KITP Program “Spintronics”
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Spin Hall Effect of Electrons and Photons

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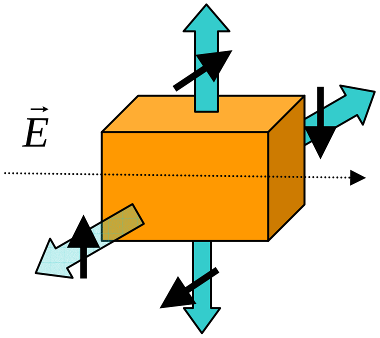
Spin Hall effect (SHE)

Electric field induces a transverse spin current.



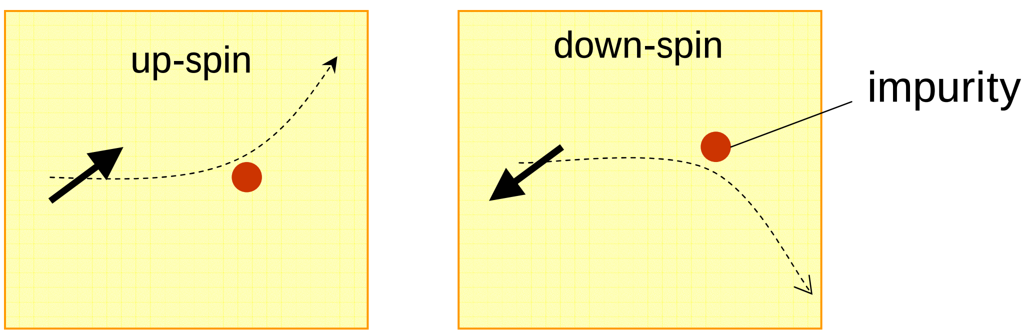
- **Extrinsic spin Hall effect**

D'yakonov and Perel' (1971)
Hirsch (1999), Zhang (2000)

impurity scattering = spin dependent (skew-scattering)

↑

Spin-orbit couping



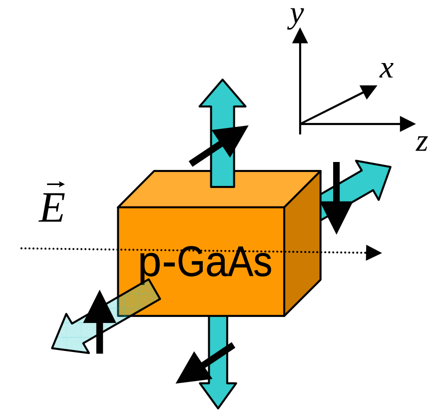
= relativistic effect

$\vec{E}$ (impurity potential) ⟶ $\vec{B}$ if seen from moving electrons,

⟶ couple with electron spin

Intrinsic spin Hall effect

- p-type semiconductors (SM, Nagaosa, Zhang, Science (2003))



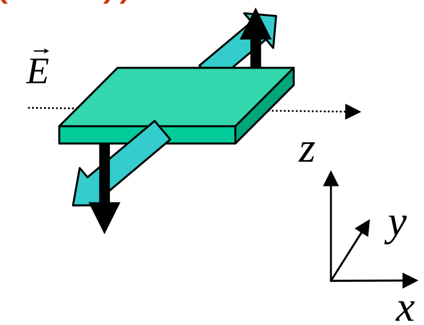
Luttinger model

$$H=\frac{\hbar^2}{2m}\left[\left(\gamma_1+\frac{5}{2}\gamma_2\right)k^2-2\gamma_2\left(\vec{k}\cdot\vec{S}\right)^2\right]$$

($\vec{S}$: spin-3/2 matrix)

- 2D n-type semiconductors in heterostructure
(Sinova, Culcer, Niu, Sinitsyn,Jungwirth, MacDonald, PRL (2004))

Rashba model



$$H=\frac{k^2}{2m}+\lambda\left(\vec{\sigma}\times\vec{k}\right)_z$$

•
•
•

Intrinsic spin Hall effect

Does not rely on impurity scattering

Berry phase in momentum space
--- multiband effect

Semiclassical eq. of motion (Sundaram,Niu,1999)

$$\begin{cases} \dot{\vec{x}} = \dfrac{1}{\hbar}\dfrac{\partial E_n(\vec{k})}{\partial \vec{k}} + \dot{\vec{k}} \times \vec{B}_n(\vec{k}) \\ \dot{\vec{k}} = -e\vec{E} \end{cases}$$

Determined from the Bloch wf.
→ Motion of a wavepacket acquires a transverse shift

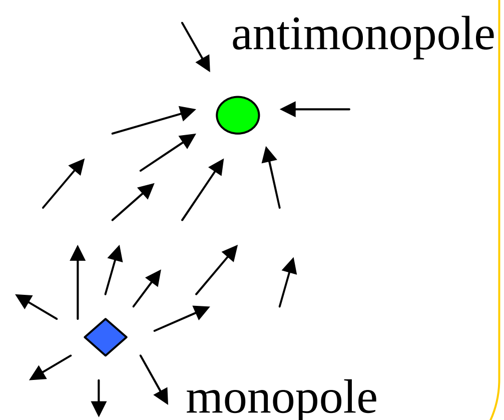
$$A_{ni}(\vec{k}) = -i\left\langle n\vec{k}\left|\frac{\partial}{\partial k_i}\right|n\vec{k}\right\rangle = -i\int_{\text{unit cell}} u^*_{n\vec{k}} \frac{\partial u_{n\vec{k}}}{\partial k_i} d^d x$$: Gauge field

($u_{n\vec{k}}$: periodic part of the Bloch wf.)

$$\psi_{n\vec{k}}(\vec{x}) = u_{n\vec{k}}(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$$

$$\vec{B}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_n(\vec{k})$$: Connection

(n : band index)



Valence band of GaAs

p-orbit (x,y,z) × (↑ , ↓)

+ spin-orbit coupling

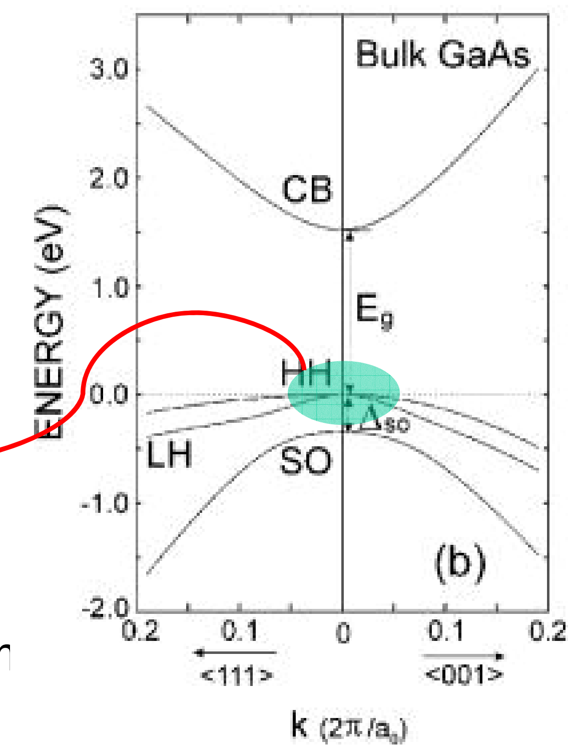
split-off band (SO)
heavy-hole band (HH)
light-hole band (LH)

doubly degenerate (Kramers)

Luttinger Hamiltonian (Luttinger(1956))

$$H = \frac{\hbar^2}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2\left(\vec{k}\cdot\vec{S}\right)^2\right]$$

($\vec{S}$: spin-3/2 r



Helicity $\lambda = \hat{k}\cdot\vec{S}$ is a good quantum number.

Helicity

$\lambda = \hat{k}\cdot\vec{S} = \pm\frac{3}{2} \Rightarrow E = \frac{\gamma_1 - 2\gamma_2}{2m}\hbar^2 k^2$: heavy hole (HH)

$\lambda = \hat{k}\cdot\vec{S} = \pm\frac{1}{2} \Rightarrow E = \frac{\gamma_1 + 2\gamma_2}{2m}\hbar^2 k^2$: light hole (LH)

Semiclassical eq. of motion

$$\hbar\dot{\vec{k}} = e\vec{E}, \quad \dot{\vec{x}} = \frac{\hbar\vec{k}}{m_\lambda} + \frac{e}{\hbar}\vec{E}\times\vec{B}^{(\lambda)}(\vec{k})$$

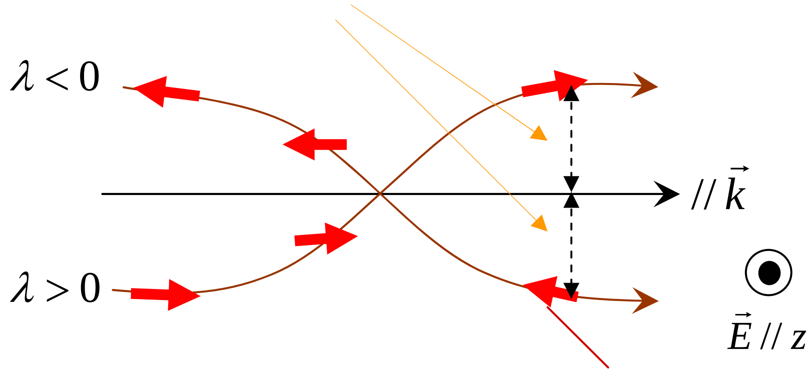
$$\vec{B}^{(\lambda)}(\vec{k}) = \lambda\left(2\lambda^2 - \frac{7}{2}\right)\frac{\vec{k}}{k^3}$$

$\lambda = \pm\frac{3}{2}$: HH, $\lambda = \pm\frac{1}{2}$: LH

$\lambda = \hat{k}\cdot\vec{S}$

(Cf. A.Zee, PRA38,1('88))

Anomalous velocity (perpendicular to $\vec{S}$ and $\vec{E}$)



Spin current (spin // x, velocity // y)

$$j_{yx}^{H} = \frac{\hbar}{3}\sum_{\lambda=\pm\frac{3}{2},\vec{k}} \dot{y}S_x n^{\lambda}(\vec{k}) = \frac{E_z k_F^H}{4\pi^2},$$

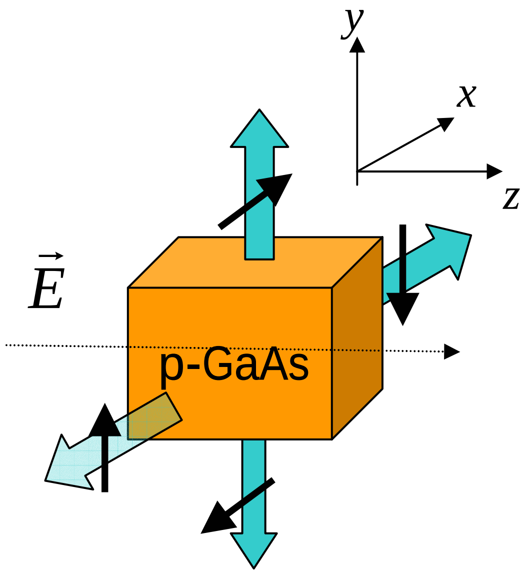
$$j_{yx}^{L} = \frac{\hbar}{3}\sum_{\lambda=\pm\frac{1}{2},\vec{k}} \dot{y}S_x n^{\lambda}(\vec{k}) = -\frac{E_z k_F^L}{12\pi^2},$$

$$\sigma_s = \frac{e}{12\pi^2}(3k_F^H - k_F^L)$$

- Quantum correction
- impurity scattering
  etc.

Missing !

Intrinsic spin Hall effect in semiconductors



$j_j^i = \sigma_s \varepsilon_{ijk} E_k$ { i: spin direction; j: current direction; k: electric field }

σ_s : even under time reversal = reactive response (dissipationless)

$$\sigma_s \approx S^i v_j$$

- Nonzero in nonmagnetic materials.

Cf. Ohm's law: $j = \sigma E$

σ : odd under time reversal = dissipative response

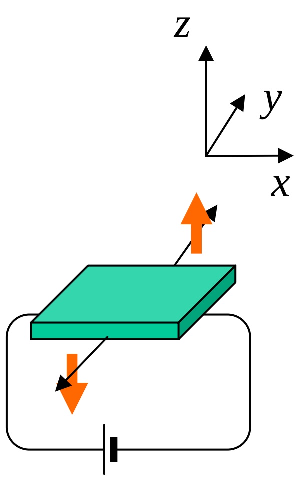
Intrinsic spin Hall effect
for 2D n-type semiconductors in heterostructure

(Sinova, Culcer, Niu, Sinitsyn, Jungwirth, MacDonald, PRL(2004))

Rashba Hamiltonian

$$H = \frac{k^2}{2m} + \lambda\left(\vec{\sigma}\times\vec{k}\right)_z$$

Structural inversion asymmetry (SIA)
Effective electric field along z



2D heterostructure

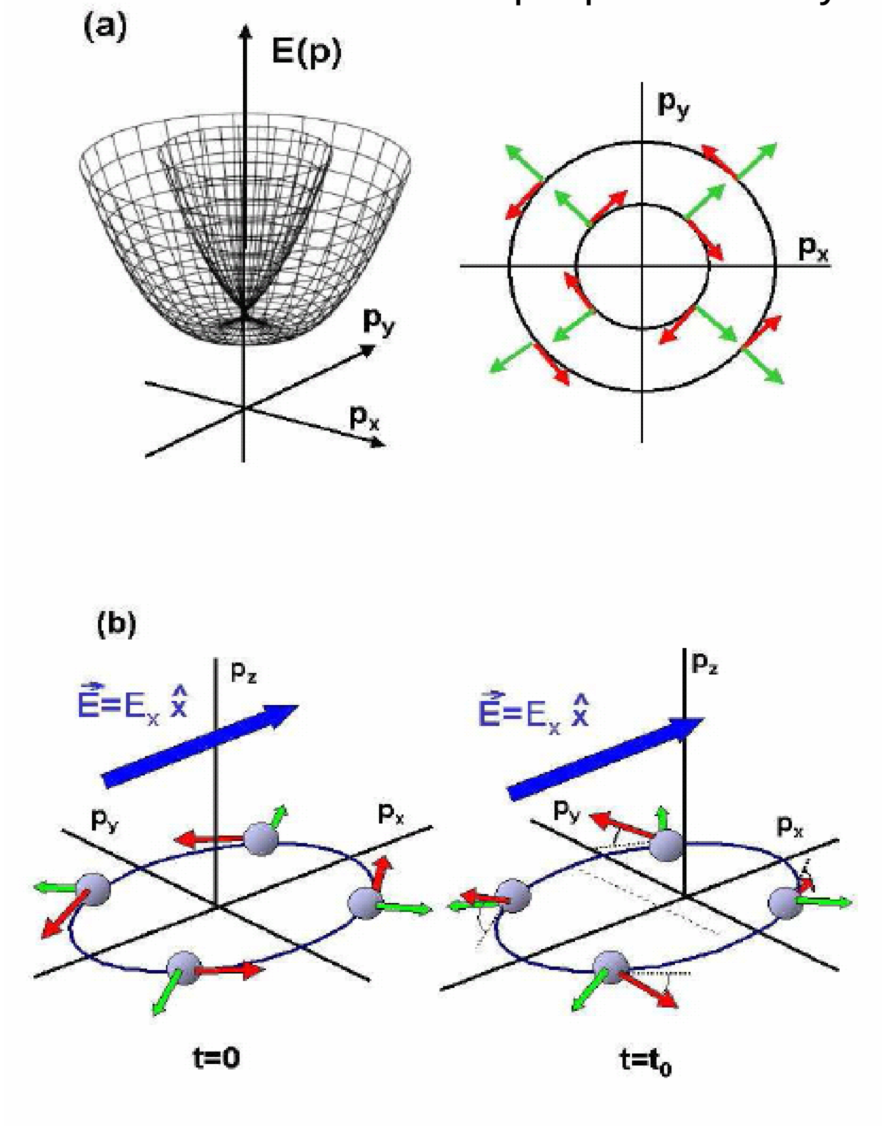
Kubo formula : $\left\langle J_x J_y^{S_z} \right\rangle \longrightarrow \sigma_s = \frac{e}{8\pi}$ (clean limit)

