Berry Phase Effects on Electronic Properties

Qian Niu

University of Texas at Austin

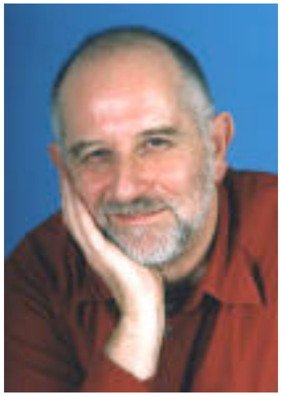
Collaborators:

D. Xiao, W. Yao, C.P. Chuu,
D. Culcer, J.R.Shi, Y.G. Yao, G. Sundaram, M.C. Chang,
T. Jungwirth, A.H.MacDonald, J. Sinova, C.G.Zeng, H. Weitering

Supported by : DOE, NSF, Welch Foundation

Outline

- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension
- Polarization and Chern-Simons forms
- Conclusion



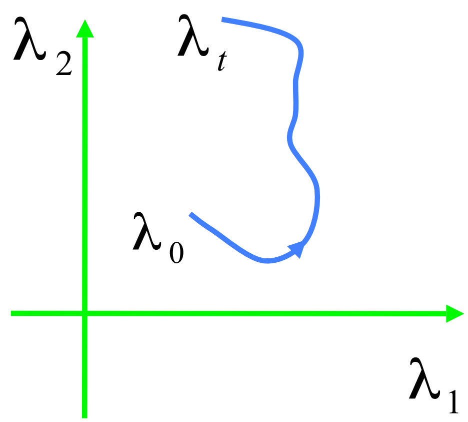
Berry Phase

In the adiabatic limit:

$$\Psi(t)=\psi_n(\lambda(t))\, e^{-i\int_0^t dt\, \varepsilon_n/\hbar}\, e^{-i\gamma_n(t)}$$

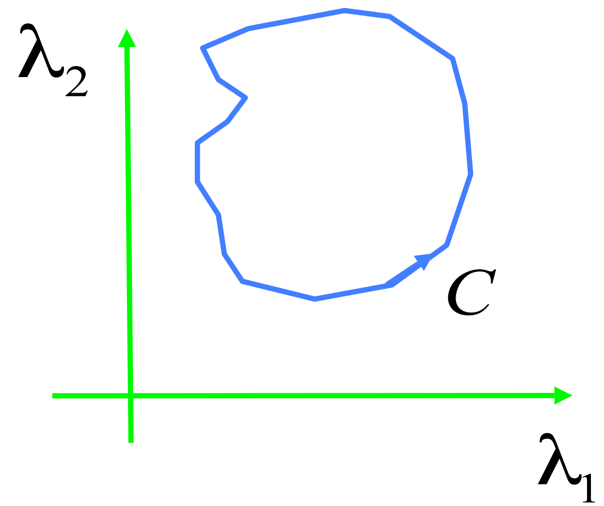
Geometric phase:

