet Dynamics

(r, k)



G. Sundaram and Q. Niu, PRB **59**, 14915 (1999)

Nonzero if either time-reversal or inversion symmetry is broken

$$\boxed{\begin{aligned} \dot{r} &= \frac{\partial \varepsilon_n(k)}{\hbar \partial k} - \dot{k} \times \Omega_n(k) \\ \hbar \dot{k} &= -eE(r) - e\dot{r} \times B(r) \end{aligned}}$$

Berry Curvature

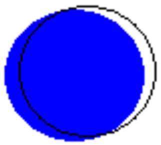
$$\Omega_n(k) = \mathrm{i}\langle \nabla_{\boldsymbol{k}} u_n(k) | \times | \nabla_{\boldsymbol{k}} u_n(k) \rangle$$

Symmetry properties

- time reversal: $\boldsymbol{\Omega}(-\mathbf{k}) = -\boldsymbol{\Omega}(\mathbf{k})$
- space inversion: $\boldsymbol{\Omega}(-\mathbf{k}) = \boldsymbol{\Omega}(\mathbf{k})$
- both: $\boldsymbol{\Omega}(\mathbf{k}) = 0$
- violation: ferromagnets, asymmetric crystals

Anomalous Hall effect

- velocity $\quad \dot{\mathbf{x}} = \dfrac{\partial \mathcal{E}}{\partial \mathbf{k}} + e\mathbf{E} \times \mathbf{\Omega},$
- distribution $\quad \mathrm{g}(\mathbf{k}) = \mathrm{f}(\mathbf{k}) + \delta\mathrm{f}(\mathbf{k})$