$J_y^{S_z} = \frac{1}{2}\left\{J_y, S_z\right\}$

independent of λ

Spin Hall effect in the Rashba model

≈ Spin precession by "k-dependent Zeeman field"



$$H=\frac{k^2}{2m}+\lambda\left(\vec{\sigma}\times\vec{k}\right)_z$$

$$\vec{B}_{eff}=\lambda(\hat{z}\times\vec{k})$$

$\vec{k}$ -dependent Zeeman field

$\vec{E}=0:$ $\vec{S}\,//\,\vec{B}_{eff}$

$\vec{E}\neq 0:$ $\vec{B}_{eff}$ varies due to electric field

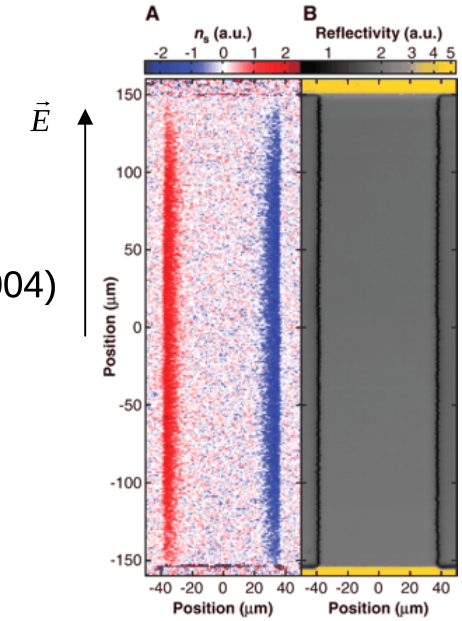
$\vec{S}$ is no longer parallel to $\vec{B}_{eff}$

⟶ **Spin precession**
→ spin Hall effect

$$\sigma_s=\frac{e}{8\pi}$$

Experiments on spin Hall effect

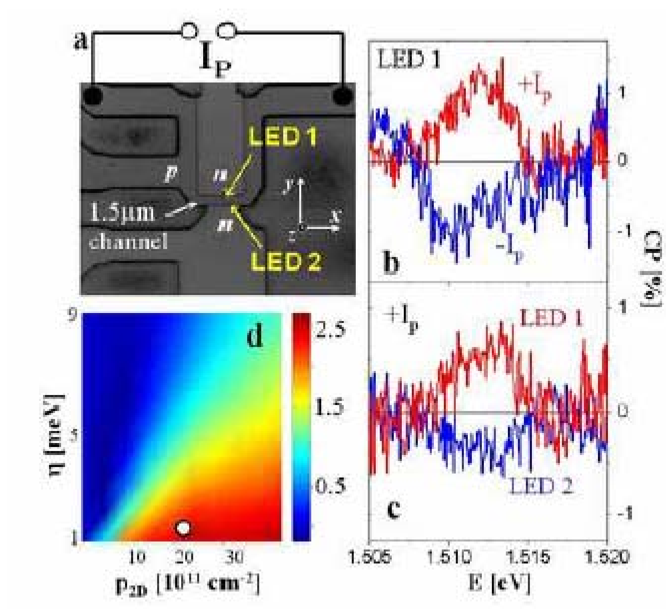
- **3D n-type**
  - Y.K.Kato, R.C.Myers, A.C.Gossard, D.D. Awschalom, Science (2004)
  - Sih et al. , Nature Physics (2005)



Spin accumulation due to spin Hall current
→ observe by Kerr effect

$\Delta_{SO} << \frac{1}{\tau}$: mostly extrinsic

- **2D p-type, spin LED**
  - J. Wunderlich, B. Kaestner, J. Sinova, T. Jungwirth, PRL (2005)



Spin-polarized holes due to spin Hall effect
→ circularly polarized light

$\Delta_{SO} >> \frac{1}{\tau}$: mostly intrinsic

(Q1): Disorder effect?

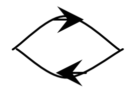
Rashba model:
(2D n-type)

$$H = \frac{k^2}{2m} + \lambda\left(\sigma_x k_y - \sigma_y k_x\right)$$

+ spinless impurities (short-range pot.)

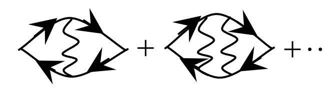
Sinova et al.(2003)

$$\sigma_S = \frac{e}{8\pi}$$



+ Vertex correction in the clean limit
(Inoue, Bauer, Molenkamp, PRB (2003))

$$\sigma_S^{\text{vertex}} = -\frac{e}{8\pi}$$



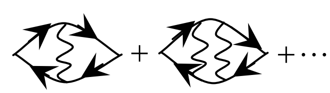
$$\sigma_S = 0$$

Inoue, Bauer, Molenkamp, PRB (2004)

- clean limit
- δ -fn. impurity

Luttinger model (3D p-type):

vertex correction=0 for δ -fn. impurities.
(Murakami, PRB (2004))

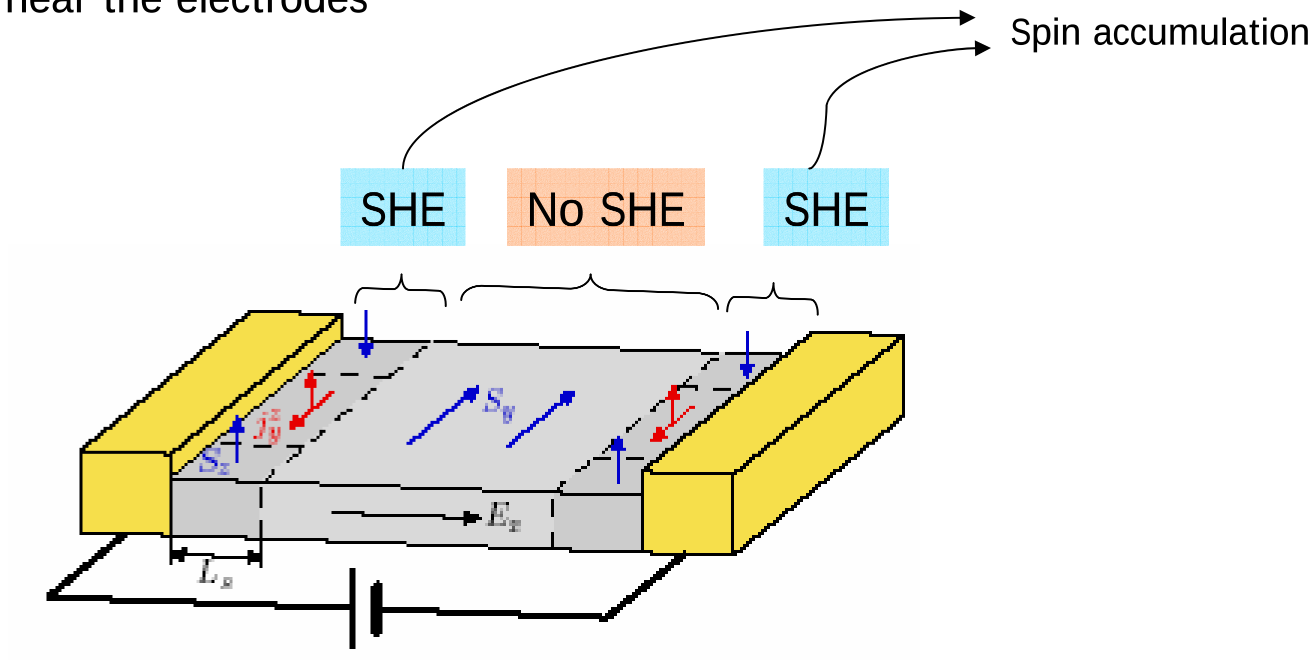


$$= 0$$

- **Calculation by Keldysh formalism** (Mishchenko, Shytov, Halperin (2004))

  Spin Hall current does not flow at the bulk – consistent with $\sigma_S = 0$

  Spin current only flows near the electrodes



SHE in disordered Rashba model -- Green's function--

$\sigma_s = 0$ in the following cases:

	$E_F\tau$	$\Delta\tau$	Potential	
Inoue, Bauer, Molenkamp (2004)	∞	∞	δ-fn.	
Mishchenko, Shytov,Halperin (2004)	any	any	δfn.	•diffusion equation
Raimondi,Schwab (2004)	∞	∞	any	•Might be nonzero for finite $E_F\tau$
Dimitrova (2004)	large	large	δ-fn	•Arbitrary dispersion (?) •Arbitrary form of Rashba coupling (?)
Liu, Lei (2004,2005)	∞	∞	any	•Zero even with Dresselhaus ('05) •Might be nonzero for T>0
Chalaev Loss (2004)	large	large	δ-fn	•Zero even with Dresselhaus. •Weak localization correction=0

Dimitrova; Chalaev,Loss : $J_s \equiv \frac{1}{2}\{v_y, S_z\} \propto \frac{dS_y}{dt} \longrightarrow \langle J_s \rangle \propto \langle \dot{S}_y \rangle = 0$ for steady state

If $J_s \propto \dot{S}_y$, spin Hall current $\langle J_s \rangle = 0$ for any type of spinless impurities.

(e.g. Rashba model)

$$\langle J_s \rangle = \frac{1}{2i}\int \frac{d\omega}{2\pi}\int \frac{d^2 p}{(2\pi)^2}\,\mathrm{tr}\left(J_s G^K\right)$$: Keldysh formalism

$$J_s \equiv \frac{1}{2}\{v_y, S_z\} = \frac{1}{4im\lambda}[H, \sigma_y]$$

$$\langle J_s \rangle = \frac{1}{2i}\frac{1}{4im\lambda}\int \frac{d\omega}{2\pi}\int \frac{d^2 p}{(2\pi)^2}\,\mathrm{tr}\left(\sigma_y \left[H, G^K\right]\right)$$

$$\left[H, G^K\right] = -ie\vec{E}\cdot\partial_{\vec{p}} G^K - \frac{i}{2}e\vec{E}\cdot\left\{\partial_{\vec{p}} H, \partial_\omega G^K\right\} - \frac{i}{2}e\vec{E}\cdot\left(\partial_{\vec{p}}\underline{\Sigma}\partial_\omega \underline{G} - \partial_\omega \underline{\Sigma}\partial_{\vec{p}}\underline{G}\right)_K + \frac{i}{2}e\vec{E}\cdot\left(\partial_{\vec{p}}\underline{G}\partial_\omega\underline{\Sigma} - \partial_\omega \underline{G}\partial_{\vec{p}}\underline{\Sigma}\right)_K - \left(\left[\underline{\Sigma}, \underline{G}\right]\right)_K$$

No contribution to $\langle J_s \rangle$

No contribution for
- 1^{st} Born
- higher Born
- weak localization corr.

for any type of spinless impurities

$$\langle J_s \rangle = 0$$

Definition of the spin current

"Spin current" is not directly measurable.

↓

Instead we can measure the spin accumulation at the edge

Does spin accumulation reflect the "bulk spin current" due to the SHE?

"Conventional" definition of the spin current operator:

$$J_s \equiv \frac{1}{2}\{v_y, S_z\}$$

not satisfy the eq. of continuity $\frac{\partial S_i}{\partial t} + \nabla \cdot J_i^{(\mathrm{spin})} = 0$

(Spin non-conservation due to spin-orbit coupling)

→ **not** directly related with spin accumulation

Conserved spin current

- Zhang, Shi, Xiao, Niu, cond-mat/0503505)
- Entin-Wohlman et al. PRL95, 086603(2005)

$$\frac{\partial}{\partial t} S_z + \vec{\nabla} \cdot \underline{J_s} = \underline{\frac{d}{dt} S_z}$$

Spin current

Local spin precession due to SO coupling
Let us write it as $-\nabla \cdot P_\tau$

Eq. of continuity for spin

$$\frac{\partial}{\partial t} S_z + \vec{\nabla} \cdot \underline{\left(J_s + P_\tau\right)} = 0$$

$\mathcal{J}_s$: conserved spin current
→ measurable as spin accumulation

Calculation of $\langle P_\tau \rangle$ in response to electric field ?

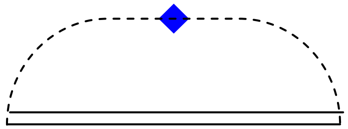
1) Spatial modulation of $\vec{E}$: $\vec{E} = (Ee^{iqy - i\omega t}, 0, 0)$

2) Calculate $\langle \dot{S}_z \rangle$

3) Calculate $\langle P_\tau \rangle$ $\quad \langle P_\tau \rangle = -\lim_{\omega \to 0} \lim_{q \to 0} \frac{1}{iq} \langle \dot{S}_z \rangle$

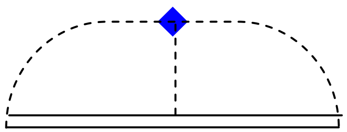
Spin Hall effect for the Rashba model -- conserved spin current $\langle \mathcal{J}_s \rangle$

- 1^{st} Born approx.



$$\langle \mathcal{J}_s \rangle_{1st} = 0$$

- 2^{nd} Born approx

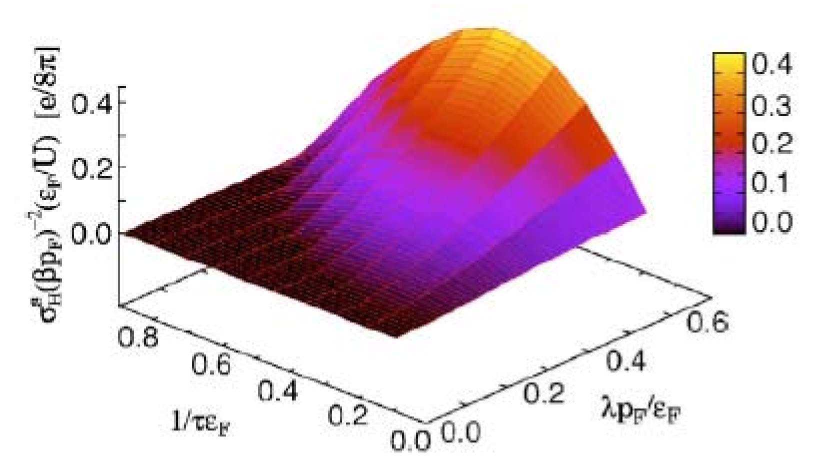


$$\langle \mathcal{J}_s \rangle_{2nd} \neq 0$$

$\sigma_s = 0$ in the clean limit

$\sigma_s = 0$ for the δ –fn. Impurity

$\sigma_s \neq 0$ for longer-ranged impurities with finite β



β : range of impurity pot.
(short but finite)

Spin Hall effect in the Rashba model

		Conventional spin current J_s	Conserved spin current $\mathcal{J}_s$
$\delta(\vec{r})$	1st	0	0
	higher	0	0
$V(\vec{p}-\vec{p}')$	1st	0	0
	higher	0	finite
$V(\vec{p},\vec{p}')$	1st	0	finite
	higher	0	finite

Depends on impurity = extrinsic.