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



Well defined for a closed path

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



Stokes theorem

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

Berry Curvature

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

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

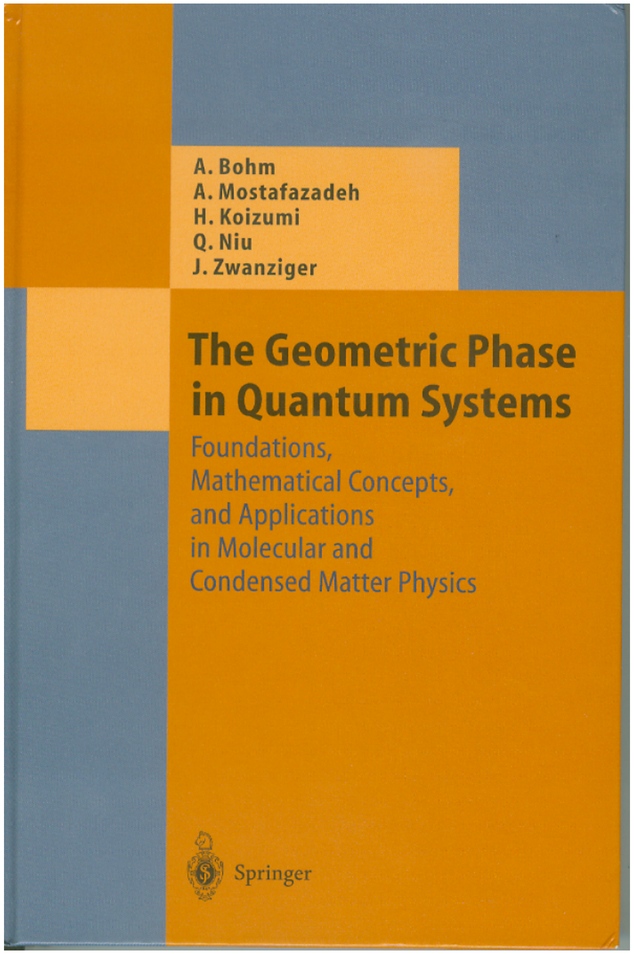
  spin dynamics,

  electron dynamics in Bloch bands

- Chern number

  quantum Hall effect,

  quantum charge pump



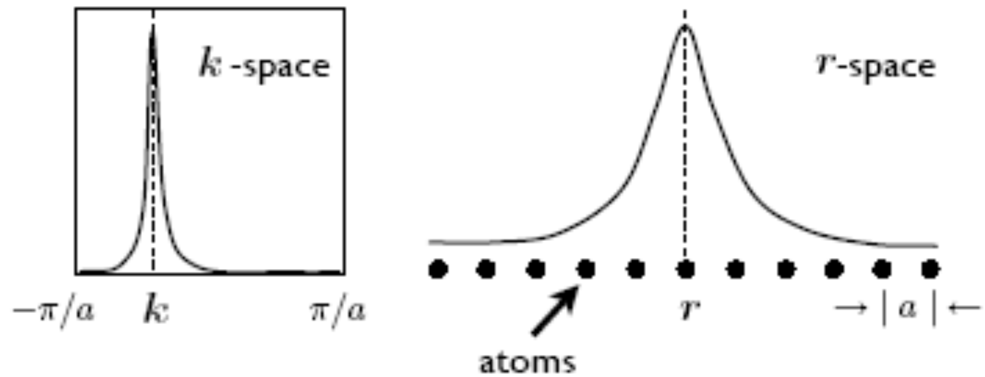
Outline

- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension
- Polarization and Chern-Simons forms
- Conclusion

Semiclassical Equations of Motion

Wave-packet Dynamics

(r, k)



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

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

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

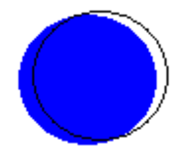
Nonzero if either time-reversal or inversion symmetry is broken