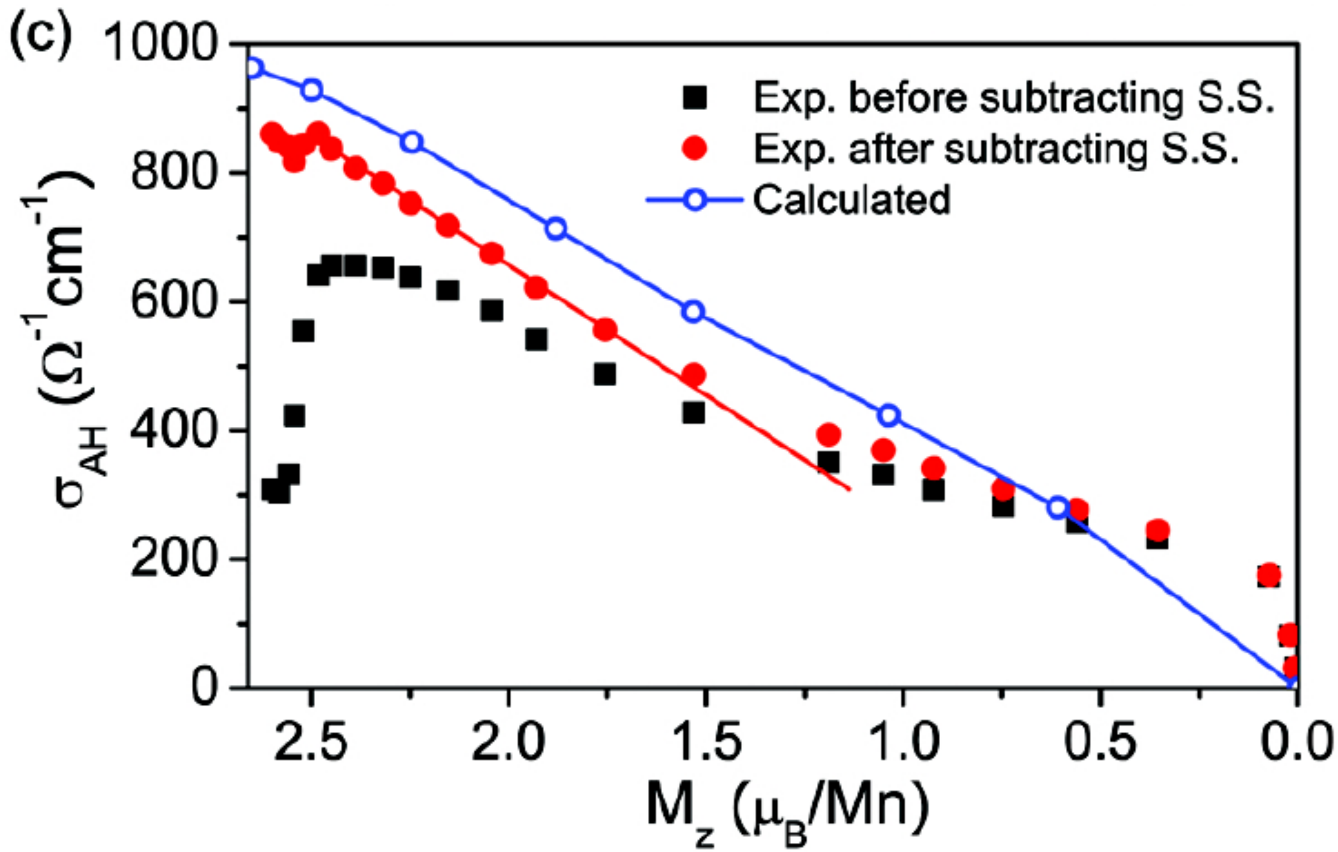


- current $\quad -e^2\,\mathbf{E} \times \int d^3\mathbf{k}\ \mathrm{f}(\mathbf{k})\,\mathbf{\Omega} - e \int d^3\mathbf{k}\ \delta\mathrm{f}(\mathbf{k})\,\dfrac{\partial \mathcal{E}}{\partial \mathbf{k}}$

Intrinsic

Experiment

Mn5Ge3 : Zeng, Yao, Niu & Weitering, PRL 2006



Intrinsic AHE in other ferromagnets

- Semiconductors, $Mn_xGa_{1-x}As$
  - Jungwirth, Niu, MacDonald , PRL (2002) , J Shi's group (2008)
- Oxides, $SrRuO_3$
  - Fang et al, Science , (2003).
- Transition metals, Fe
  - Yao et al, PRL (2004),Wang et al, PRB (2006), X.F. Jin's group (2008)
- Spinel, $CuCr_2Se_{4-x}Br_x$
  - Lee et al, Science, (2004)

Honeycomb with Asymmetry

MoS2, etc.

- Energy bands

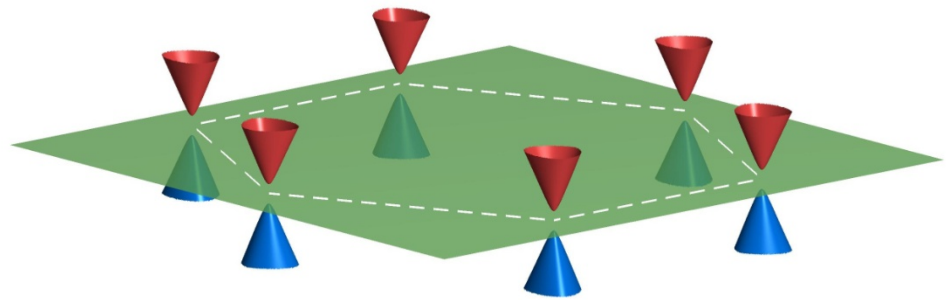
$$\varepsilon(q) = \pm\sqrt{\Delta^2 + 3t^2q^2/4}$$