Nonzero for general spin-orbit-coupled system

(Q2) SHE in insulators

A) Spin Hall insulator SM, Nagaosa, Zhang, PRL 93, 156804 (2004)

: no edge states

B) Quantum Spin Hall systems : edge states

- Kane, Mele, PRL95, 146802, 226801('05)
- Bernevig, Zhang, PRL96,106802 ('06)
- Qi, Wu, Zhang, cond-mat/0505308
- Onoda, Nagaosa, PRL 95,106601 ('05)
- Xu, Moore, cond-mat/0508291
- Wu, Bernevig, Zhang, PRL96,106401('06)

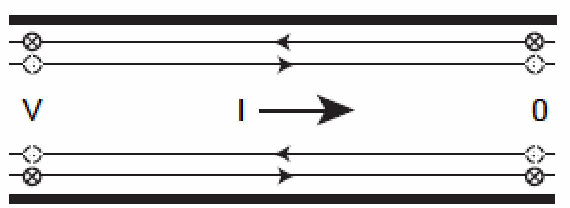
- **helical spin current at the edge**

Outline

Calculate spin Hall conductivity σ_s

← Streda formula (cf. QHE)

- Relation with edge states
- Candidate materials



Spin Hall effect and Streda formula

Středa formula for Hall effect

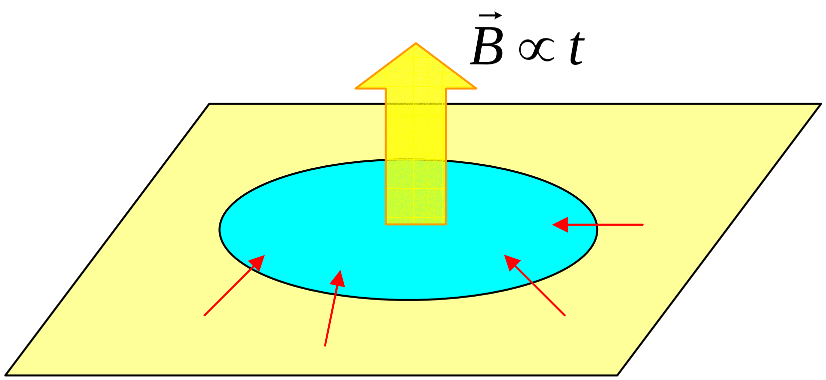
Středa (1982)

$$\sigma_{xy} = \sigma_{xy}^{I} + \sigma_{xy}^{II} \quad \begin{cases} \sigma_{xy}^{I} = \dfrac{ie^2}{2}\mathrm{Tr}\left[v_i \dfrac{1}{E_F - H + i0} v_j \delta(E_F - H) - \mathrm{h.c.} \right] \\ \sigma_{xy}^{II} = e \left.\dfrac{\partial N}{\partial B}\right|_{E_F} \end{cases}$$

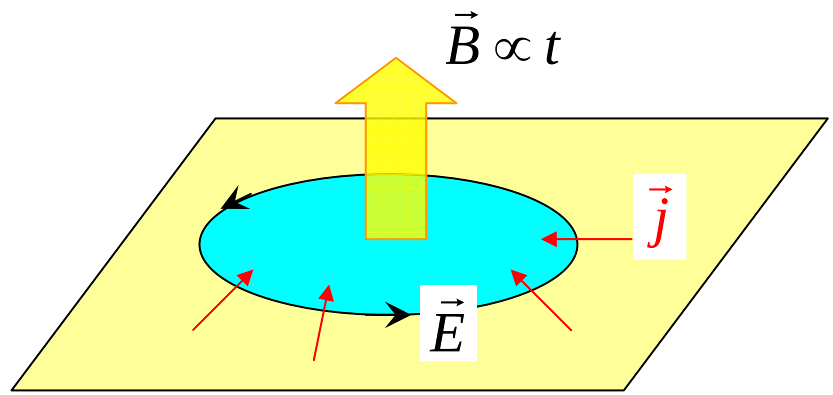
σ_{xy}^{I} : intraband (Fermi level)
zero for insulator

σ_{xy}^{II} : interband
can be nonzero for insulator

(N : Number of states below E_F)



$\left.\dfrac{\partial N}{\partial B}\right|_{E_F}$ **electrons flow in.**



$$j = E \underbrace{e \left.\frac{\partial N}{\partial B}\right|_{E_F}}_{\sigma_{xy}}$$: Hall current

Středa formula for spin Hall effect

Expected result

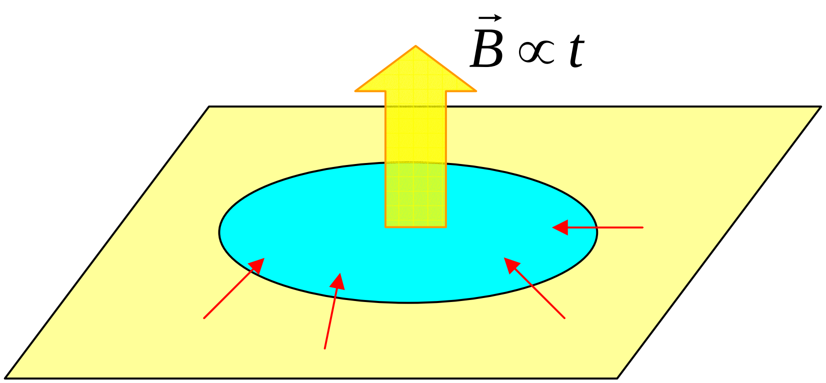
$$\sigma_s = \sigma_s^I + \sigma_s^{II}$$

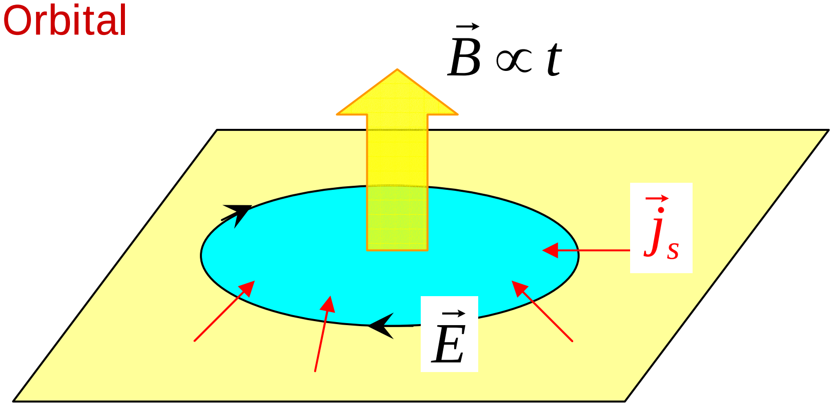
σ_s^I : intraband (Fermi level)
zero for insulator

$$\sigma_s^{II} = \left.\frac{\partial S_z}{\partial B}\right|_{E_F}$$

Spin
: interband
Orbital

Spin-orbital susceptibility
← spin-orbit coupling





$\left.\frac{\partial S_z}{\partial B}\right|_{E_F}$ **spins flow in.**

$$j_s = E \left.\frac{\partial S_z}{\partial B}\right|_{E_F}$$: spin Hall current

σ_s

“Středa-like” formula for spin Hall effect

Yang, Chang, PRB73,073304 (2006)

$$\sigma_{sH} = \sigma^{I}_{sH} + \sigma^{II}_{sH},$$

- **intraband** (Fermi level) -- zero for insulator

$$\sigma^{I}_{sH} = -\frac{i\hbar\Omega}{2}\int d\varepsilon \frac{\partial f(\varepsilon)}{\partial \varepsilon}\mathrm{Tr}\left[j^z_y G^+(\varepsilon) j_x \delta(\varepsilon - H) - j^z_y \delta(\varepsilon - H) j_x G^-(\varepsilon)\right],$$

- **interband** -- nonzero for insulator

$$\sigma^{II}_{sH} = \sigma^{II,(c)}_{sH} + \sigma^{II,(n)}_{sH},$$

$$\sigma^{II,(c)}_{sH} = \frac{e}{4\pi i\,\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\left\{s_z G^+(xv_y - yv_x)G^+ - s_z G^-(xv_y - yv_x)G^-\right\}, = -\left.\frac{\partial S_z}{\partial B}\right|_{\mu,T},$$

$$\sigma^{II,(n)}_{sH} = -\frac{i\hbar^2 e}{4\pi\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\left\{\dot{s}_z\left[(G^+)^2 v_x G^+ v_y G^+ + G^+ v_y G^+ v_x (G^+)^2 - \mathrm{H.\ c.}\right]\right\}$$
$$-\frac{\hbar e}{8\pi\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\left\{\dot{s}_z\left[G^+[y, v_x](G^+)^2 + (G^+)^2[y, v_x]G^+ + \mathrm{H.\ c.}\right]\right\}.$$

← Spin non-conservation
unwanted terms

Definition of spin current

"Conventional" spin current

$$J_s \equiv \frac{1}{2}\{v_y, S_z\}$$

not satisfy the eq. of continuity $\frac{\partial S_i}{\partial t} + \nabla \cdot J_s = 0$

→ **not** directly related with spin accumulation

Conserved spin current

- Shi, Zhang, Xiao, Niu, PRL96,076604 (2006)
- Entin-Wohlman et al. PRL95, 086603(2005)

$$\frac{\partial}{\partial t} S_z + \vec{\nabla} \cdot J_s = \frac{d}{dt} S_z$$

Spin current ($\vec{\nabla} \cdot J_s$)

Local spin precession due to SO coupling ($\frac{d}{dt} S_z$)

write it as $-\nabla \cdot P_\tau$

Eq. of continuity for spin

$$\frac{\partial}{\partial t} S_z + \vec{\nabla} \cdot \left(J_s + P_\tau\right) = 0$$

$\mathcal{J}_s$: conserved spin current

- conserve
- satisfy Onsager relation
- have conjugate force

Středa formula for spin Hall effect

$$\sigma_{sH} = \sigma_{sH}^{(I)} + \sigma_{sH}^{(II)}$$

- **intraband** -- zero for insulator

$$\sigma_{sH}^{(I)} = \frac{ie}{8\pi V}\int d\varepsilon \frac{df}{d\varepsilon}\mathrm{tr}\Big[(G_+ - G_-)\cdot\big([H,s_z]G_+\{v_x,y\} - \{v_x,y\}G_-[H,s_z] - 2[H,s_z y]G_+ v_x + 2v_x G_-[H,s_z y] + [y,[s_z,v_x]]\big)\Big]$$

- **interband** -- nonzero for insulator

$$\sigma_{sH}^{(I)} = \frac{ie}{8\pi V}\int d\varepsilon\ f(\varepsilon)\mathrm{tr}\big(2s_z G_+(yv_x - xv_y)G_+ - (+\leftrightarrow -)\big) = \frac{1}{V}\frac{ds_z}{dB_{\mathrm{orb.}}}$$

Cf. N. Sugimoto et al., cond-mat/0503475 (to appear in PRB)
P19.00009

For insulators ...

$$\sigma_s = \frac{1}{V}\frac{dS_z}{dB_{\mathrm{orb}}} = \frac{1}{V}\frac{dL_z}{dB_{\mathrm{Zeeman}}}$$

: Středa formula for spin Hall effect

"orbital-spin" susceptibility

How to calculate orbital magnetization?

$$\rightarrow\quad M = \frac{1}{2c(2\pi)^3}\,\mathrm{Im}\sum_n \int_{\varepsilon_{n\vec{k}}\le\mu} d\vec{k}\,\langle \partial_{\vec{k}} u_{n\vec{k}} | \times (H + \varepsilon_{n\vec{k}} - 2\mu) | \partial_{\vec{k}} u_{n\vec{k}} \rangle$$

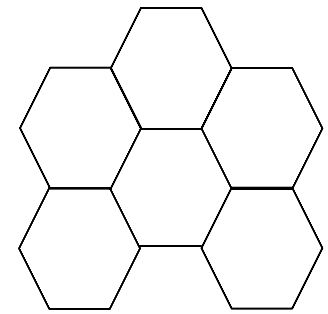
- Resta et al., ChemPhysChem 6, 1815 (2005)
- Xiao et al., PRL 95, 137204 (2005)
- Thonhauser et al., PRL 95, 137205 (2005)
- Ceresoli et al., cond-mat/0512142

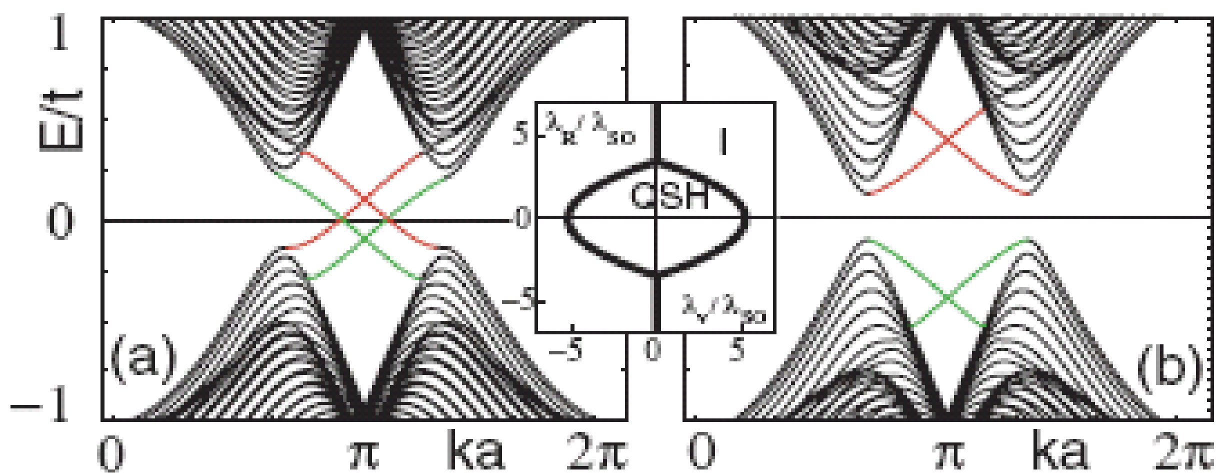
Honeycomb-lattice model for the QSHS

C. L. Kane and E. J. Mele, PRL **95,** 146802 ,226801 (2005)

$$H = t\sum_{\langle ij\rangle} c_i^+ c_j + i\lambda_{SO}\sum_{\langle\langle ij\rangle\rangle} v_{ij} c_i^+ s^z c_j + i\lambda_R \sum_{\langle ij\rangle} c_i^+ \left(\vec{s}\times\vec{d}_{ij}\right)_z c_j + \lambda_v \sum_i \xi_i c_i^+ c_i$$

kinetic — Spin-orbit — Rashba — Staggered on-site energy



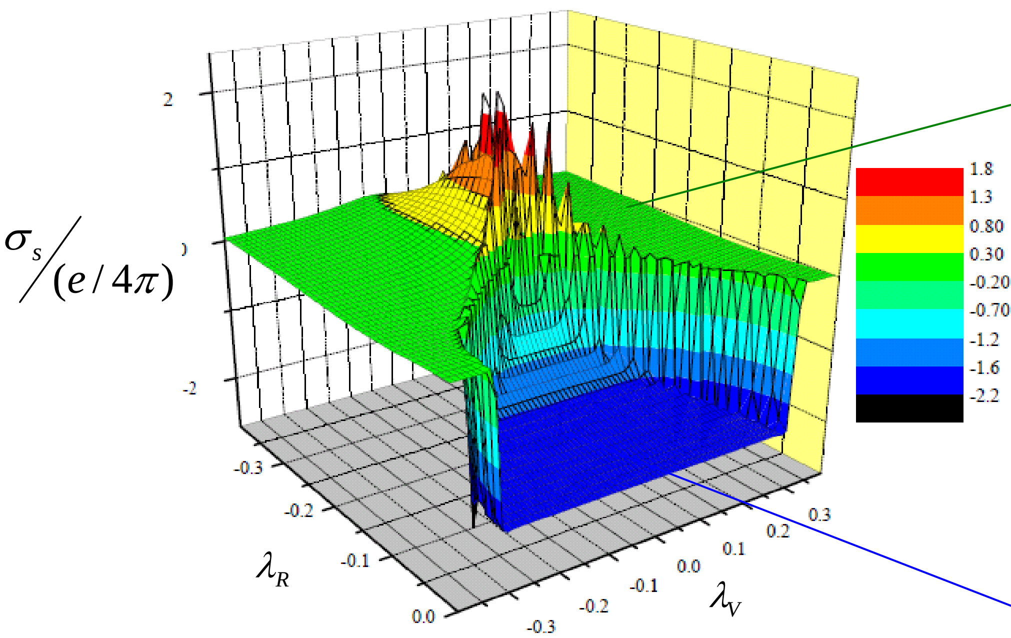


Z$_2$ topological index

Quantum spin Hall system (QSHS)

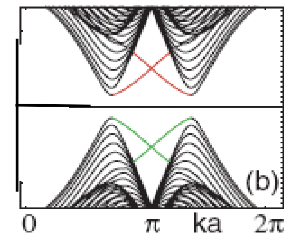
Spin Hall insulator (SHI)

Numerical calculation of σ_s for Kane-Mele model .