Berry Curvature

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

Anomalous Hall effect

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

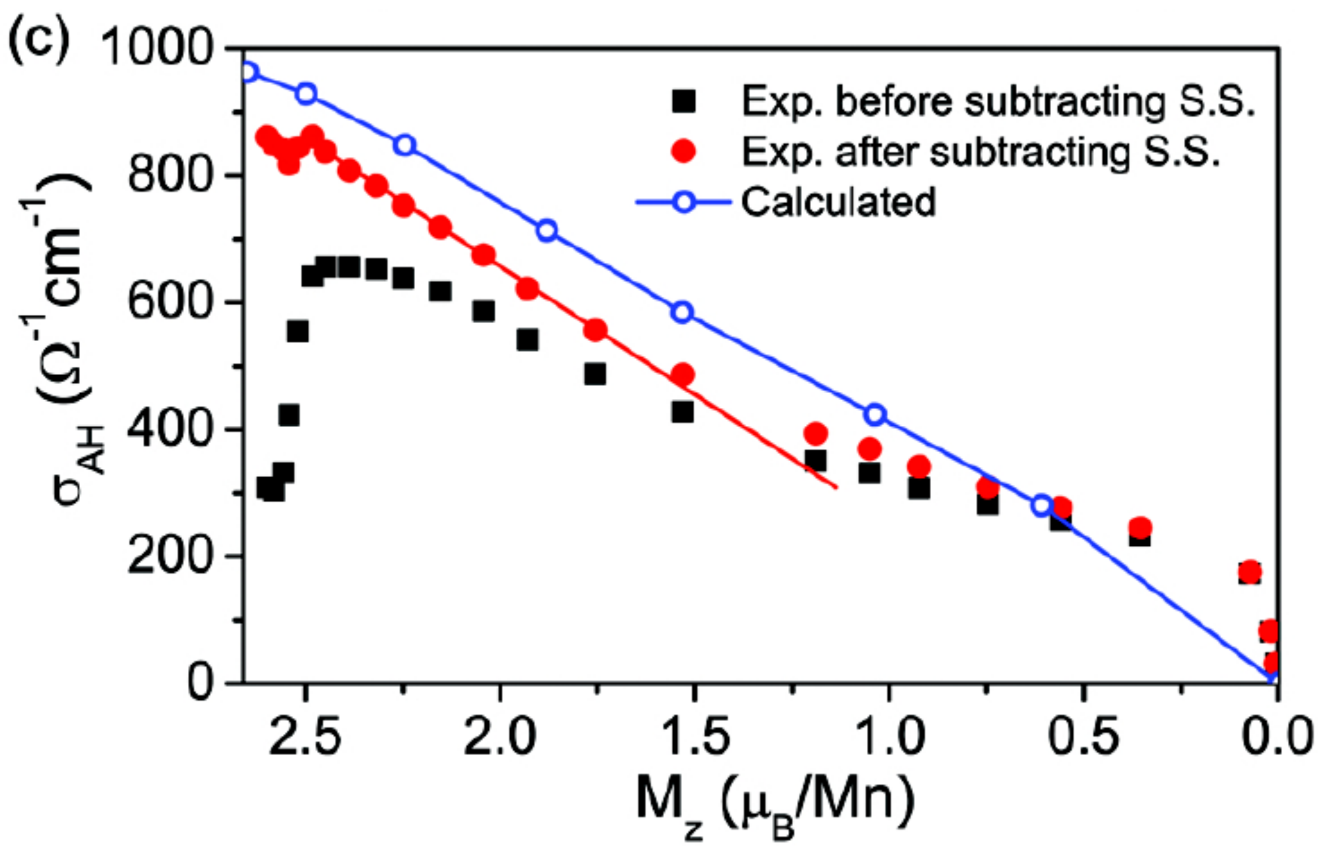


- current $$-e^2 \mathbf{E} \times \int d^3\mathbf{k}\; f(\mathbf{k})\, \mathbf{\Omega} - e \int d^3\mathbf{k}\; \delta f(\mathbf{k}) \frac{\partial \mathcal{E}}{\partial \mathbf{k}}$$

Intrinsic

Recent experiment

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



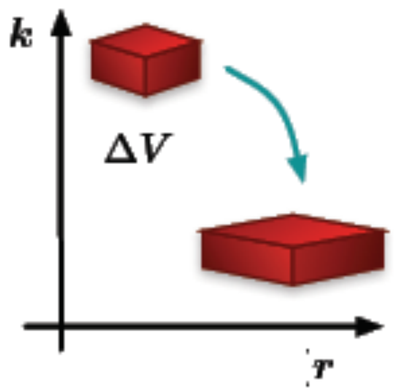
Intrinsic AHE in other ferromagnets

- 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)

Outline

- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension
- Polarization and Chern-Simons forms
- Conclusion

Phase Space Density of States



Evolution of a phase space volume

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

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

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

Free energy: $$\begin{aligned} F &= -\frac{1}{\beta}\sum_{\boldsymbol{k}} \log(1+e^{-\beta(\tilde{\varepsilon}-\mu)}) \\ &= -\frac{1}{\beta}\int \frac{d\boldsymbol{k}}{(2\pi)^3}\left(1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}\right)\log(1+e^{-\beta(\tilde{\varepsilon}-\mu)}) \end{aligned}$$

