Berry Phase Effects on Electronic Properties

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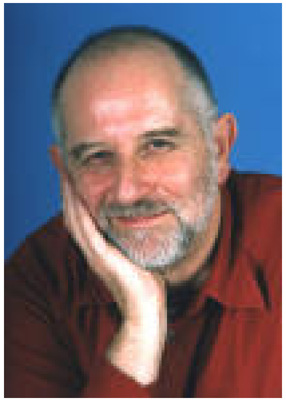
Outline

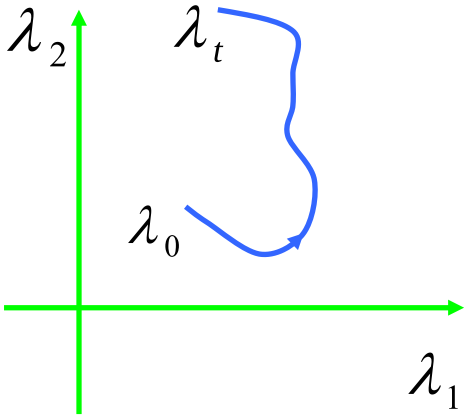
- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension
- Quantization of semiclassical dynamics
- Conclusion



Berry Phase

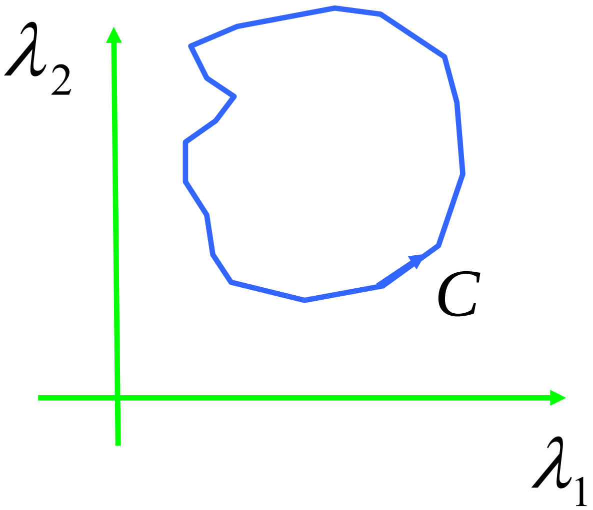
In the adiabatic limit: $\Psi(t) = \psi_n(\lambda(t))\; e^{-i\int_0^t dt\, \varepsilon_n/\hbar}\; e^{-i\gamma_n(t)}$