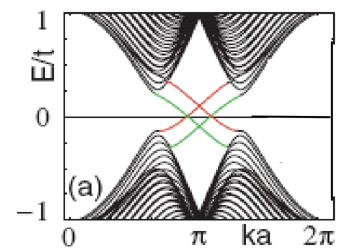
Spin Hall insulator (SHI)

$\sigma_s \approx 0$



Quantum spin Hall system (QSHS)

$\sigma_s \approx 2 \cdot \frac{-e}{4\pi}$



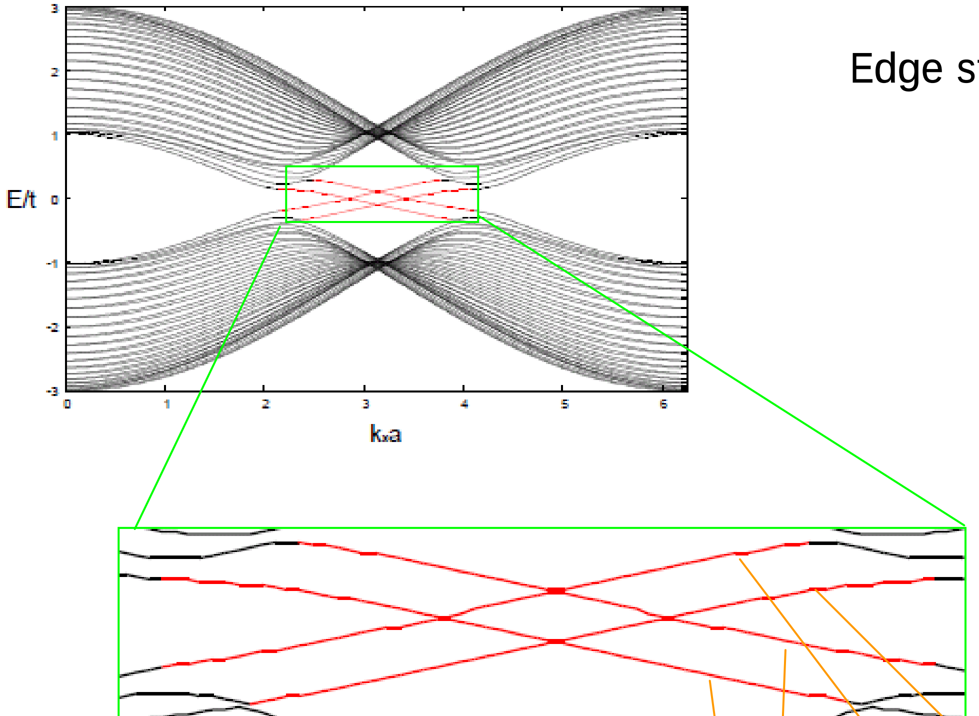
edge states

- deviation from $\frac{e}{4\pi}$ - quantization

→ enhanced near QSHS-SHI phase boundary

= Band crossing

Spin polarization for bulk & edge states

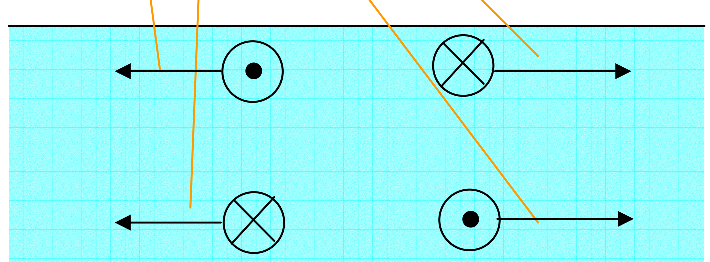


Edge states :almost fully polarized $\left(\geq 0.95 \cdot \frac{\hbar}{2} \right)$

$$\sigma_s = \frac{e}{2\pi\hbar}\left(\langle S_z \rangle_L - \langle S_z \rangle_R \right)\Big|_{E_F}$$

Kane, Mele, PRL95 (2005)
Sheng et al., cond-mat/0603054

$$\Rightarrow \quad \sigma_s \approx 2 \cdot \frac{e}{4\pi}$$



Helical spin current

Candidate materials for QSHE ?

- Graphene → Kane-Mele model ?

  Estimate for spin-orbit coupling

  $\Delta \approx 0.2\mathrm{meV}$ (Kane,Mele, PRL95,226801 ('05))

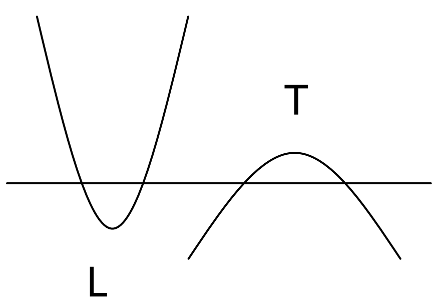
  $\Delta \approx 0.001\mathrm{meV}$ (Sinitsyn et al, cond-mat/0602598) : very small!

QSHE requires $\Delta >> 1/\tau$ { • sample quality • low temperature

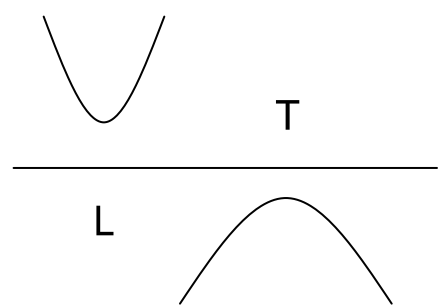
---

- Bi – semimetal { hole pocket at T point; 3 electron pockets at L points }

$Bi_{1-x}Sb_x$ -- insulator (semiconductor) for x>0.07



Semimetal (x<0.07)



Semiconductor (0.07<x)

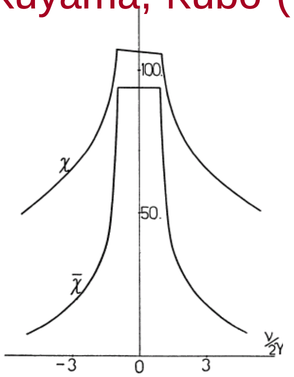
$Bi_{1-x}Sb_x$ as a candidate material for QSHE

- **Enhanced diamagnetic susceptibility in Bi and $Bi_{1-x}Sb_x$**

Interband matrix elements due to spin-orbit coupling

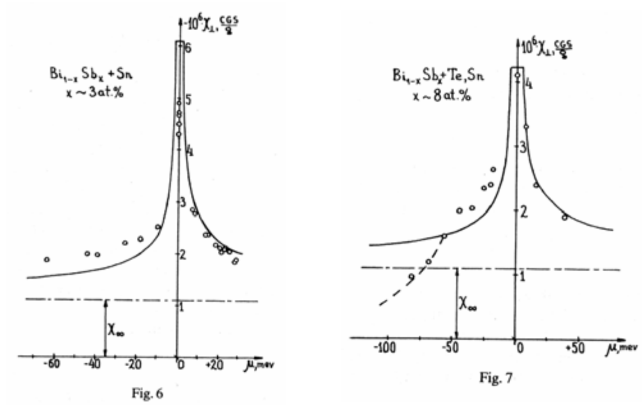
Theory

Fukuyama, Kubo (1970)



Experiment

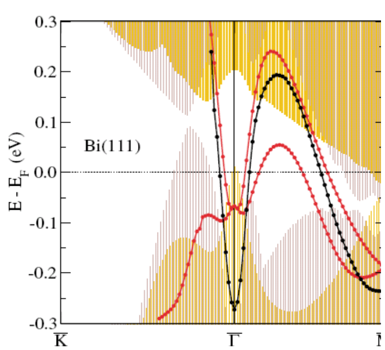
Brandt, Semenov, Falkovsky (1977)



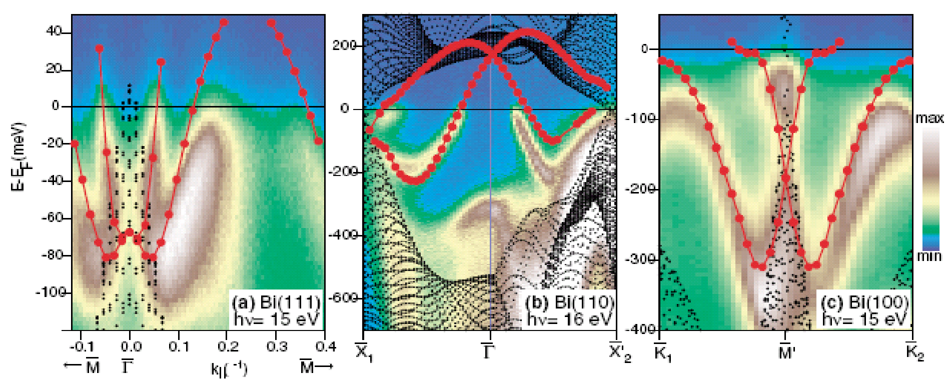
- **Surface states of Bi -- large spin splitting --**

Large spin splitting in Bi (111)

Koroteev et al., PRL93, 046403 ('04).



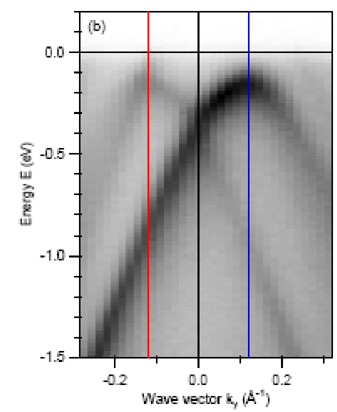
(Calc.)



(Exp.)

Large spin splitting (~1eV) in Bi/Ag(111)

Ast et al., cond-mat/0509509

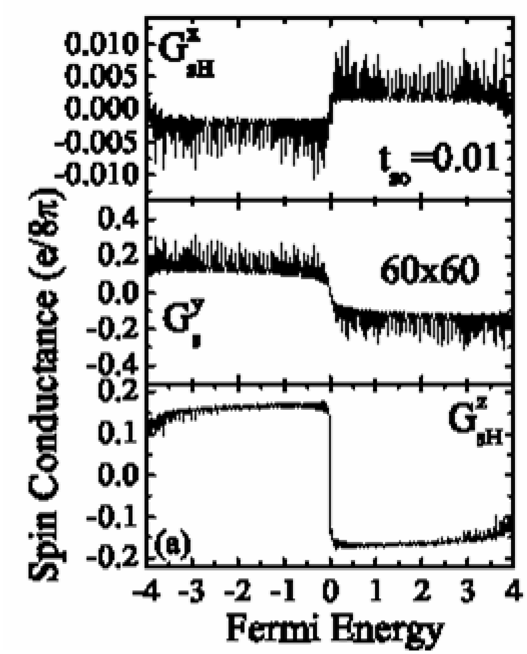


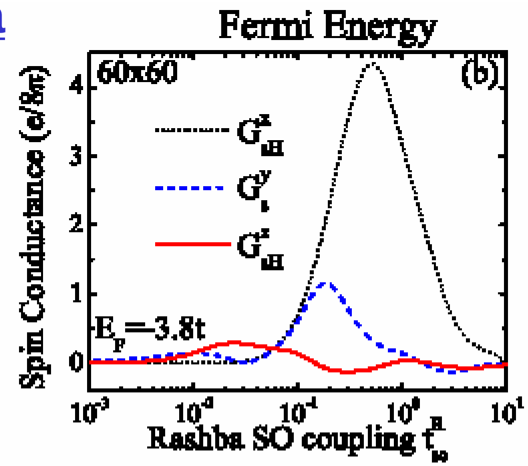
(Q3) Is “spin Hall current” observable?

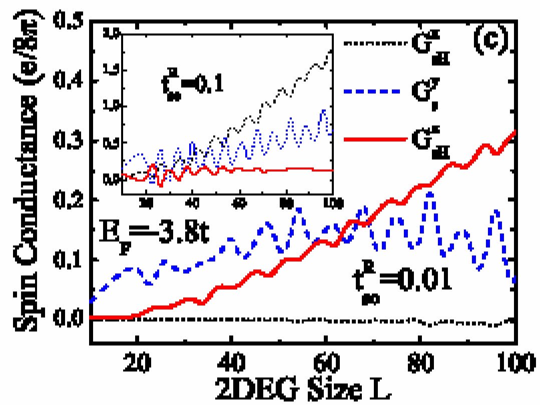
Landauer-Büttiker formula

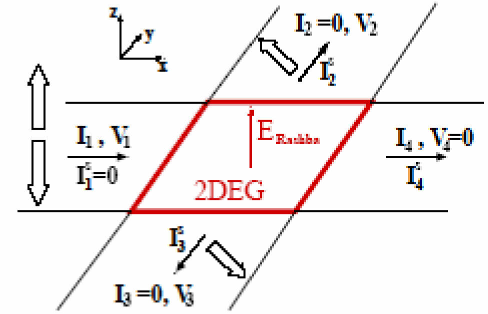
Nikolic et al., PRB (’04)

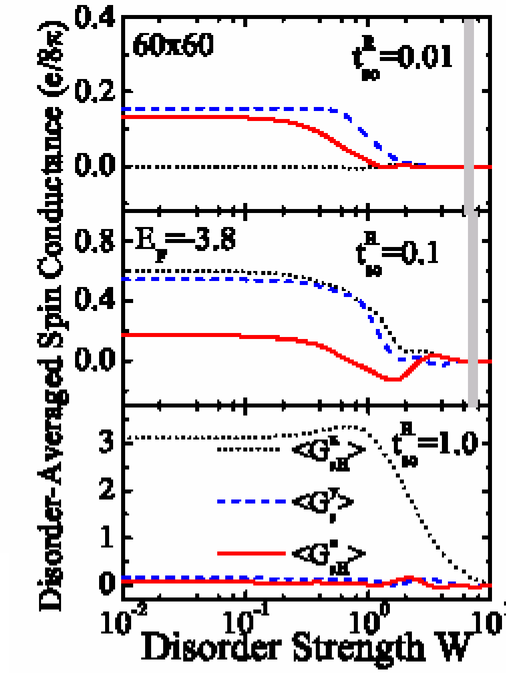
Sheng et al.., PRL(’04)





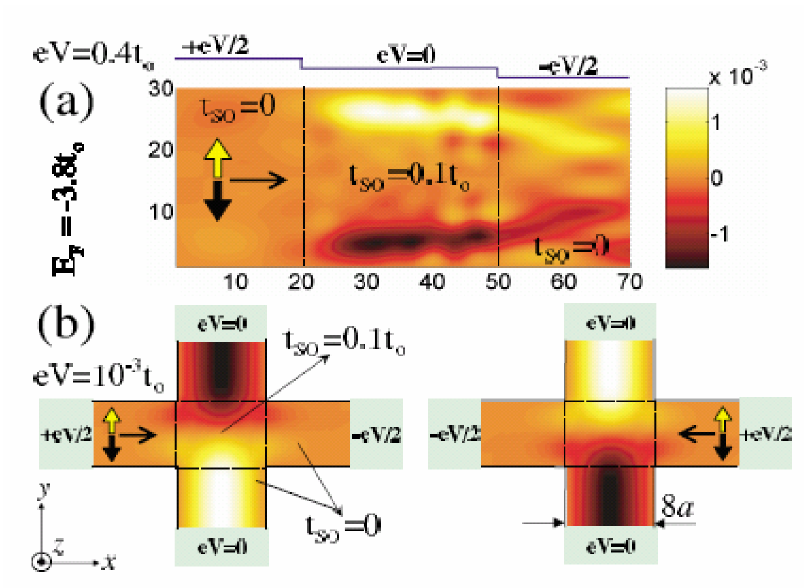




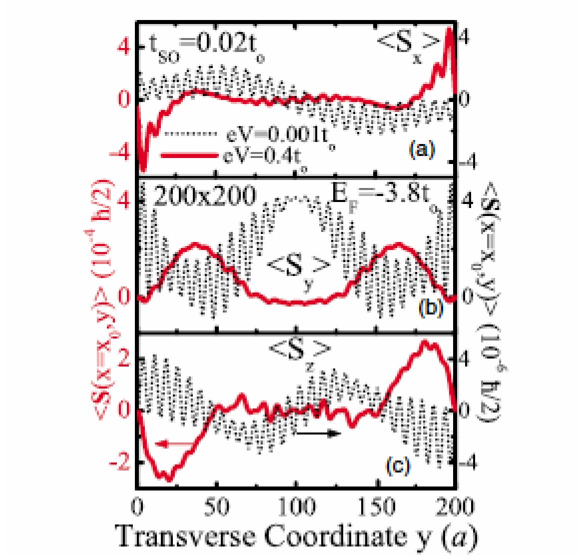


Nikoliç, Souma, Zârbo, Sinova, PRL (2005)

Landauer-Keldysh

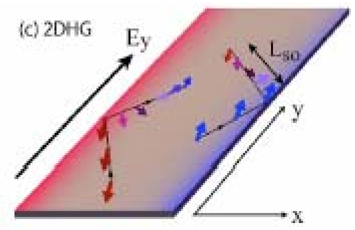


Spin current flows into the leads.