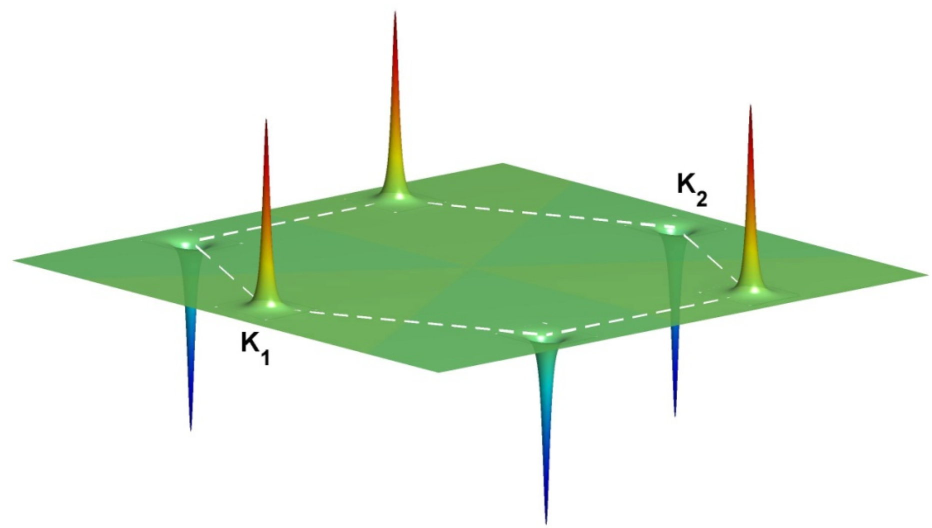
- Berry curvature

$$\Omega(q) = \pm\tau_z \frac{3a^2\Delta t^2}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}}$$