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



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

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

Berry connection

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

Geometric phase

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

Chern number

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

Magnetic field

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

Vector potential

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

Aharonov-Bohm phase

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

Dirac monopole

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

Applications

- Berry phase

  interference,

  energy levels,

  polarization in crystals

- Berry curvature

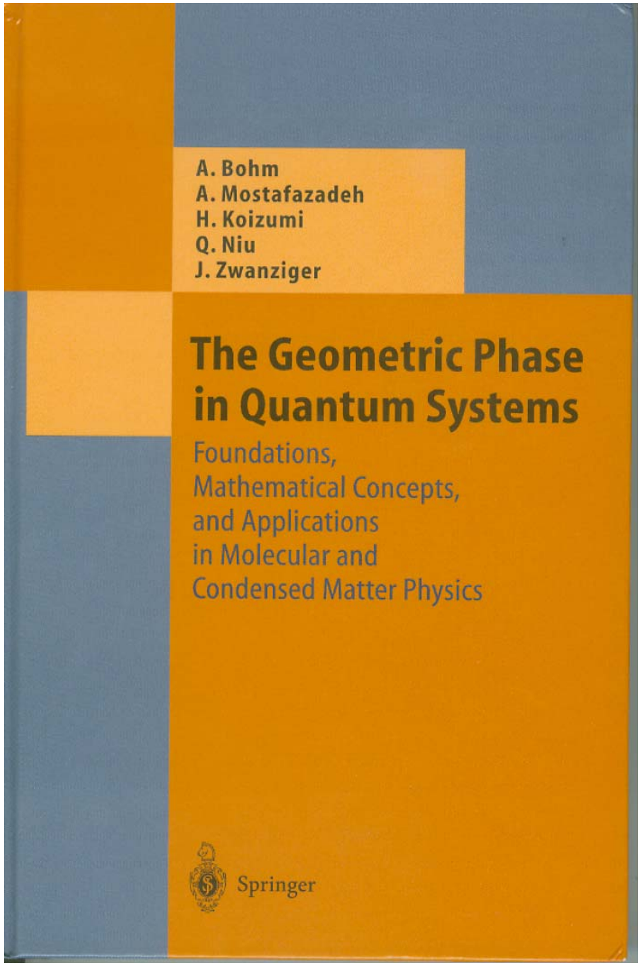
  spin dynamics,

  electron dynamics in Bloch bands

- Chern number

  quantum Hall effect,

  quantum charge pump



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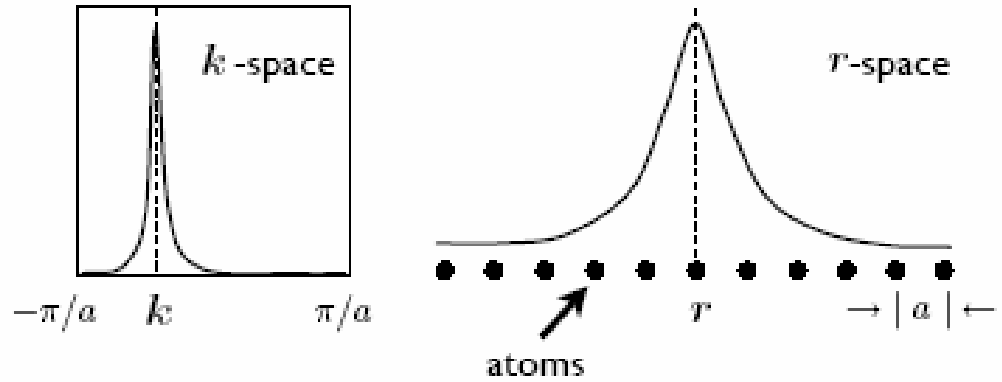
Semiclassical Equations of Motion

Wave-packet Dynamics

(r, k)



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

Nonzero if either time-reversal or inversion symmetry is broken

$$\dot{r} = \frac{\partial \varepsilon_n(k)}{\hbar \partial k} - \dot{k} \times \Omega_n(k)$$

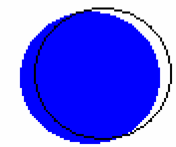
$$\hbar \dot{k} = -eE(r) - e\dot{r} \times B(r)$$