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

Anomalous Thermoelectric Transport

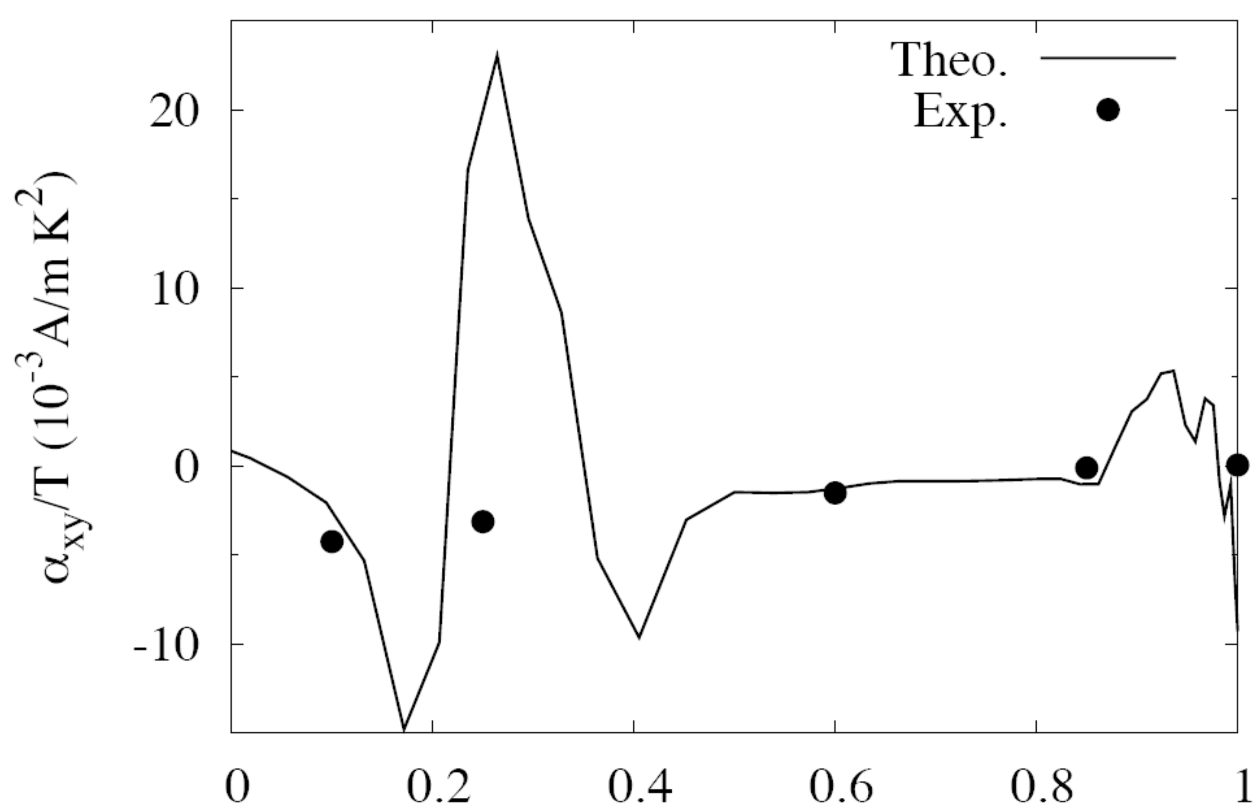
- Berry phase correction to magnetization

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

- 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 $CuCr_2Se_{4-x}Br_x$



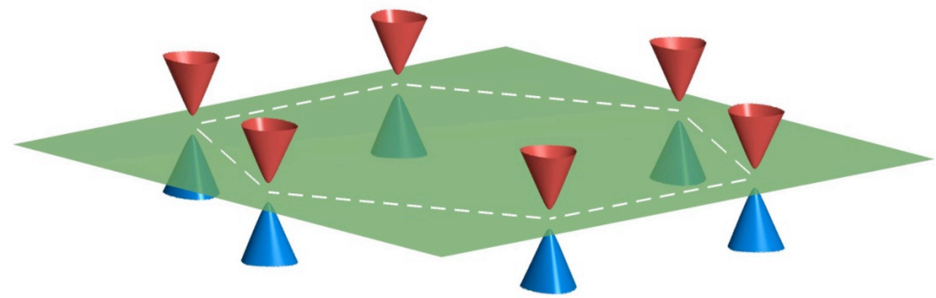
Outline

- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension
- Polarization and Chern-Simons forms
- Conclusion