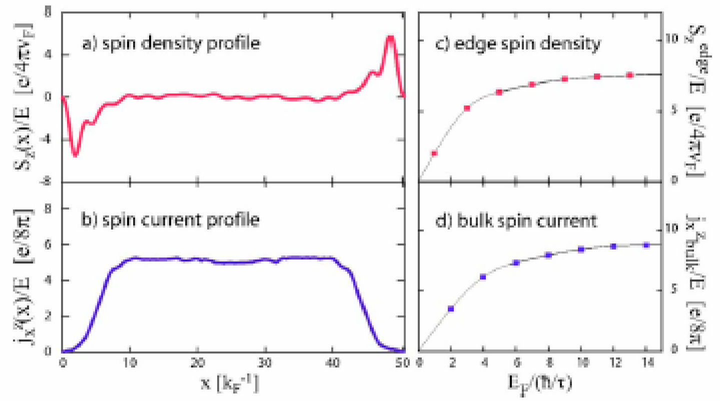


Nonequilibrium spin accumulation

Nomura et al., PRB('05)

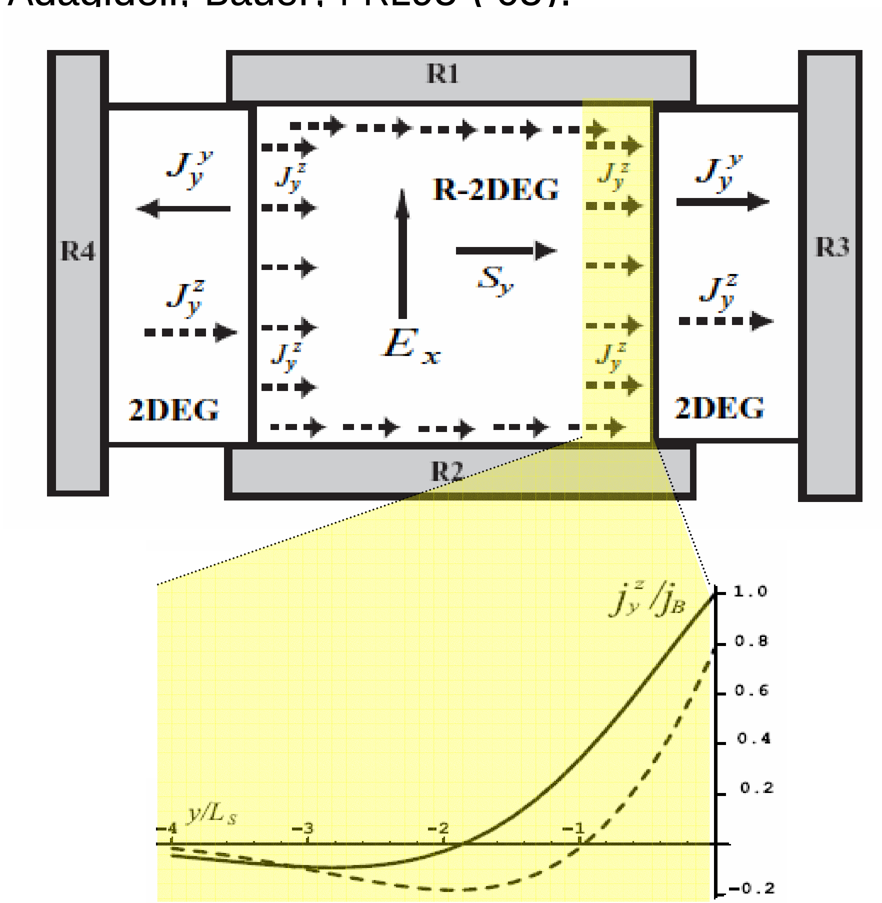


Conventional spin current well agrees with the spin accumulation at the edge

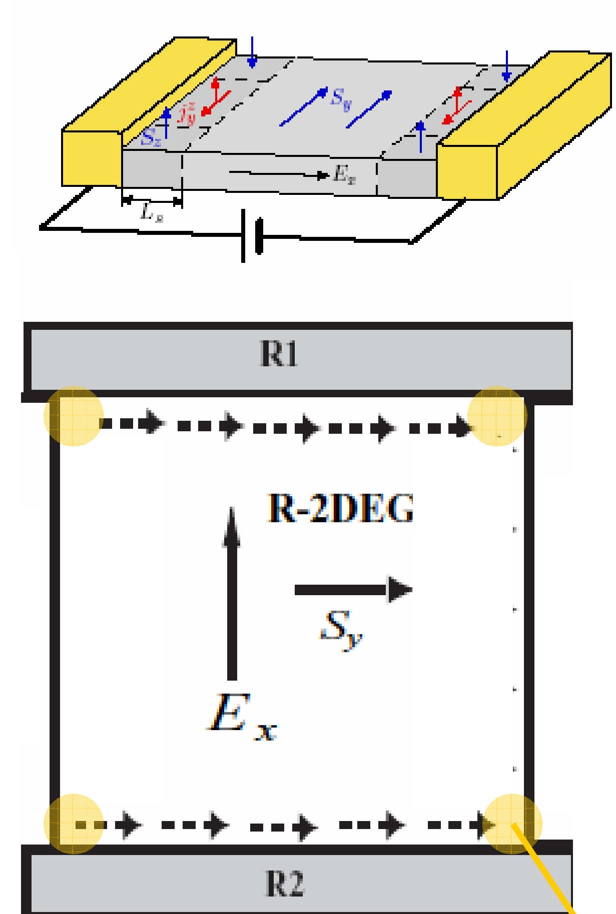


Bulk vs. edge

Adagideli, Bauer, PRL95 ('05).



Mishchenko,Shytov,Halperin, PRL('04)



No bulk spin Hall effect

but

Spin Hall current flows into the leads.

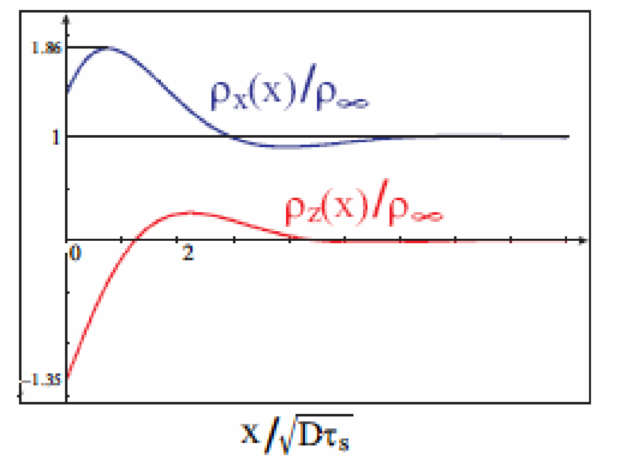
$\left(\frac{e}{8\pi} \right.$ in the clean limit $\left. \right)$

Presence of leads is essential.

Spin accumulation

Galitski,Burkov, Das Sarma, cond-mat/0601677

Spin accumulation depends on the nature of the boundary



Hall effect of light

- Anomalous velocity due to Berry phase

  → interference of waves in wavepackets ($\vec{k}$ and $\vec{k}+\delta\vec{k}$)

  Common in every wave phenomenon.

How about "light" ?

↓

YES!

Hall effect of light

Hall effect of light

Onoda, SM, Nagaosa, Phys. Rev. Lett.93, 083901 (2004)

-- Analog of the spin Hall effect --

Semiclassical eq. of motion

$$\begin{cases} \dot{\vec{r}} = v(\vec{r})\hat{k} + \dot{\vec{k}} \times \langle z | \vec{\Omega}(\vec{k}) | z \rangle \\ \dot{\vec{k}} = -k \nabla v(\vec{r}) \\ |\dot{z}\rangle = -i\dot{\vec{k}} \cdot \vec{\Lambda}(\vec{k}) | z \rangle \end{cases}$$

Shift of a trajectory of light beam
"Hall effect of light"

Geometrical optics
"Fermat's principle"

Polarization change

Chiao,Wu('86) : theory
Tomita,Chiao('86) : experiment

$v(\vec{r}) = \dfrac{c}{n(\vec{r})}$: slowly varying

$|z\rangle$: polarization

$\vec{\Lambda}(\vec{k})$: gauge field

$\vec{\Omega}(\vec{k})$: Berry curvature

In the vacuum

$$\vec{\Omega}(\vec{k}) = \frac{\vec{k}}{k^3} \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

→ Left circular pol.
→ right

in the helicity basis

Eigen-equations

$$\begin{aligned}\overleftrightarrow{\epsilon}(\boldsymbol{r})\partial_t \boldsymbol{\Phi}^E_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t) &= \boldsymbol{\nabla}\times\boldsymbol{\Phi}^H_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t),\\ \overleftrightarrow{\mu}(\boldsymbol{r})\partial_t \boldsymbol{\Phi}^H_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t) &= -\boldsymbol{\nabla}\times\boldsymbol{\Phi}^E_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t),\\ \boldsymbol{\nabla}\overleftrightarrow{\epsilon}(\boldsymbol{r})\boldsymbol{\Phi}^E_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t) &= \boldsymbol{\nabla}\overleftrightarrow{\mu}(\boldsymbol{r})\boldsymbol{\Phi}^H_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t)=0,\end{aligned}$$

Bloch wf.

$$\boldsymbol{\Phi}^I_{n\lambda\boldsymbol{k}}(\boldsymbol{r},t) = e^{-iE_{n\boldsymbol{k}}t}\boldsymbol{\Phi}^I_{n\lambda\boldsymbol{k}}(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}-iE_{n\boldsymbol{k}}t}}{\sqrt{2E_{n\boldsymbol{k}}}}\boldsymbol{U}^I_{n\lambda\boldsymbol{k}}(\boldsymbol{r}),$$

$$I = E \text{ or } H.$$

Gauge field

$$\begin{aligned}\boldsymbol{\Lambda}_{n\boldsymbol{k}} &= \frac{1}{2}\left[\boldsymbol{\Lambda}^E_{n\boldsymbol{k}}+\boldsymbol{\Lambda}^H_{n\boldsymbol{k}}\right],\\ \left[\boldsymbol{\Lambda}^E_{n\boldsymbol{k}}\right]_{\lambda\lambda'} &= -i\langle U^E_{n\lambda\boldsymbol{k}}|\overleftrightarrow{\epsilon}|\boldsymbol{\nabla}_{\boldsymbol{k}}U^E_{n\lambda'\boldsymbol{k}}\rangle,\\ \left[\boldsymbol{\Lambda}^H_{n\boldsymbol{k}}\right]_{\lambda\lambda'} &= -i\langle U^H_{n\lambda\boldsymbol{k}}|\overleftrightarrow{\mu}|\boldsymbol{\nabla}_{\boldsymbol{k}}U^H_{n\lambda'\boldsymbol{k}}\rangle,\end{aligned}$$

(Berry) curvature

$$\boldsymbol{\Omega}_{n\boldsymbol{k}} = \boldsymbol{\nabla}_{\boldsymbol{k}}\times\boldsymbol{\Lambda}_{n\boldsymbol{k}}+i\boldsymbol{\Lambda}_{n\boldsymbol{k}}\times\boldsymbol{\Lambda}_{n\boldsymbol{k}}.$$

Anomalous velocity causes a transverse shift at the interface

Onoda, SM, Nagaosa, PRL93, 083901 (2004)

Anomalous velocity due to Berry phase

$$\dot{\vec{r}} = v(\vec{r})\frac{\vec{k}}{k} + \boxed{\dot{\vec{k}} \times (z|\vec{\Omega}_{\vec{k}}|z)}$$

$$\dot{\vec{k}} = -k\nabla v(\vec{r})$$

Isotropic medium

$$\vec{\Omega}(\vec{k}) = \frac{\vec{k}}{k^3}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

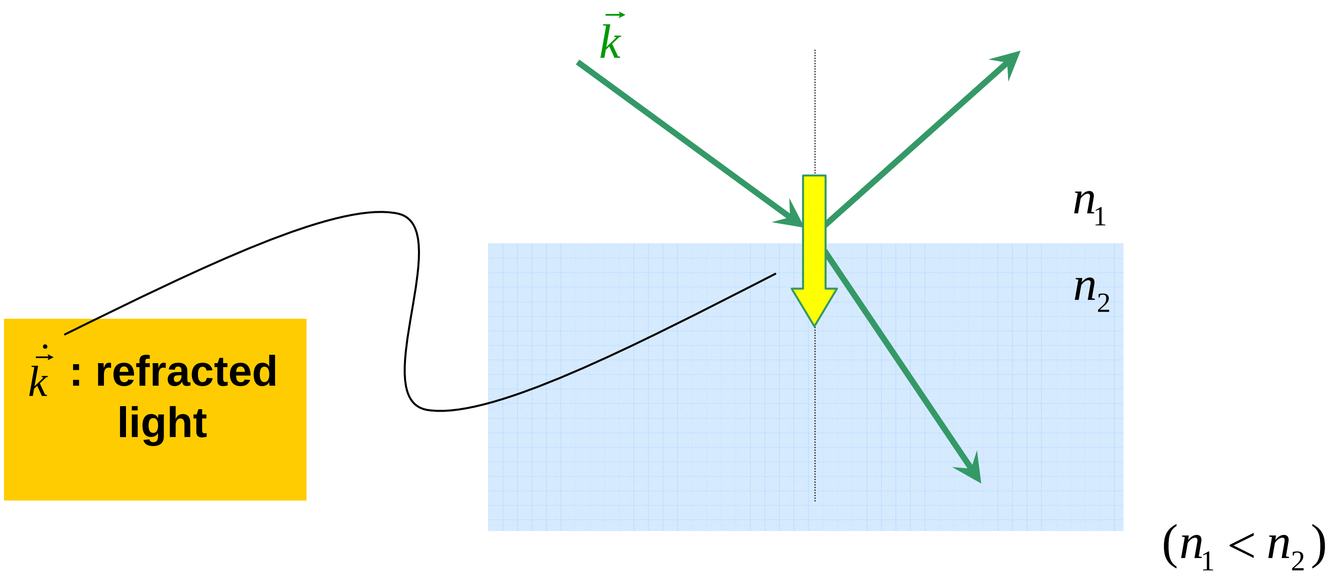
→ Left circular pol.
→ Right circular pol.

in the helicity basis

For refracted light,

→ Anomalous velocity = ⊙
→ Anomalous velocity = ⊗

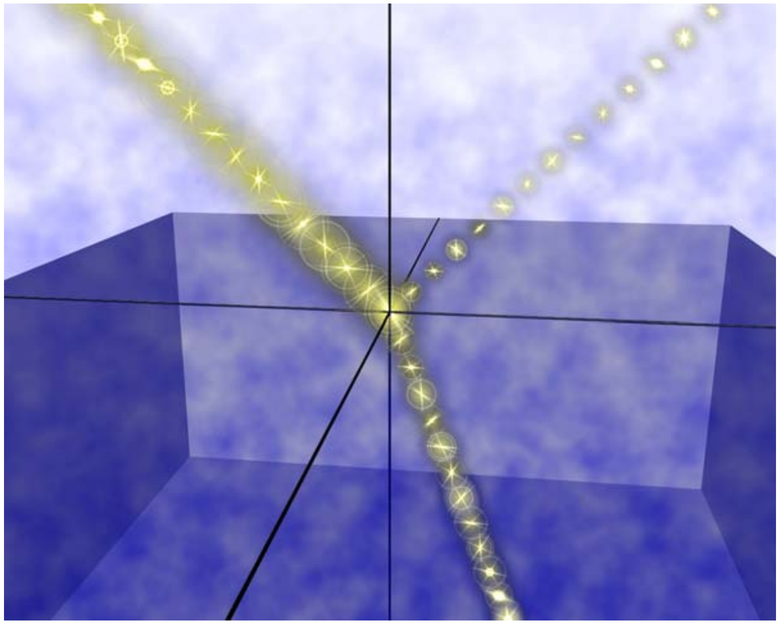
= transverse shift



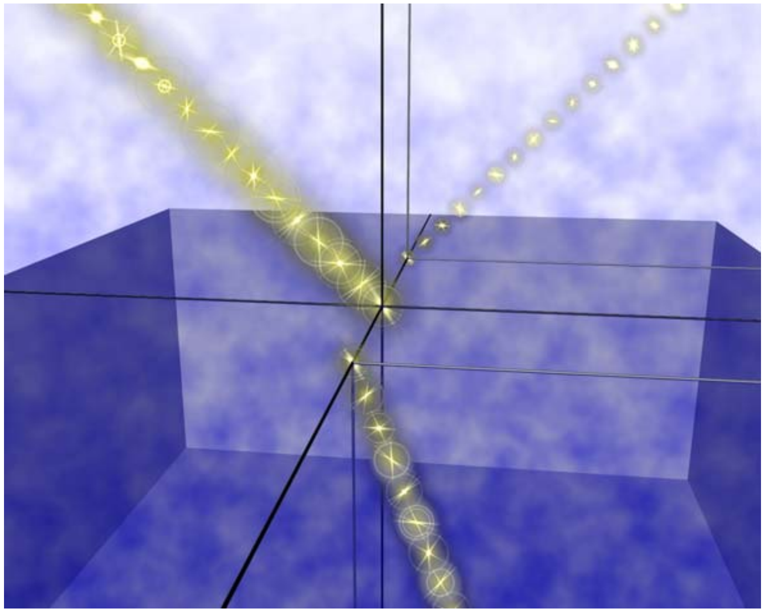
(For reflected light, the direction is opposite.)