Berry Curvature

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

Anomalous Hall effect

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

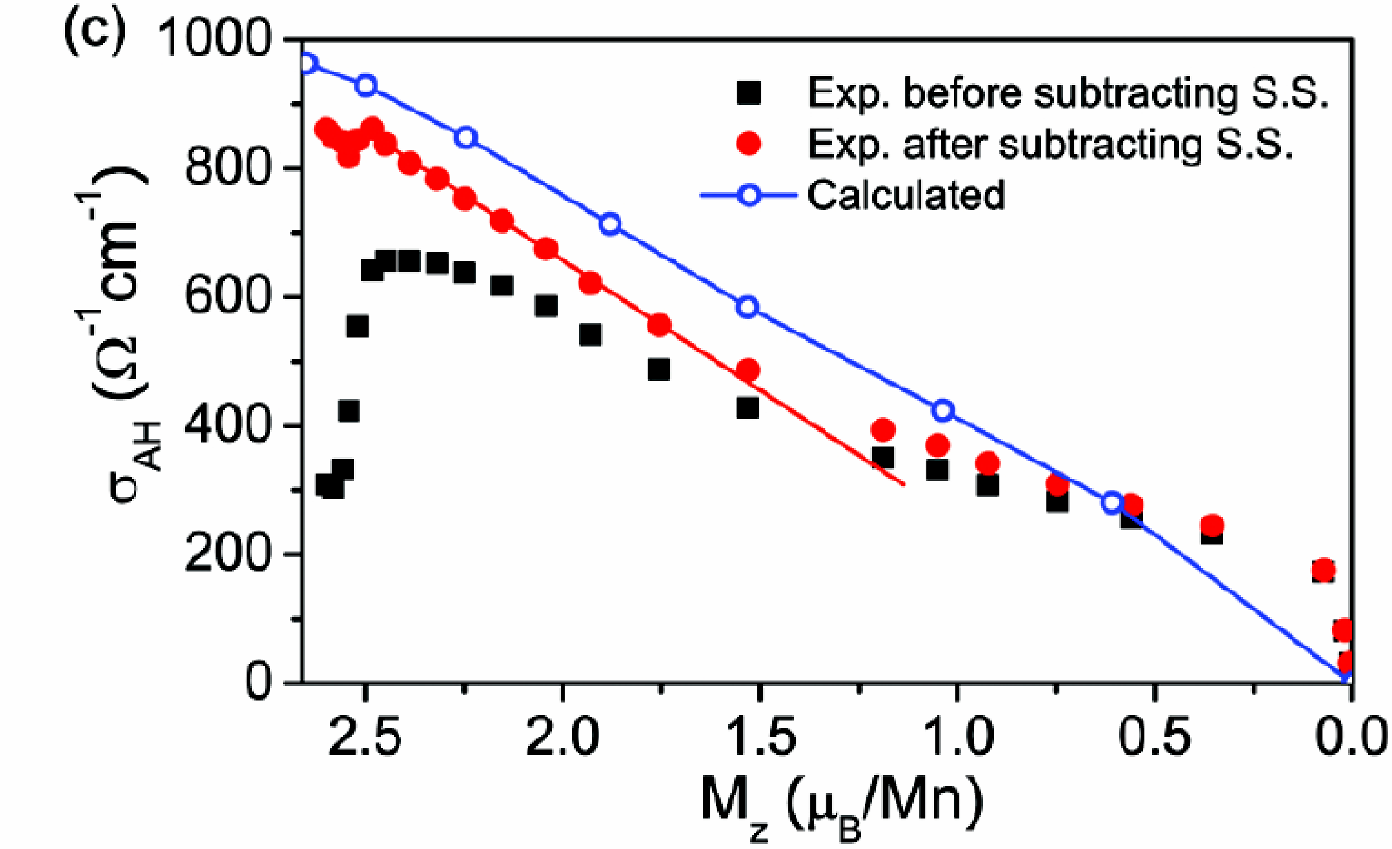


- current $$-e^2\,\mathbf{E}\times\int d^3\mathbf{k}\;\mathrm{f}(\mathbf{k})\,\mathbf{\Omega} - e\int d^3\mathbf{k}\;\delta\mathrm{f}(\mathbf{k})\,\frac{\partial \mathcal{E}}{\partial \mathbf{k}}$$

Intrinsic

Recent experiment

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



Intrinsic AHE in other ferromagnets

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

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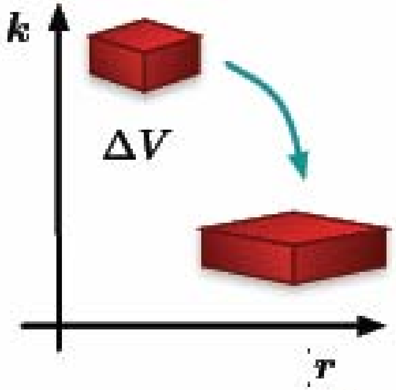
Phase Space Density of States



Evolution of a phase space volume

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

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

Liouville's theorem breaks down

Density of States

$$D_n(\boldsymbol{r}, \boldsymbol{k}) = (2\pi)^{-d}(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}_n)$$