Graphene without inversion symmetry

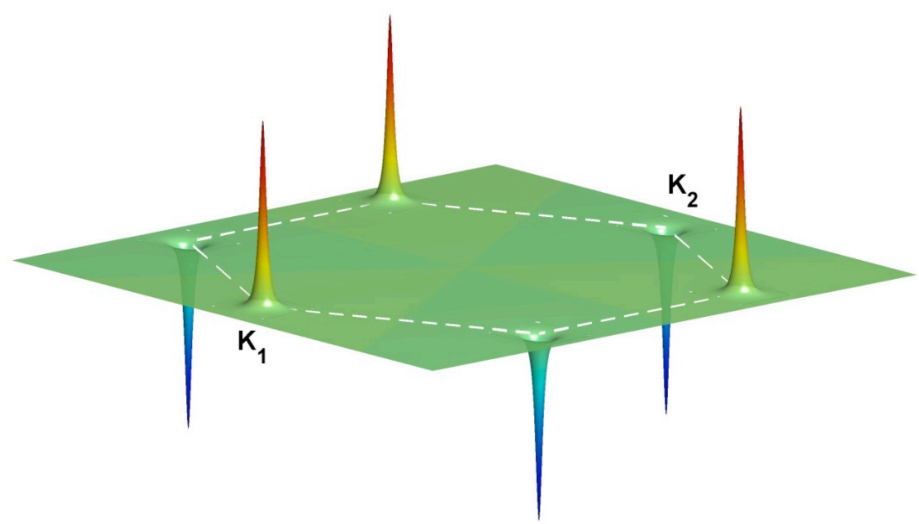
- Graphene on SiC: Dirac gap 0.28 eV
- Energy bands

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



- Berry curvature

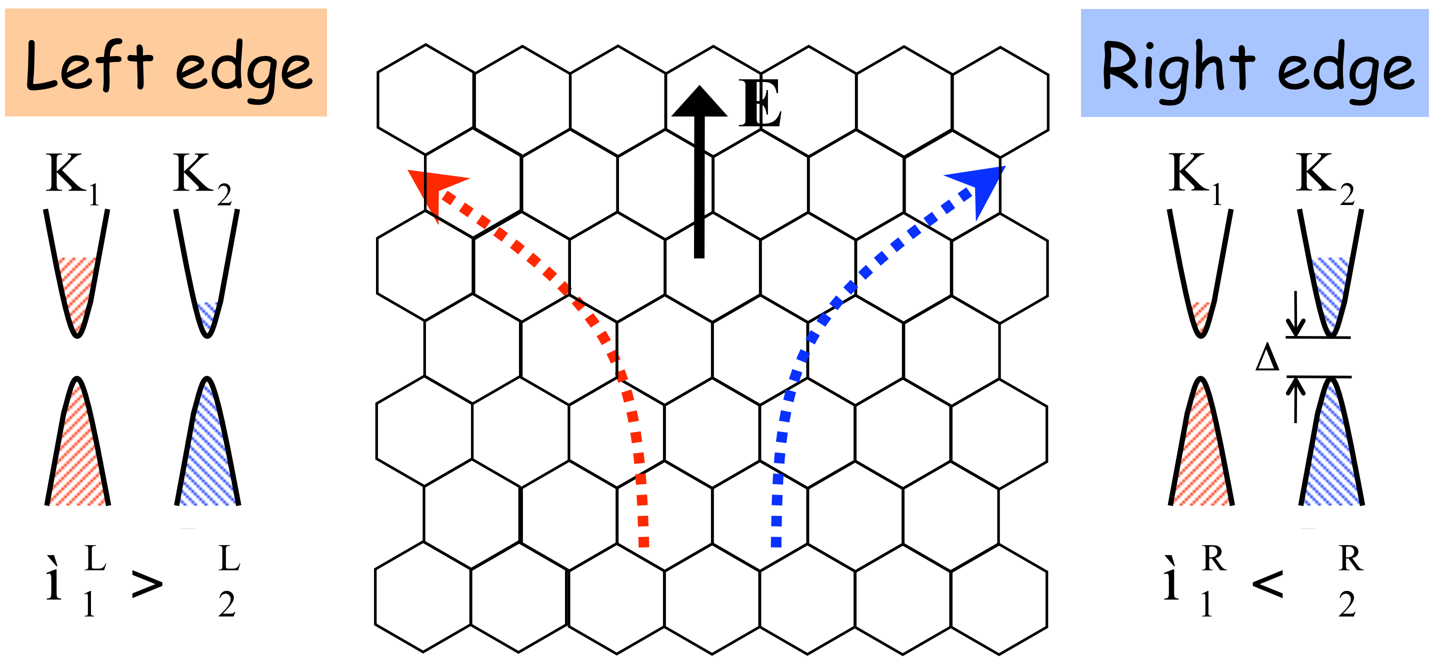
$$\Omega(\boldsymbol{q}) = \pm\tau_z \frac{3a^2\Delta t^2}{2(\Delta^2 + 3q^2a^2t^2)^{3/2}}$$