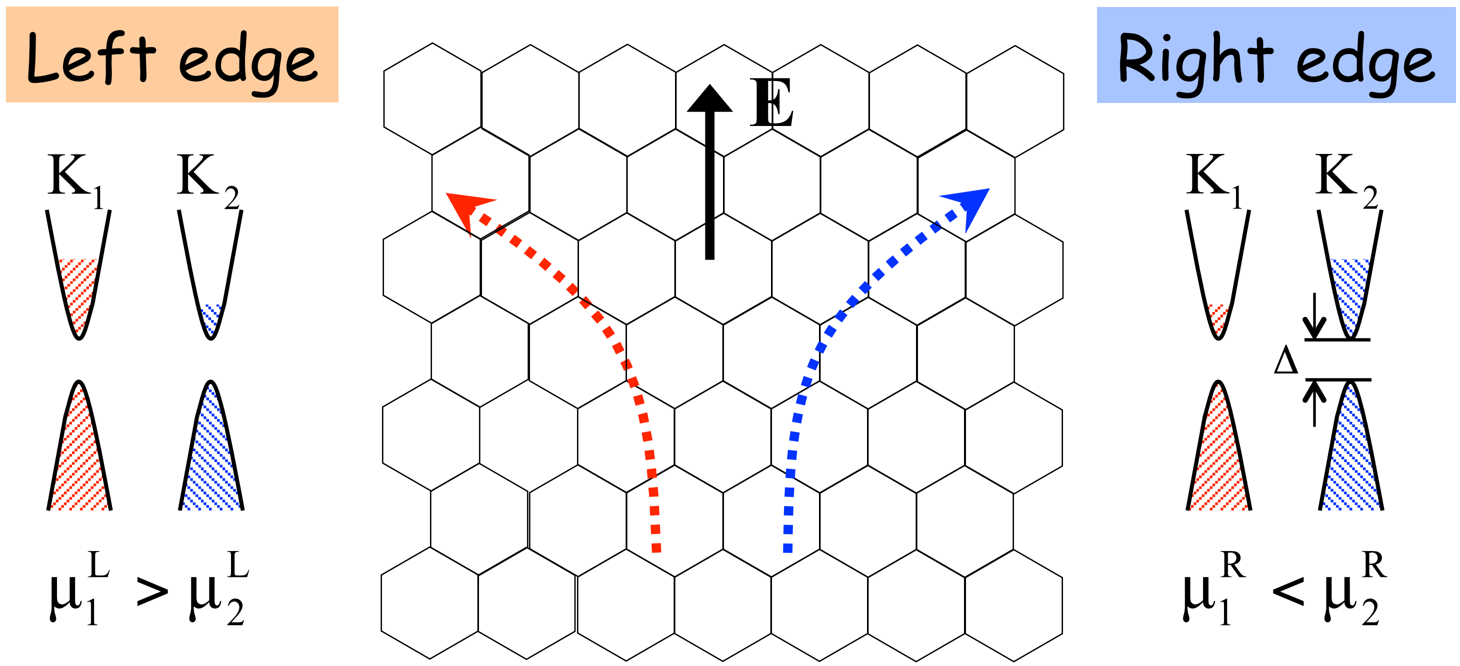
- Orbital moment

$$m(q) = \frac{e}{\hbar}\varepsilon(q)\Omega(q)$$





Valley Hall Effect
And edge magnetization



Valley polarization induced on side edges

Edge magnetization:

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Degenerate bands

- Internal degree of freedom η
- Non-abelian Berry curvature $\mathcal{F}$
- Non-abelian Berry connection $\mathcal{R}$
- Magnetic moment $\dfrac{e}{2m}\mathcal{L}$

$$\hbar \dot{\mathbf{k}}_c = -e\mathbf{E} - e\dot{\mathbf{r}}_c \times \mathbf{B},$$

$$\hbar \dot{\mathbf{r}}_c = \frac{1}{\mathrm{i}}\eta^\dagger \left[\mathrm{i}\frac{\partial}{\partial \mathbf{k}_c} + \mathcal{R}, \mathcal{H} \right] \eta - \hbar \dot{\mathbf{k}}_c \times \eta^\dagger \mathcal{F} \eta,$$

$$\mathrm{i}\hbar \dot{\eta} = \left(\frac{e}{2m}\mathcal{L}\cdot\mathbf{B} - \hbar \dot{\mathbf{k}}_c \cdot \mathcal{R} \right) \eta,$$

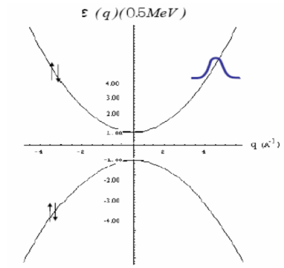
Cucler, Yao & Niu, PRB, 2005
Shindou & Imura, Nucl. Phys. B, 2005
Chang & Niu, 2008 (review)

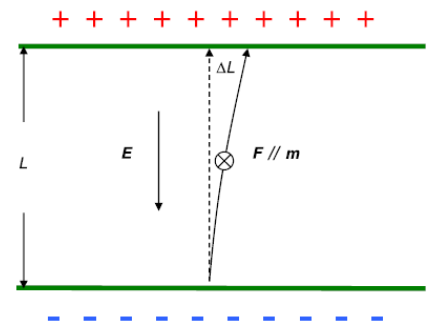
Applications

- Dirac bands

$$\mathcal{R} = \frac{\lambda_c^2}{2\gamma(\gamma+1)}\mathbf{q}\times\boldsymbol{\sigma},$$

$$\mathcal{F} = -\frac{\lambda_c^2}{2\gamma^3}\left(\boldsymbol{\sigma} + \lambda_c^2\frac{\mathbf{q}\cdot\boldsymbol{\sigma}}{\gamma+1}\mathbf{q}\right)$$





- Semiconductor bands

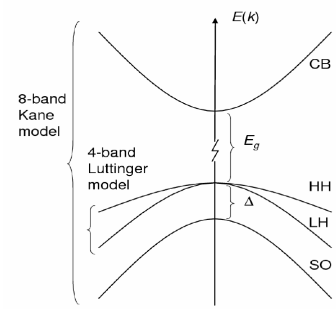


TABLE I: Berry connection, Berry curvature, and orbital angular momentum of the wavepacket in three disjoint subspaces of the 8-band Kane model. Only the leading order (in k) terms are shown. E_g and Δ are the conduction-valence band gap and the spin-orbit gap. σ and J are the spin-1/2 and spin-3/2 angular momentum matrices, and $V = \hbar\langle S|p_x|X\rangle/m_0$.