Thermal dynamic quantity

$$\bar{Q} = \sum_n \int \mathrm{d}\boldsymbol{k}\, D_n(\boldsymbol{k}) f_n(\boldsymbol{k}) Q_n(\boldsymbol{k})$$

(homogenous system)

Orbital magnetization

Xiao et al, PRL 2005, 2006

Definition: $$\boldsymbol{M} = -\Big(\frac{\partial F}{\partial \boldsymbol{B}}\Big)_{\mu,T}$$

Free energy: $$F = -\frac{1}{\beta}\sum_{\boldsymbol{k}} \log(1 + e^{-\beta(\tilde{\varepsilon}-\mu)})$$

$$= -\frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^3}(1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})\log(1 + e^{-\beta(\tilde{\varepsilon}-\mu)})$$

Our Formula:

$$\boldsymbol{M}(\boldsymbol{r}) = \int \frac{d\boldsymbol{k}}{(2\pi)^3} f(\boldsymbol{r},\boldsymbol{k})\boldsymbol{m}(\boldsymbol{k}) + \frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})\log(1 + e^{-\beta(\varepsilon-\mu)})$$

Anomalous Thermoelectric Transport

- Berry phase correction

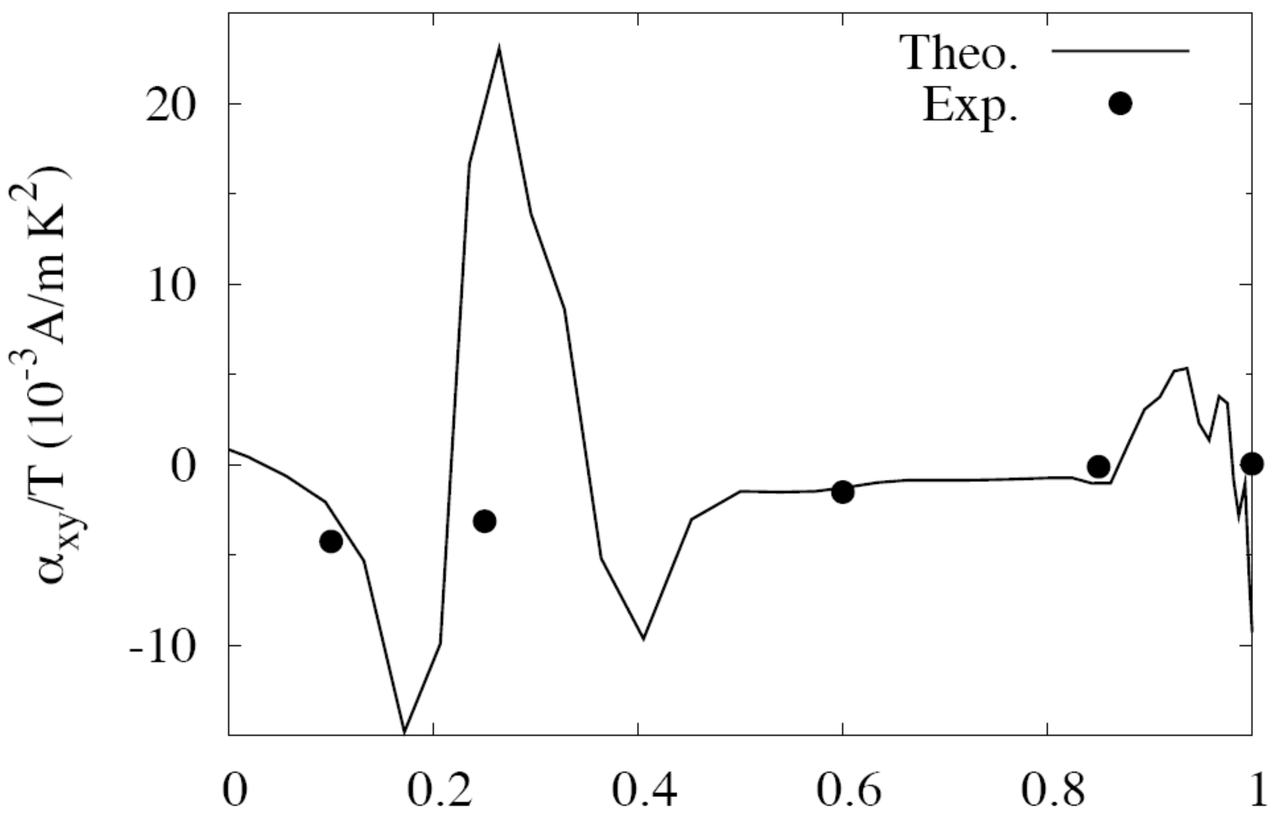
$$\boldsymbol{M} = \int \mathrm{d}\boldsymbol{k}\, f(\boldsymbol{k})\boldsymbol{m}(\boldsymbol{k}) + k_B T \int \mathrm{d}\boldsymbol{k}\, \frac{e}{\hbar}\boldsymbol{\Omega} \log(1 + e^{-\beta(\varepsilon-\mu)})$$
$$= \boldsymbol{M}_{\mathrm{moment}} + \boldsymbol{M}_{\mathrm{free}}$$