- 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:

Outline

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

Degenerate bands

- Internal degree of freedom: η
- Non-abelian Berry curvature: $\mathcal{F}$
- Useful for spin transport studies

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

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

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

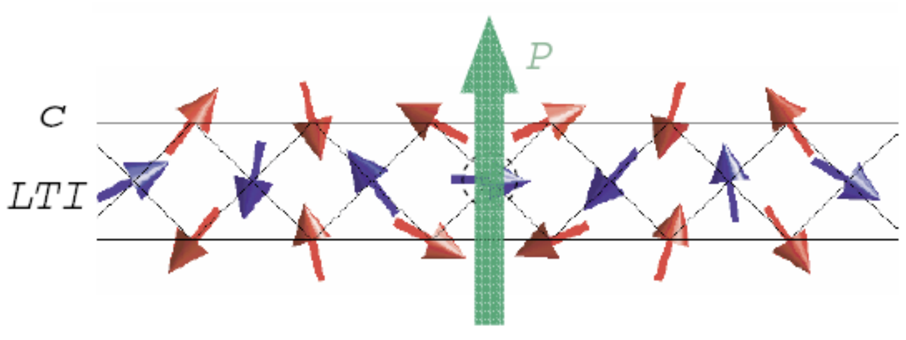
Cucler, Yao & Niu, PRB, 2005
Shindou & Imura, Nucl. Phys. B, 2005
Chuu, Chang & Niu, 2006

Outline

- Berry phase and its applications
- Anomalous velocity
- Anomalous density of states
- Graphene without inversion symmetry
- Nonabelian extension: spin transport
- Polarization and Chern-Simons forms
- Conclusion

Electrical Polarization

- A basic materials property of dielectrics
  - To keep track of bound charges
  - Order parameter of ferroelectricity
  - Characterization of piezoelectric effects, etc.
- **A multiferroic problem:** electric polarization induced by inhomogeneous magnetic ordering



G. Lawes et al, PRL (2005)

Polarization as a Berry phase

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{j} = 0$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{P} = -\rho$$

$$\boldsymbol{P} = \int_0^T dt\, \boldsymbol{j}(\lambda, \dot{\lambda})$$

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

King-Smith and Vanderbilt (1993):

$$\boldsymbol{P}^{\text{KS-V}} = -e \sum_n \int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \langle u_{n\boldsymbol{k}} | i \boldsymbol{\nabla}_{\boldsymbol{k}} | u_{n\boldsymbol{k}} \rangle$$

Led to great success in first principles calculations

Inhomogeneous order parameter

- Make a local approximation and calculate Bloch states

|u>= |u(m,k)>, m = order parameter

- A perturbative correction to the KS-V formula

$$\delta \boldsymbol{P}^{\text{KS-V}} = 2e \sum_n \int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \, \text{Im}\langle \delta u_{n\boldsymbol{k}} | \boldsymbol{\nabla}_{\boldsymbol{k}} u_{n\boldsymbol{k}} \rangle$$

Perturbation from the gradient

- A topological contribution (Chern-Simons)

$$P_\alpha^{(2)} = e \int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \left(\mathcal{A}_\alpha^k \nabla_\beta^r \mathcal{A}_\beta^k + \mathcal{A}_\beta^k \nabla_\alpha^k \mathcal{A}_\beta^r + \mathcal{A}_\beta^r \nabla_\beta^k \mathcal{A}_\alpha^k \right)$$

$$\mathcal{A}_\alpha^k = \langle u | i \nabla_\alpha^k | u \rangle \ , \quad \mathcal{A}_\alpha^r = \langle u | i \nabla_\alpha^r | u \rangle$$

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

Polarization and Chern-Simons forms