Transverse shift

linear polarization



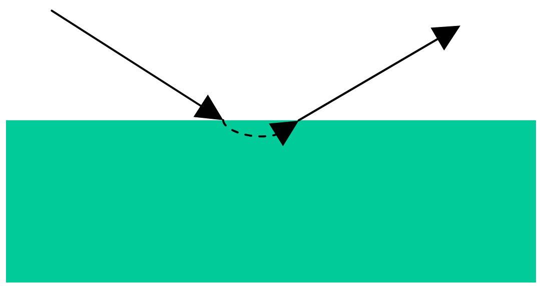
Left circular polarization



Shift of light beam in interface reflection / refraction

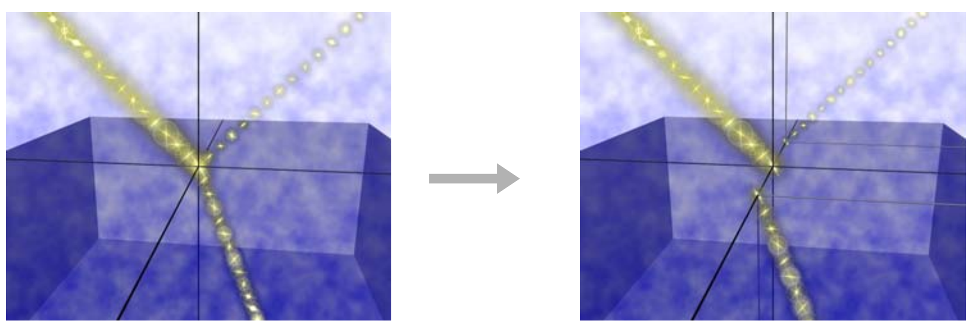
Goos-Hänchen shift

Shift within the incident plane
Different shift for s-pol. and p-pol.



Imbert shift

Shift perpendicular to the incident plane.
Opposite shift for right and left circular polarization.



Theory: Fedorov (1955)
Experiment: Imbert(1972)

Magnitude of the shift $\approx \lambda$
Width of the beam is much larger → not easy to observe.

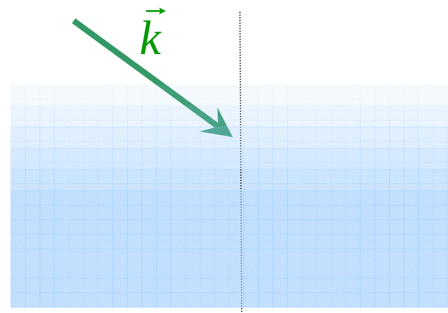
Calculation of the shift

Semiclassical eq. of motion can describe "gradual interface"

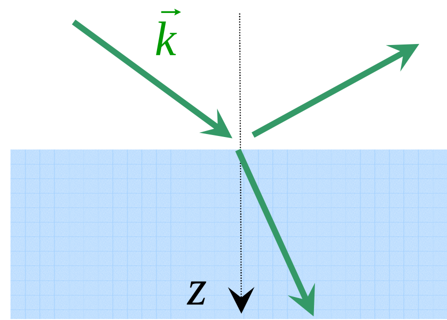
$$\dot{\vec{r}} = v(\vec{r})\hat{k} + \dot{\vec{k}} \times \langle z | \vec{\Omega}(\vec{k}) | z \rangle$$

$$\dot{\vec{k}} = -k\nabla v(\vec{r})$$

$$|\dot{z}\rangle = -i\dot{\vec{k}} \cdot \vec{\Lambda}(\vec{k}) | z \rangle$$



It cannot describe "sharp interface"
in particular the splitting into transmitted & reflected beams.



Instead we use the conservation of the total angular momentum (TAM).

$$\vec{j} = \vec{r} \times \vec{k} + \langle z | \sigma_3 | z \rangle \hat{k}$$: z-component is conserved due to rotational symmetry

Assumption: j_z is conserved for reflected and transmitted light beam, respectively.

$$j_z^I = j_z^R = j_z^T$$

According to Bliokh and Bliokh, PRL (2006),...

PRL 96, 073903 (2006) PHYSICAL REVIEW LETTERS week ending 24 FEBRUARY 2006

Conservation of Angular Momentum, Transverse Shift, and Spin Hall Effect in Reflection and Refraction of an Electromagnetic Wave Packet

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(Received 16 August 2005; published 23 February 2006)

We present a solution to the problem of reflection and refraction of a polarized Gaussian beam on the interface between two transparent media. The transverse shifts of the beams' centers of gravity are calculated. They always satisfy the total angular momentum conservation law for beams, but, in general, do not satisfy the conservation laws for individual photons as a consequence of the lack of the "which path" information in a two-channel wave scattering. The field structure for the reflected and refracted

Conservation of angular momentum

- $j_z^{(i)} = R^2 j_z^{(r)} + T^2 \dfrac{n_2 \mu_1 \cos\theta'}{n_1 \mu_2 \cos\theta} j_z^{(t)}.$: for whole beam → correct
- $j_z^{(i)} = j_z^{(r)}, \qquad j_z^{(i)} = j_z^{(t)}.$: for individual photon → **incorrect!**

As is shown later, it is not true!

$$|z\rangle \propto |p\rangle + m|s\rangle$$

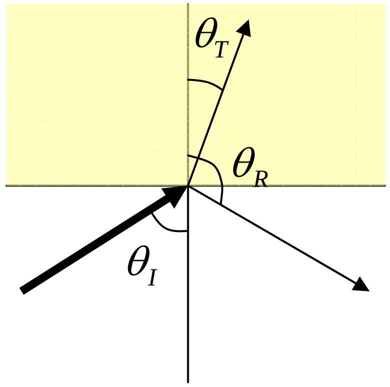
p-pol. s-pol.

$m = i$: left circular pol.

$m = -i$: right circular pol.

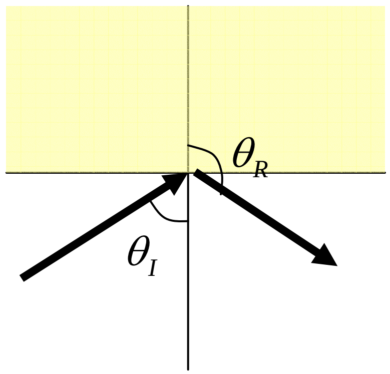
Transverse shift in partial refraction/reflection

$$\delta y^A = \frac{2\,\mathrm{Im}\,m}{k\sin\theta_I}\left[\frac{(A_s/A_p)\cos\theta_A}{1+(A_s/A_p)^2\,|m|^2} - \frac{\cos\theta_I}{1+|m|^2}\right] \quad (A = R, T)$$



Transverse shift in total reflection

$$\delta y^R = \frac{-2\cos\theta_I}{k\sin\theta_I}\,\frac{\left(\mathrm{Re}(A_p^* A_p)+1\right)\mathrm{Im}\,m + \mathrm{Re}\,m\,\mathrm{Im}(A_p^* A_p)\,\mathrm{Re}\,m}{1+|m|^2}$$

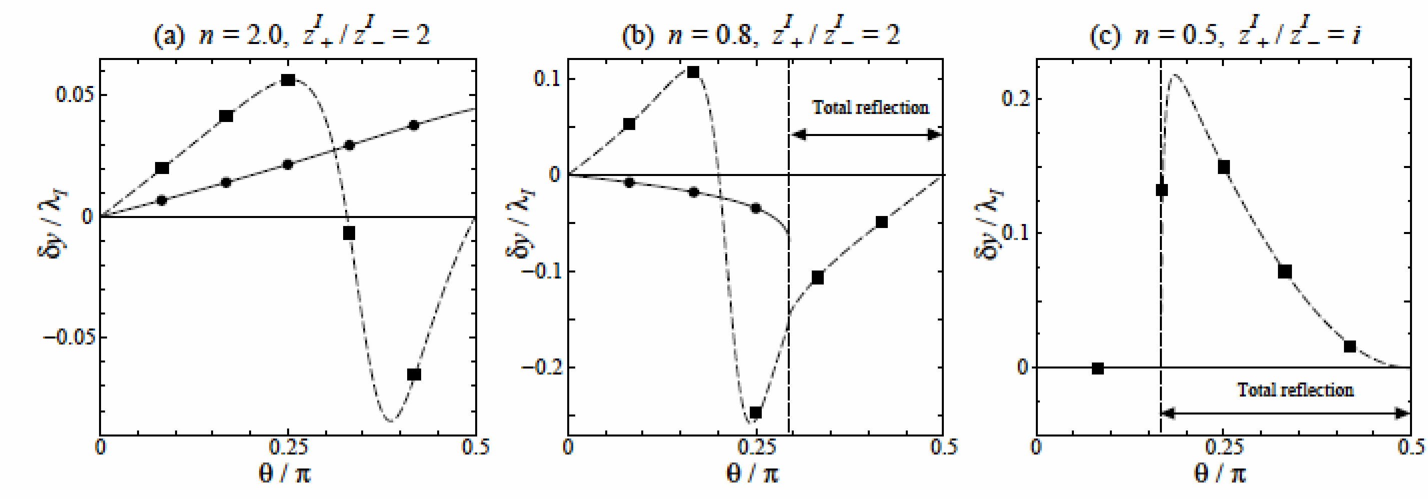


Identical with calculation of the shift by Maxwell eq. by Fedoseev ('91).

Transverse shift: Numerical results

Elliptic polarization

Linear polarization



— : Transmitted beam

– – : Reflected beam

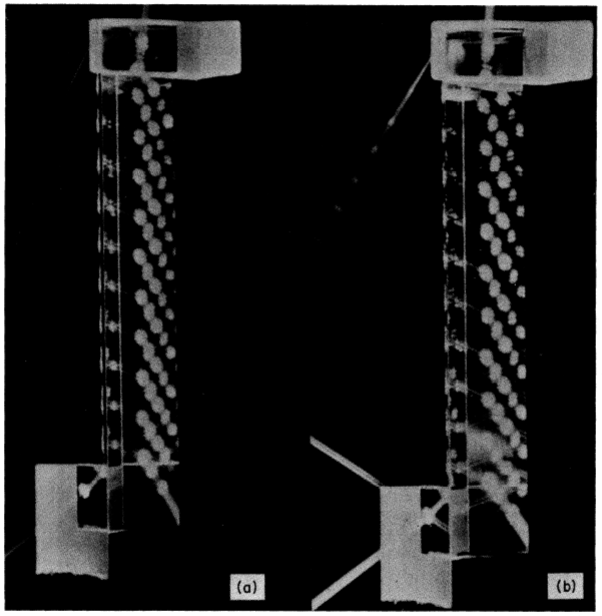
■ ● : numerical simulation

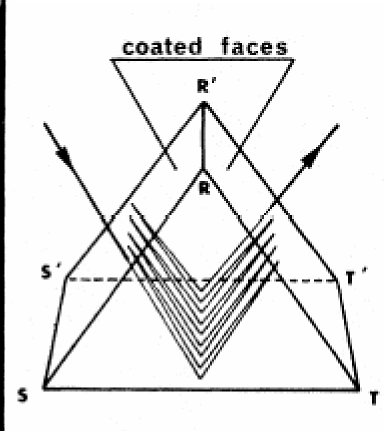
(i) TAM conservation for individual photons
(ii) Analytic calculation with Maxwell eq.
(iii) Numerical simulation

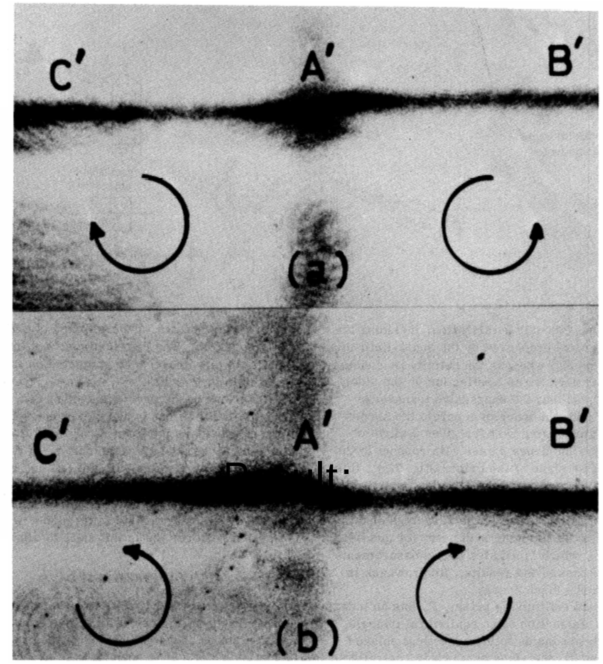
} Identical results

Experiments: transverse shift on total reflection (Imbert shift)

Imbert, PRD5, 787 (1972)

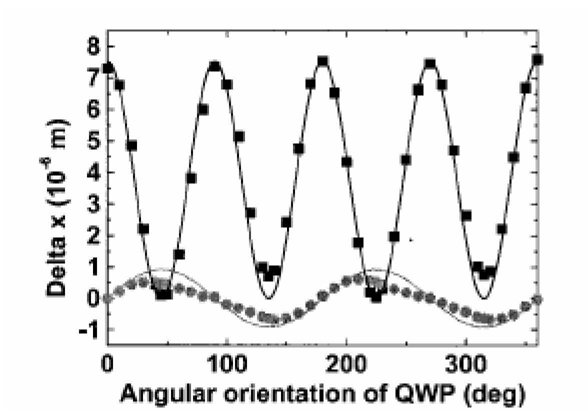






28 total reflections

Pillon et al. Appl. Opt. (2004)



Good agreement with theory.

Photonic crystals and Berry phase

Electrons in condensed matter:

Periodic lattice enhances the Hall effect by orders of magnitude

Will the "Hall effect of light" enhanced in photonic crystals?

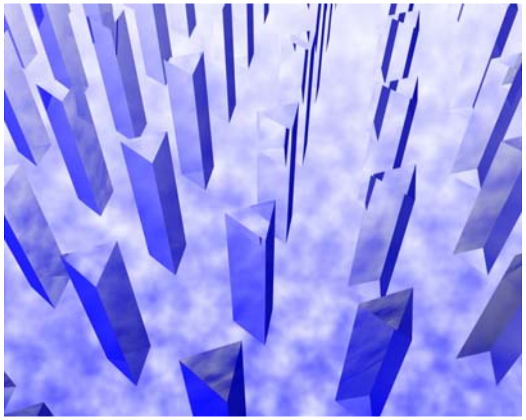
→ YES!