- Thermoelectric transport

$$\boldsymbol{j}^{\mathrm{tr}} = -e \int \mathrm{d}\boldsymbol{k}\, g(\boldsymbol{r}, \boldsymbol{k})\dot{\boldsymbol{r}} - \boldsymbol{\nabla} \times \boldsymbol{M}_{\mathrm{free}}$$

Anomalous Nernst Effect in $CuCr_2Se_{4-x}Br_x$

Lee, *et al*, Science 2004; PRL 2004, Xiao et al, PRL 2006



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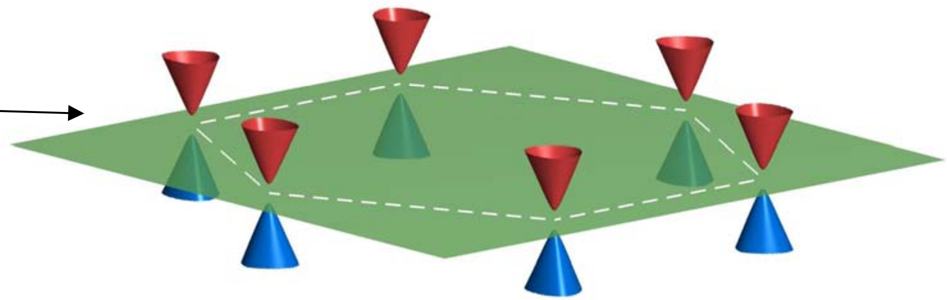
Graphene without inversion symmetry

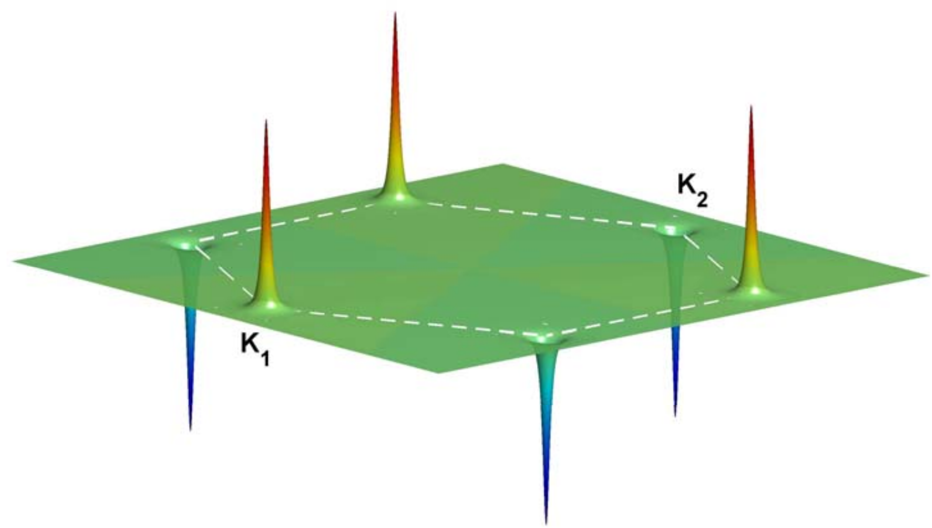
- Graphene on SiC: Dirac gap 0.28 eV
- Energy bands