	conduction band	HH-LH band	split-off band
$\mathcal{R}$	$\frac{V^2}{3}\left[\frac{1}{E_g^2}-\frac{1}{(E_g+\Delta)^2}\right]\sigma\times\mathbf{k}$	$-\frac{V^2}{3E_g^2}J\times\mathbf{k}$	$-\frac{V^2}{3}\frac{1}{(E_g+\Delta)^2}\sigma\times\mathbf{k}$
$\mathcal{F}$	$\frac{2V^2}{3}\left[\frac{1}{E_g^2}-\frac{1}{(E_g+\Delta)^2}\right]\sigma$	$-\frac{2V^2}{3E_g^2}J$	$-\frac{2V^2}{3}\frac{1}{(E_g+\Delta)^2}\sigma$
$\mathcal{L}$	$-\frac{2m_0}{3\hbar}V^2\left(\frac{1}{E_g}-\frac{1}{E_g+\Delta}\right)\sigma$	$-\frac{2m_0}{3\hbar}\frac{V^2}{E_g}J$	$-\frac{2m_0}{3\hbar}\frac{V^2}{E_g}\sigma$

Quantization of semiclassical dynamics

- Physical variables are not canonical
  - because of Berry curvature and magnetic field
- Canonical variables are not physical
  - Generalization of Peierls substitution
  - Gauge dependent

$$\mathbf{r} = \mathbf{r}_c - \mathbf{R}(\mathbf{k}_c) - \mathbf{G}(\mathbf{k}_c),$$

$$\mathbf{p} = \hbar\mathbf{k}_c - e\mathbf{A}(\mathbf{r}_c) - \frac{e}{2}\mathbf{B} \times \mathbf{R}(\mathbf{k}_c)$$

where $G_\alpha(\mathbf{k}_c) \equiv (e/\hbar)(\mathbf{R} \times \mathbf{B}) \cdot \partial\mathbf{R}/\partial k_{c\alpha}$.

M.C. Chang and QN (2008)

Effective Quantum Mechanics

- Wavepacket energy $\mathcal{H}(\mathbf{r}_c, \mathbf{k}_c) = E_0(\mathbf{k}_c) - e\phi(\mathbf{r}_c) + \frac{e}{2m}\boldsymbol{\mathcal{L}}(\mathbf{k}_c) \cdot \mathbf{B}$
- Energy in canonical variables

Spin-orbit

$$E(\mathbf{r}, \mathbf{p}) = E_0(\boldsymbol{\pi}) - e\phi(\mathbf{r}) + e\mathbf{E} \cdot \mathbf{R}(\boldsymbol{\pi}) + \frac{e}{2m}\mathbf{B} \cdot \left[\mathbf{L}(\boldsymbol{\pi}) + 2\mathbf{R} \times m\frac{\partial E_0}{\partial \boldsymbol{\pi}}\right].$$

$\pi = \mathrm{p} + e\mathbf{A}(\mathrm{r})$

Spin & orbital moment

Yafet term

- Quantum theory

[r, p] = ih/2p

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Polarization as a Berry Phase

- Thouless (1983): found adiabatic current in a crystal in terms of a Berry curvature in (k,t) space.