(Example) 2D photonic crystals (PC)

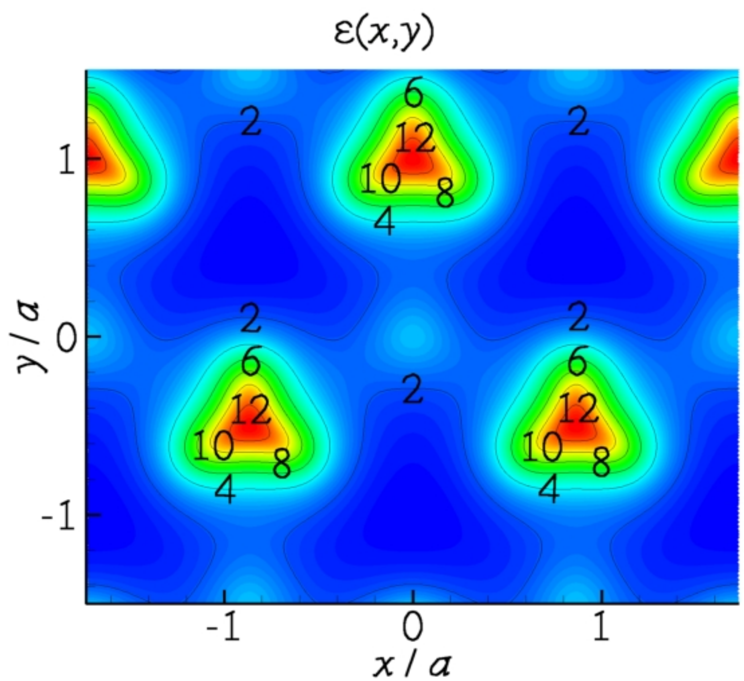
<u>**Caution**</u> :

Berry curvature is zero for 2D PC with inversion symmetry.

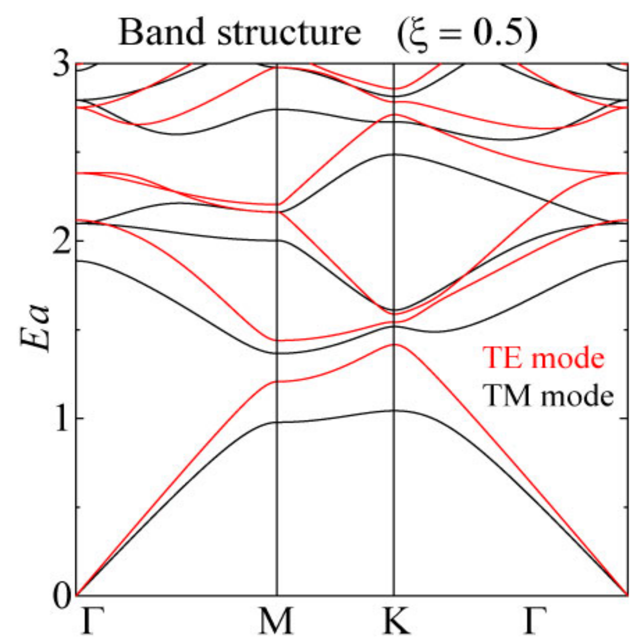
We use a 2D PC without inversion symmetry.



Simulation : Dielectric constant and its band structure



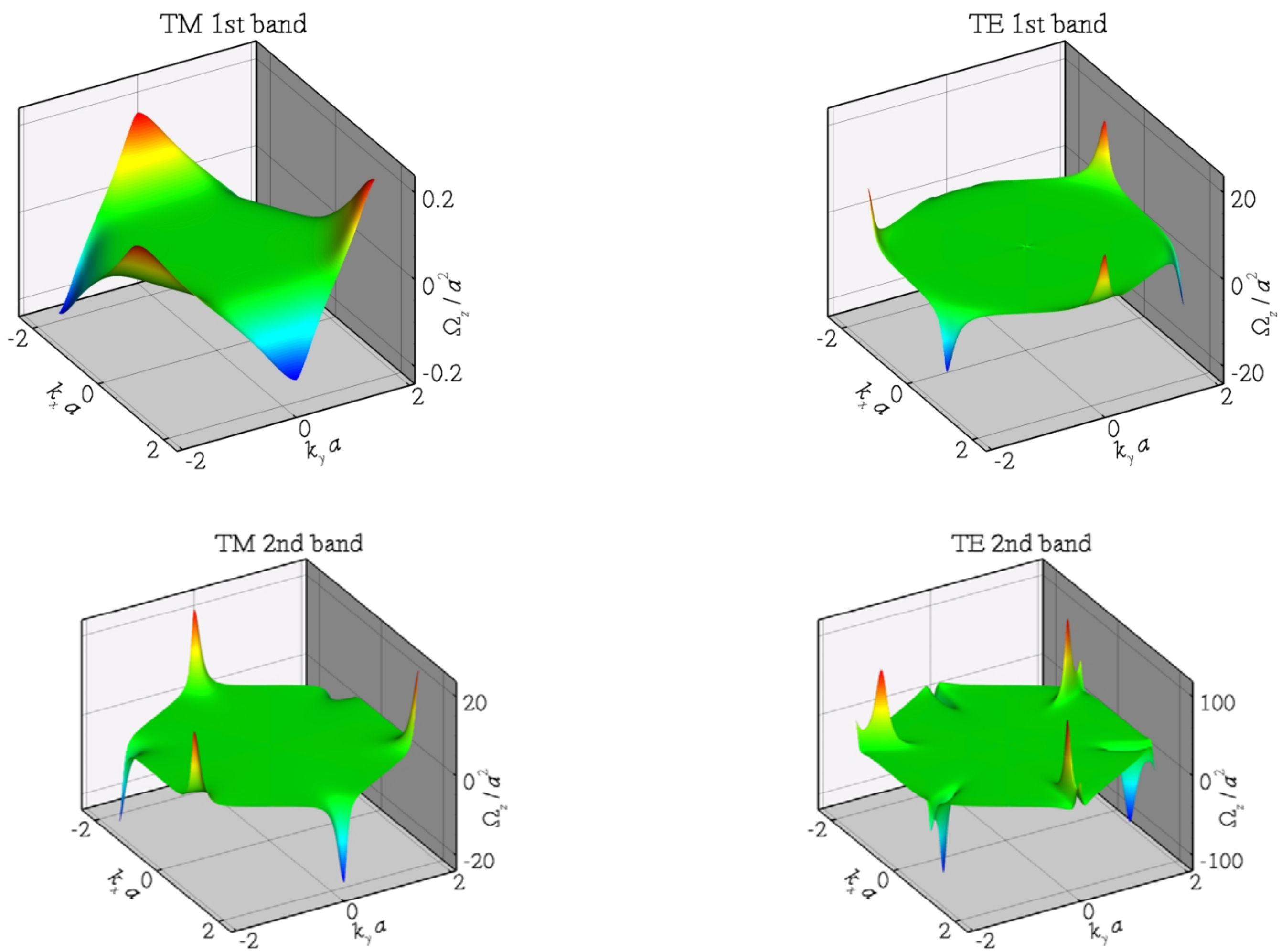
Dielectric constant



Photonic band structure

Onoda, SM, Nagaosa, Phys. Rev. Lett.93, 083901 (2004)

Berry phase in photonic crystals



Large Berry curvature when the band approach other bands in energy

Enhancement of Berry curvature in photonic crystals

• vacuum : $\left|\vec{\Omega}_{\vec{k}}\right| \approx \dfrac{1}{k^2}$ ⟶ Shift $\approx \lambda$ very small (e.g.: Imbert shift)

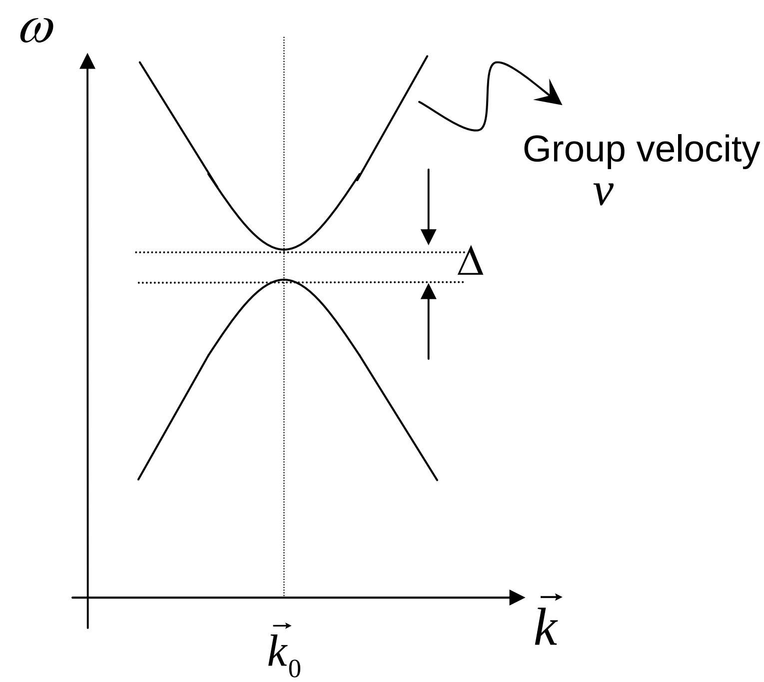
• photonic crystals:

$$\Omega_z \approx \frac{v^2 \Delta}{\left(\Delta^2 + v^2 (\vec{k} - \vec{k}_0)^2\right)^{3/2}}$$

⟶ maximum at the gap : $\Omega_z \approx \dfrac{v^2}{\Delta^2}$

Maximum shift of the beam $\dfrac{v}{\Delta}$

Bigger for smaller gap



Trajectory of light beam in photonic crystals

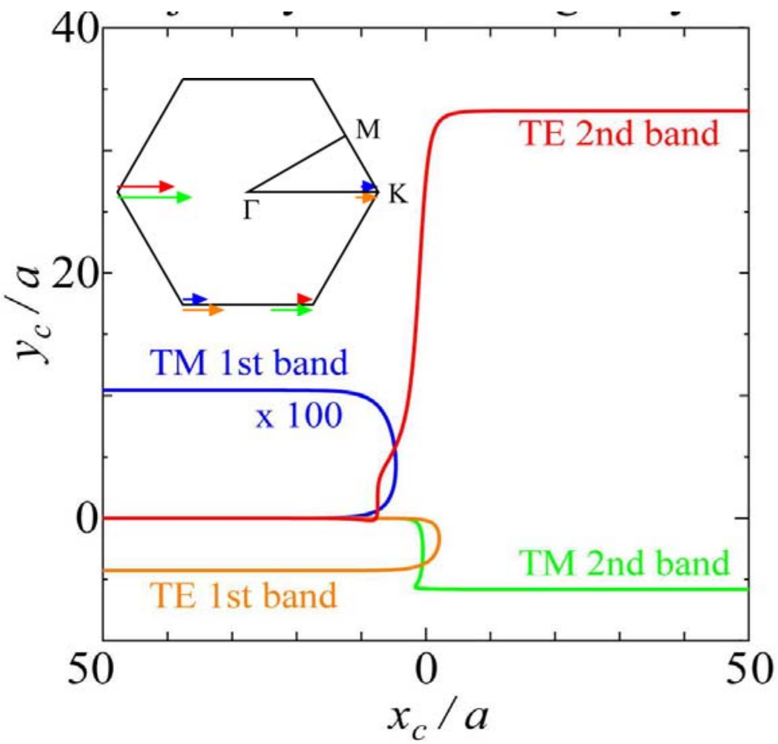
To see the anomalous velocity $\dot{\vec{k}} \times (z|\vec{\Omega}_{\vec{k}}|z)$
$\vec{k}$ should change in time.

(In addition to periodic modulation of $\varepsilon(\vec{r})$),
slow 1D modulation needed

slow 1D modulation near x=0

larger ε for larger x

Simulation



Large shift !!

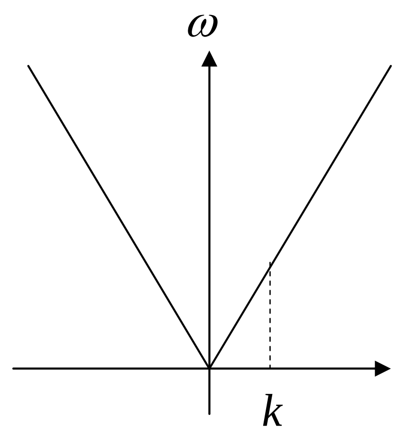
Onoda, SM, Nagaosa, Phys. Rev. Lett.93, 083901 (2004)

Shift of the light beam $\approx$ Distance from a monopole in k space

- Vacuum: monopole at k=0

(shift) $\approx \lambda <<$ (width of the beam)

Small shift

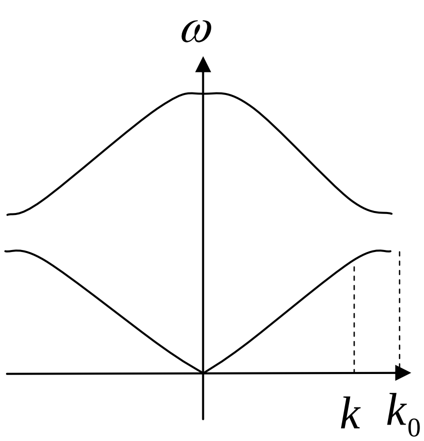


- Photonic crystal: monopole at band-touching points k_0

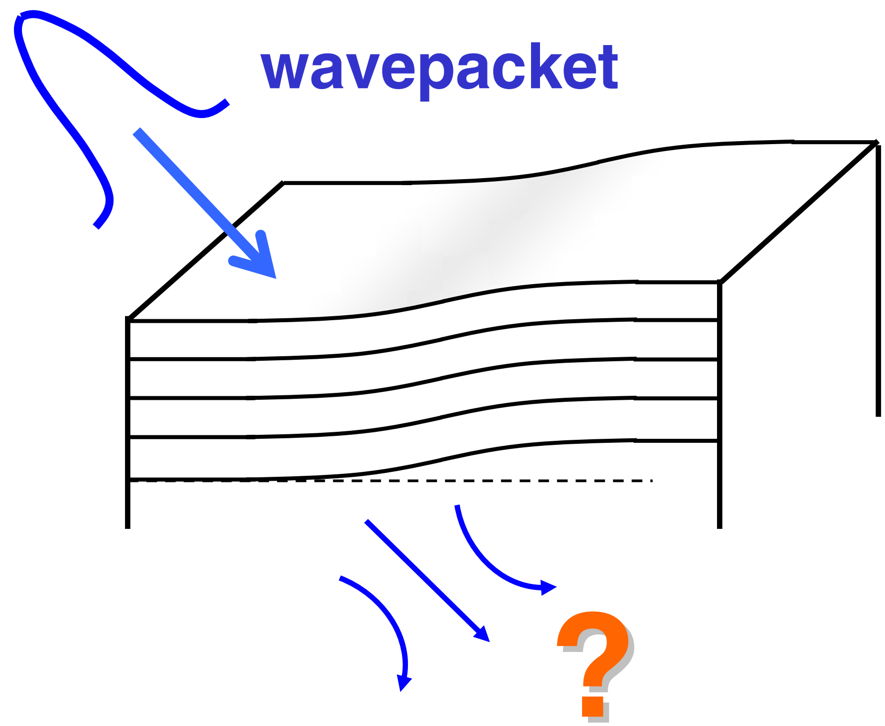
(shift) $\approx \dfrac{1}{|\vec{k}-\vec{k}_0|}$

(width of the beam) $>> \dfrac{1}{|\vec{k}|}$

Shift can be large
(if we use the beam near k_0)



Enhanced shift of X ray trajectory by crystal deformation



Equations of motion for wavepackets including **spatial modulation** of the potential.