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



- Berry curvature

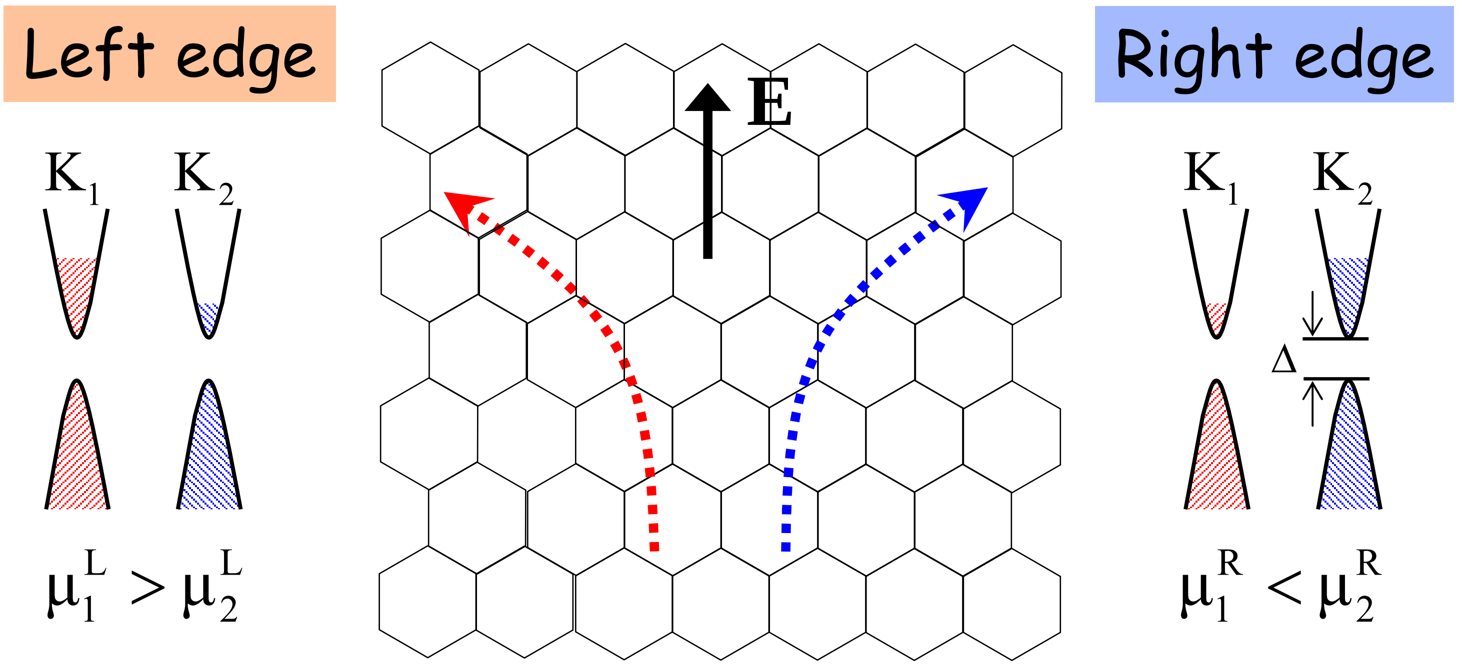
$$\Omega(\boldsymbol{q}) = \pm\tau_z \frac{3a^2\Delta t^2}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}}$$



- 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: $\mathcal{F}$
- Useful for spin transport studies