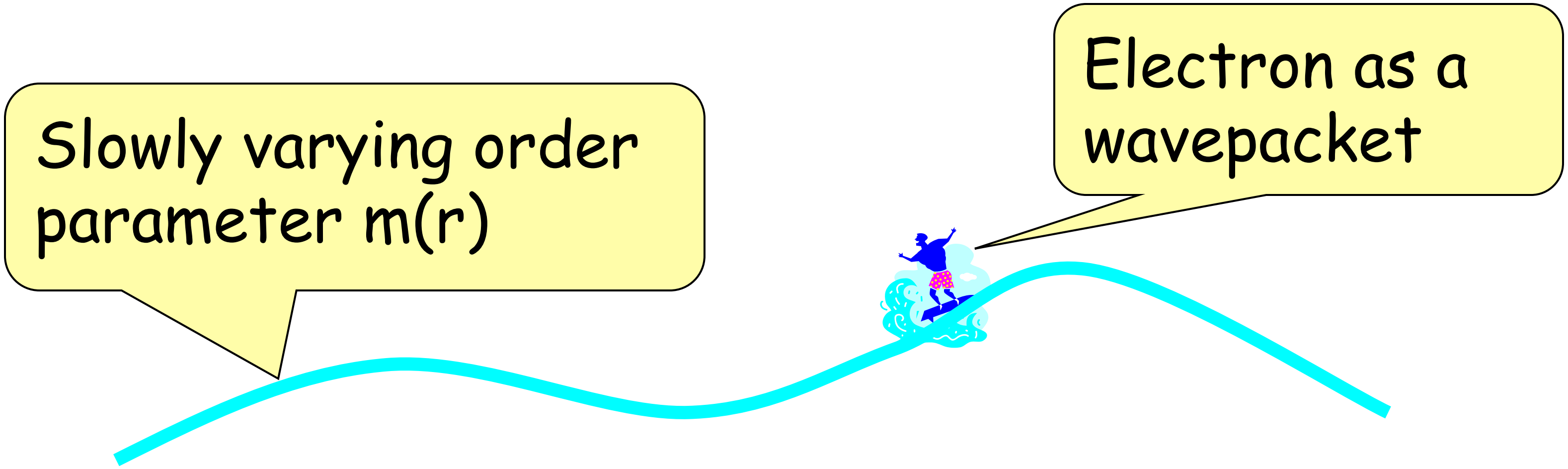
- King-Smith and Vanderbilt (1993):

$$\boxed{\boldsymbol{P} = e\int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d}\, i\left\langle u(\boldsymbol{k}) \middle| \frac{\partial u(\boldsymbol{k})}{\partial \boldsymbol{k}} \right\rangle \Bigg|_{\mathrm{intial}}^{\mathrm{final}}}$$

  » u(k): Bloch function amplitudes

- Led to great success in first principles calculations

Motion driven by inhomogeneity



Expand the wavepacket in the Bloch function basis of the local Hamiltonian $\mathcal{H}_c[\boldsymbol{m}(\boldsymbol{r}_c);\lambda]$

Find the semiclassical dynamics of the wavepacket center in the presence of inhomogeneity

Calculate the adiabatic current due to change in the control parameter and find the polarization

Semiclassical Dynamics

Equations of motion

$$\dot{r}_\alpha = \nabla^k_\alpha \varepsilon - \Omega^{kr}_{\alpha\beta}\dot{r}_\beta - \Omega^{kk}_{\alpha\beta}\dot{k}_\beta - \dot{\lambda}\Omega^{k\lambda}_\alpha ,$$
$$\dot{k}_\alpha = -\nabla^r_\alpha \varepsilon + \Omega^{rr}_{\alpha\beta}\dot{r}_\beta + \Omega^{rk}_{\alpha\beta}\dot{k}_\beta + \dot{\lambda}\Omega^{r\lambda}_\alpha$$

Berry connection
(vector potential)

$$\mathcal{A}^k_\alpha = \langle u|i\nabla^k_\alpha|u\rangle , \qquad \mathcal{A}^r_\alpha = \langle u|i\nabla^r_\alpha|u\rangle$$

Berry curvature
(magnetic field)

$$\Omega^{kr}_{\alpha\beta} = \nabla^k_\alpha \mathcal{A}^r_\beta - \nabla^r_\beta \mathcal{A}^k_\alpha$$

M.-C. Chang & QN, PRB (1996); G. Sundaram & QN, PRB (1999)

Polarization

Find adiabatic current for filled bands of electrons
and integrate

$$\boxed{\boldsymbol{P} = -e \int_{\mathrm{BZ}} d\boldsymbol{k} \int_0^T dt\, D(\boldsymbol{k}, \boldsymbol{r})\dot{\boldsymbol{r}}}$$