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

$$\hbar \dot{\mathbf{r}}_c = \eta^\dagger \left[\frac{D}{D\mathbf{k}}, \mathcal{H} \right] \eta - \hbar \dot{\mathbf{k}}_c \times \eta^\dagger \mathcal{F} \eta,$$

$$i\hbar \frac{D\eta}{Dt} = \mathcal{H}\eta.$$

Cucler, Yao & Niu, PRB, 2005
Shindou & Imura, Nucl. Phys. B, 2005
Chuu, Chang & Niu, 2006

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Quantization by Canonization

- Physical variables are not canonical
  - because of Berry curvature and magnetic field

- Canonical variables
  - 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 $G_\alpha \equiv 1/2(\partial\mathbf{R}/\partial k^\alpha)\cdot(\mathbf{R}\times\mathbf{B})$.

M.C. Chang and QN (2007)

Effective Hamiltonian

- Wavepacket energy

$$H(\mathbf{r}_c, \mathbf{k}_c) = E_0(\mathbf{k}_c) - e\phi(\mathbf{r}_c) + \frac{e}{2m}\mathbf{B}\cdot\mathcal{L}(\mathbf{k}_c)$$

- Energy in canonical variables

Peierls substitution

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

Spin-orbit

$$\begin{aligned} H(\mathbf{r}, \mathbf{p}) &= E_0(\pi) - e\phi(\mathbf{r}) + e\mathbf{E}\cdot\mathcal{R}(\pi) \\ &+ \frac{e}{2m}\mathbf{B}\cdot\left[\mathcal{L}(\pi) + 2\mathcal{R}\times m\frac{\partial E_0}{\partial \mathbf{p}}\right] \end{aligned}$$

Spin & orbital moment

Yafet term

- Quantum theory

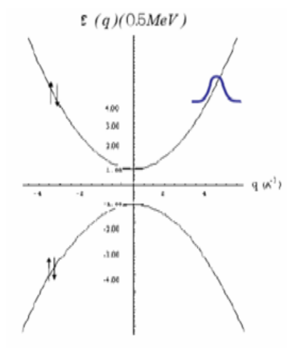
$[\, r, p \,] = ih/2\pi$

Applications

- Dirac bands:

  Reproduces Pauli Hamiltonian with spin-orbit coupling

- Semiconductor bands



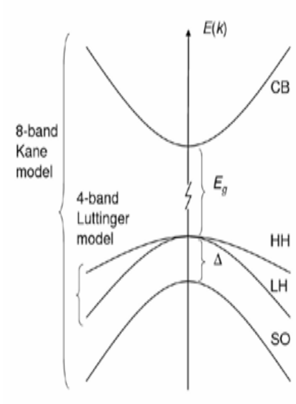


TABLE I: Berry connection, Berry curvature, and orbital angular momentum of the wavepacket in three disjoint subspaces of the 8-band Kane model. Only the leading order (in k) terms are shown. E_g and Δ are the conduction-valence band gap and the spin-orbit gap, σ and J are the spin-1/2 and spin-3/2 angular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

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

Extension of 4-band Luttinger model:

$$H(\mathbf{r},\mathbf{p}) = E_0(\pi,\mathbf{J}) - e\phi(\mathbf{r}) + \alpha_H \mathbf{E}\cdot\mathbf{J}\times\pi + 2\kappa\mu_B\mathbf{B}\cdot\mathbf{J}$$

Conclusion

Berry phase

A unifying concept with many applications

Anomalous velocity

Hall effect from a ‘magnetic field’ in k space.

Anomalous density of states

Berry phase correction to orbital magnetization
anomalous thermoelectric transport

Graphene without inversion symmetry

valley dependent orbital moment
valley Hall effect

Nonabelian extension for degenerate bands

Quantization of semiclassical dynamics

Physical variables are non-canonical
Generalized Peierlse substitution

Take home message

To account all effects linear in E & B, it is necessary and sufficient to know the Berry curvature and orbital moment.

Let's calculate their band structures!