Density of states:

$$D(\boldsymbol{r}, \boldsymbol{k}) = \frac{1}{(2\pi)^d}(1 + \Omega^{kr}_{\alpha\alpha})$$

Di Xiao, Junren Shi & QN, PRL, 2005

$$P_\alpha = -e \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \int_0^T dt \Big[\nabla^k_\alpha \varepsilon + \Big(\Omega^{kr}_{\beta\beta} \nabla^k_\alpha \varepsilon - \Omega^{kr}_{\alpha\beta} \nabla^k_\beta \varepsilon + \Omega^{kk}_{\alpha\beta} \nabla^r_\beta \varepsilon \Big) - \dot{\lambda} \Omega^{k\lambda}_\alpha - \dot{\lambda} \Big(\Omega^{kr}_{\beta\beta} \Omega^{k\lambda}_\alpha - \Omega^{kr}_{\alpha\beta} \Omega^{k\lambda}_\beta + \Omega^{kk}_{\alpha\beta} \Omega^{r\lambda}_\beta \Big) \Big]$$

The 0th Order Contribution

- In the absence of inhomogeneity

$$P_\alpha^{(0)} = e \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \int_0^1 d\lambda \, \Omega_\alpha^{k\lambda}$$

- King-Smith and Vanderbilt (under periodic gauge):

$$P_\alpha^{(0)} = e \int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \mathcal{A}_\alpha^{k}$$

- Uncertain quantum: Berry phase is defined up to 2p:

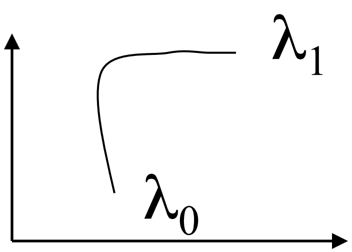
$$\Delta P_x^{(0)} = \frac{e}{a_y a_z}$$

The 1st Order Contribution
Xiao et al PRL 2009

- To 1st order in the gradient of order parameter

$$P_\alpha^{(1)} = e\int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d}\int d\lambda\left(\Omega^{kr}_{\beta\beta}\Omega^{k\lambda}_{\alpha} - \Omega^{kr}_{\alpha\beta}\Omega^{k\lambda}_{\beta} + \Omega^{kk}_{\alpha\beta}\Omega^{r\lambda}_{\beta}\right)$$

- Two-point formula:



$$P_\alpha^{(1)} = e\int_{\mathrm{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d}\left(\mathcal{A}^k_\alpha \nabla^r_\beta \mathcal{A}^k_\beta + \mathcal{A}^k_\beta \nabla^k_\alpha \mathcal{A}^r_\beta + \mathcal{A}^r_\beta \nabla^k_\beta \mathcal{A}^k_\alpha\right)\Big|_0$$

Chern-Simons field in (k_a, k_b, r_b) space

Electric Polarization by B field

- Treat vector potential in Hamiltonian as an inhomogeneity.
- Spatial derivative becomes k derivative

$$\boldsymbol{k} \rightarrow \boldsymbol{k} + e\boldsymbol{a} \qquad\qquad \partial_x \rightarrow \partial_x a_i \partial_{k_i}$$

$$\langle P_x^{(\mathrm{in})} \rangle = \frac{Be^2}{\hbar} \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\, \epsilon_{ijk}\, \mathrm{Tr}[\mathcal{A}_i \partial_j \mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i \mathcal{A}_j \mathcal{A}_k] \quad (6)$$

Polarziation induced by a magnetic field
PRL (2009): Essin, Moore, Vanderbilt

Conclusions

- Berry phase is a unifying concept
- Berry curvature in space-time
  - Electromagnetic like fields
  - e.g. Ferro-Josephson effect
- Berry curvature in momentum space
  - Anomalous velocities
  - e.g. Anomalous Hall effect
- Non-abelian generalization
  - Spin transport
  - Effective quantum theory
- Berry curvature in phase space
  - Polarization and Chern-Simons form
  - Polarization induced by magnetic field