Equations of motion for wavepackets

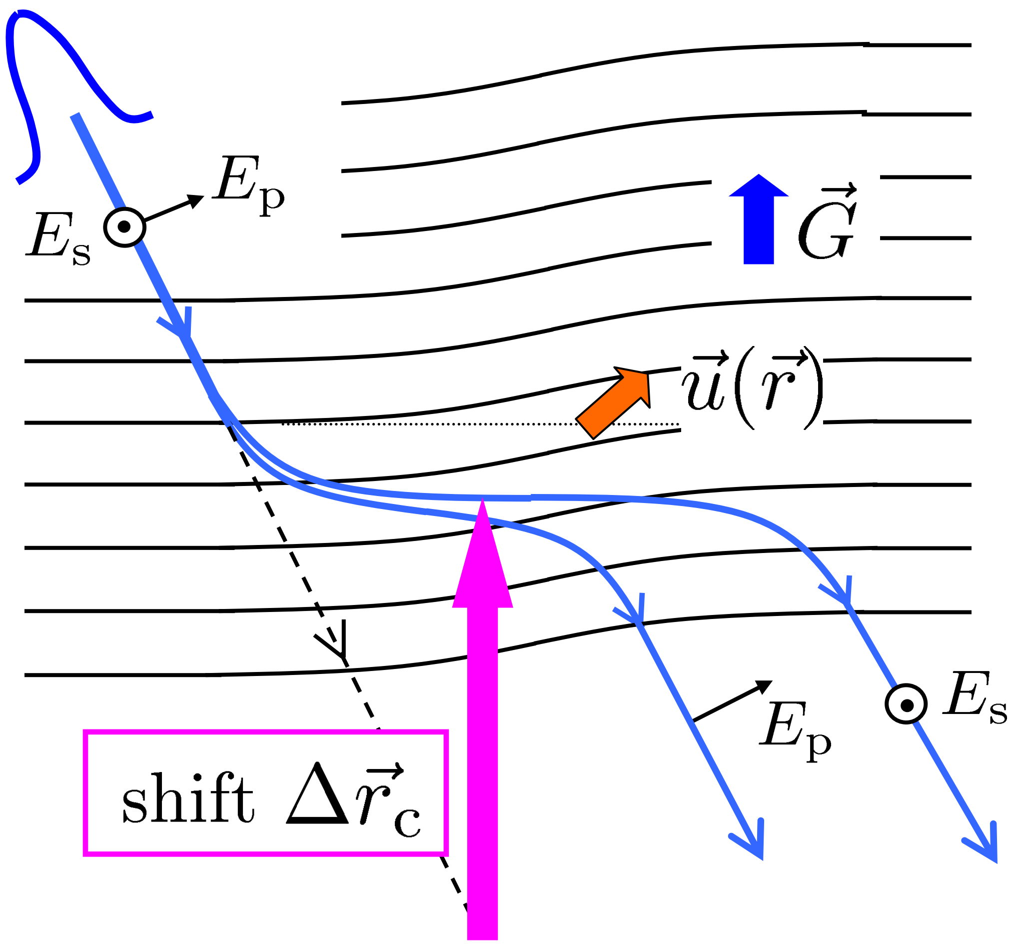
- Sundaram and Niu, PRB **59**, 14915(1999).
- Onoda, Murakami and Nagaosa, PRL **93**, 083901(2004).

Answer **Deformation displaces the wavepacket.**

Deformation

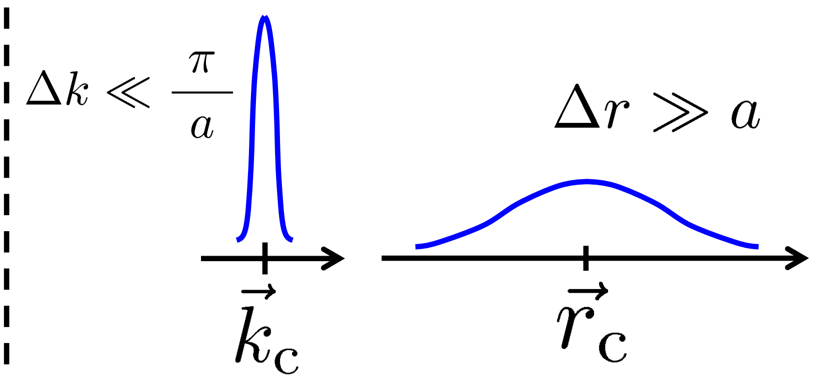
Atomic position: $\vec{r} \longrightarrow \vec{r} + \vec{u}(\vec{r})$

Wavefunction: $\vec{\Gamma}(\vec{r}) \longrightarrow \vec{\Gamma}(\vec{r} - \underline{\underline{\vec{u}(\vec{r}_c)}})$



Wavepacket

$$W(\vec{k}_c, \vec{r}_c, t) = \int \frac{d\vec{k}}{(2\pi)^3} \underline{\underline{w(\vec{k}, \vec{k}_c, t)}} \vec{\Gamma}_{n\vec{k}z_c}(\vec{r}_c)$$



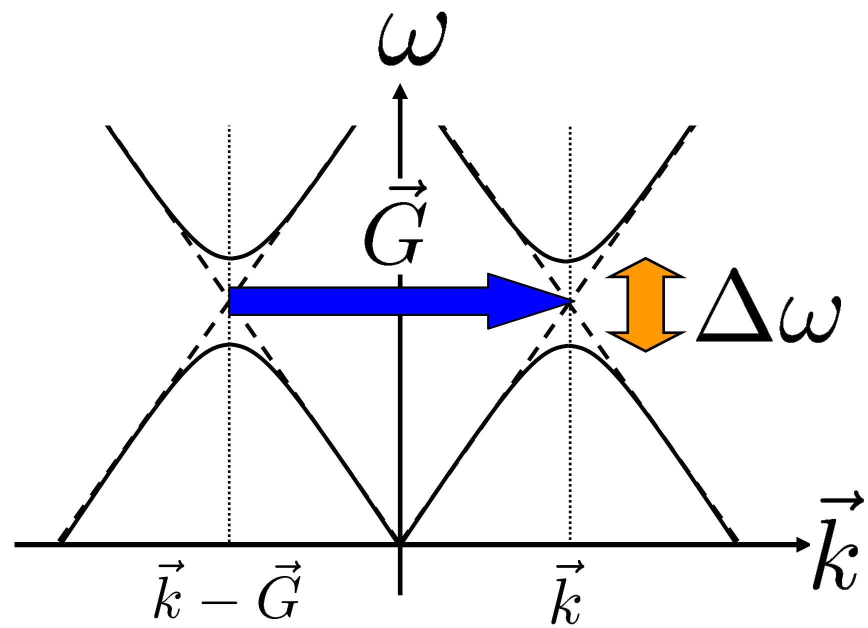
Sawada, SM, Nagaosa, Phys. Rev.Lett. 96,154802 (2006)

Two-wave approximation

Size of the **gap**

$$\frac{\Delta\omega}{\omega} \approx 10^{-6}$$

for x-ray in crystals.



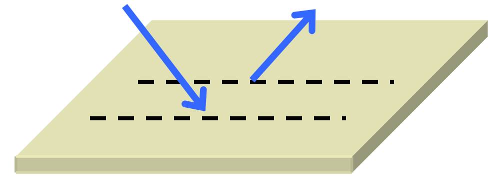
- Only two waves ($\vec{k}$ and $\vec{k} - \vec{G}$) is enough

→ can calculate analytically

Role of each term

$\vec{v}_g$: group velocity

"Hall effect" **(Onoda *et al.*)**



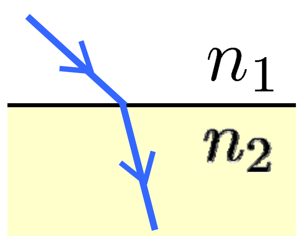
$$\begin{cases} \dot{\vec{r}}_c = \dfrac{\partial \omega_n}{\partial \vec{k}_c} - \Omega_{\vec{k}\vec{k}} \cdot \dot{\vec{k}}_c - \Omega_{\vec{k}\vec{r}} \cdot \dot{\vec{r}}_c + \Omega_{t\vec{k}} & \text{(Shift)} \\ \dot{\vec{k}}_c = -\dfrac{\partial \omega_n}{\partial \vec{r}_c} + \Omega_{\vec{r}\vec{r}} \cdot \dot{\vec{r}}_c + \Omega_{\vec{r}\vec{k}} \cdot \dot{\vec{k}}_c - \Omega_{t\vec{r}} & \text{(Refraction)} \end{cases}$$

(Lorentz force)

Geometrical optics

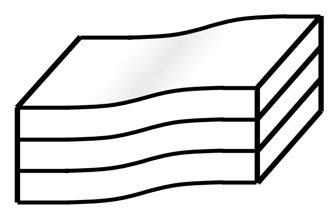
Snell's law

$$\frac{d}{ds}\left[n(\vec{r})\frac{d\vec{r}}{ds}\right] = \text{grad } n(\vec{r})$$



Deformation

Let's calculate!

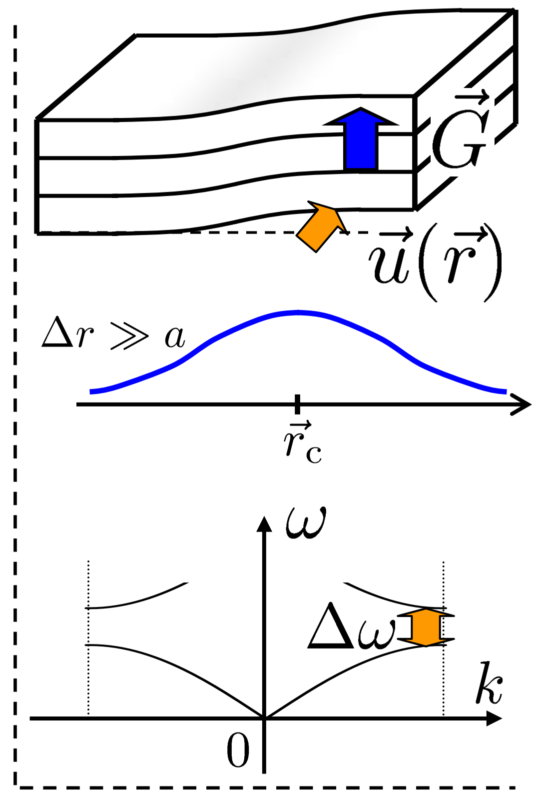


Formula for the shift

$$(\Omega_{\vec{k}\vec{r}})_{\alpha\gamma} = -\frac{\partial u_\beta}{\partial r_\gamma}\frac{\partial \mathcal{A}_{\mathrm{r}\beta}}{\partial k_\alpha}$$

Two-wave approx.
in $|\vec{k}| \simeq |\vec{k}-\vec{G}|$.

$$\simeq \pm\frac{1}{2}\frac{G_\alpha G_\beta}{k^2}\frac{\omega}{\Delta\omega}$$



Integrate the EOM for center position:

$$\dot{\vec{r}}_{\mathrm{c}} = \vec{v}_{\mathrm{g}} - \Omega_{\vec{k}\vec{r}}\cdot\dot{\vec{r}}_{\mathrm{c}}$$

$\int_0^t dt$

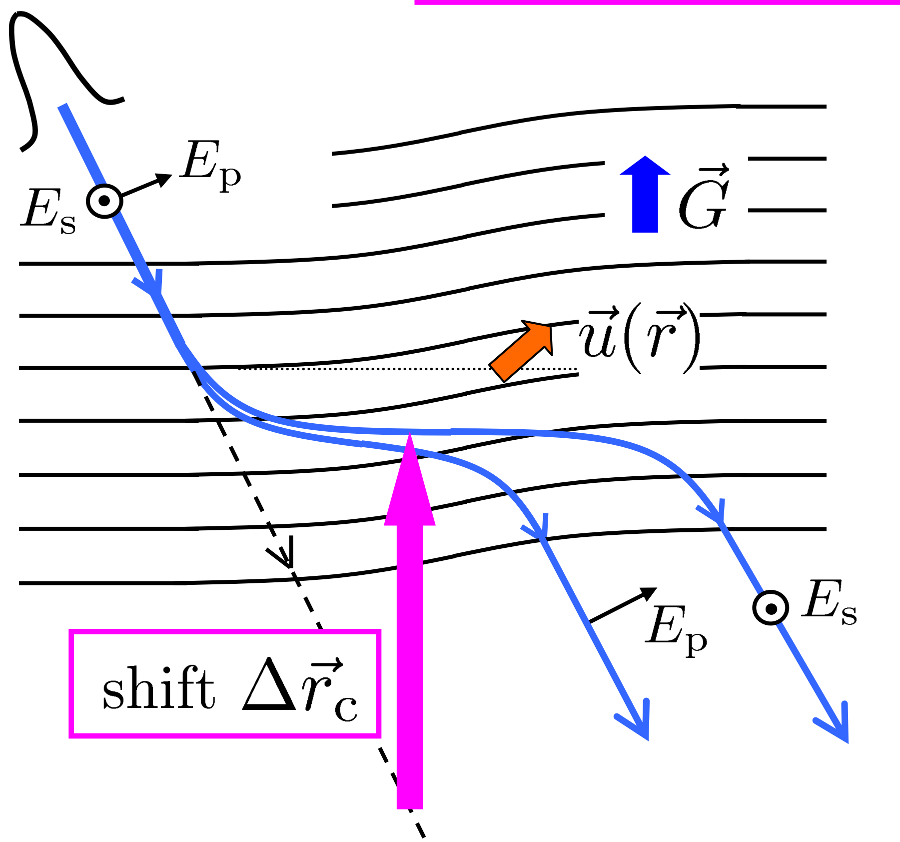
$$r_{\mathrm{c}\alpha} - r_{0\alpha} = v_{\mathrm{g}\alpha}t + \int(\Omega_{\vec{k}\vec{r}}\cdot\dot{\vec{r}}_{\mathrm{c}})_\alpha dt$$

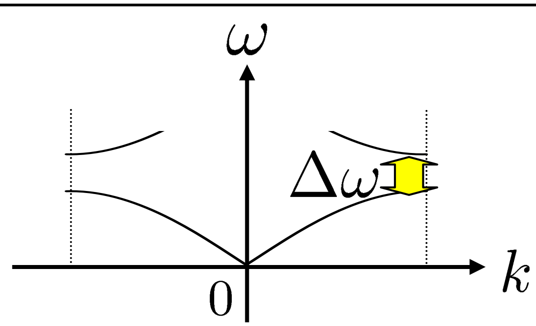
$$= v_{\mathrm{g}\alpha}t + \int\frac{\partial u_\beta}{\partial r_\gamma}\frac{\partial \mathcal{A}_{\mathrm{r}\beta}}{\partial k_\alpha}\dot{r}_\gamma dt = v_{\mathrm{g}\alpha}t + \frac{\partial \mathcal{A}_{\mathrm{r}\beta}}{\partial k_\alpha}\int d\vec{u}_\beta$$

$$\vec{r}_{\mathrm{c}} - \vec{r}_0 = \vec{v}_{\mathrm{g}}t \pm \vec{G}\Big[\vec{G}\cdot\Big(\vec{u}(\vec{r}_{\mathrm{c}}) - \vec{u}(\vec{r}_0)\Big)\Big]\frac{\omega}{2\Delta\omega}\frac{1}{k^2}$$

Trajectory

$$\vec{r}_c - \vec{r}_0 = \vec{v}_g t \pm \vec{G}\left[\vec{G}\cdot\left(\vec{u}(\vec{r}_c) - \vec{u}(\vec{r}_0)\right)\right]\frac{\omega}{2\Delta\omega}\frac{1}{k^2}$$





Displacement $\Delta\vec{r}_c$ is

- parallel to $\vec{G}$
- maximum when $\vec{u} \parallel \vec{G}$
- $\pm$ for lower and upper bands
- magnified by a factor $\dfrac{\omega}{\Delta\omega}$

$\sim 10^6$

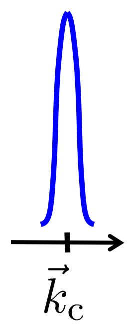
Sawada, SM, Nagaosa, Phys. Rev.Lett. 96,154802 ('06)

Realistic estimate

$$\vec{r}_{\rm c} - \vec{r}_0 = \vec{v}_{\rm g} t \pm \vec{G}\left[\vec{G}\cdot\left(\vec{u}(\vec{r}_{\rm c}) - \vec{u}(\vec{r}_0)\right)\right]\frac{\omega}{2\Delta\omega}\frac{1}{k^2}$$

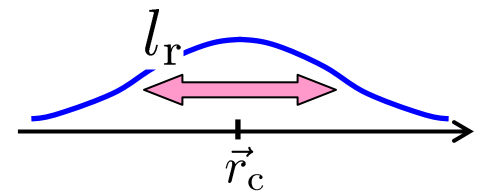
- deformation
  $|\vec{u}(\vec{r})| \sim 0.1\ \mathrm{nm}$

- width in *k*-space
  $\dfrac{\Delta k}{k} \sim \dfrac{\Delta\omega}{\omega} \sim 10^{-6}$



uncertainty principle

- width in real space
  $l_{\rm r} \sim 0.1\ \mathrm{mm}$



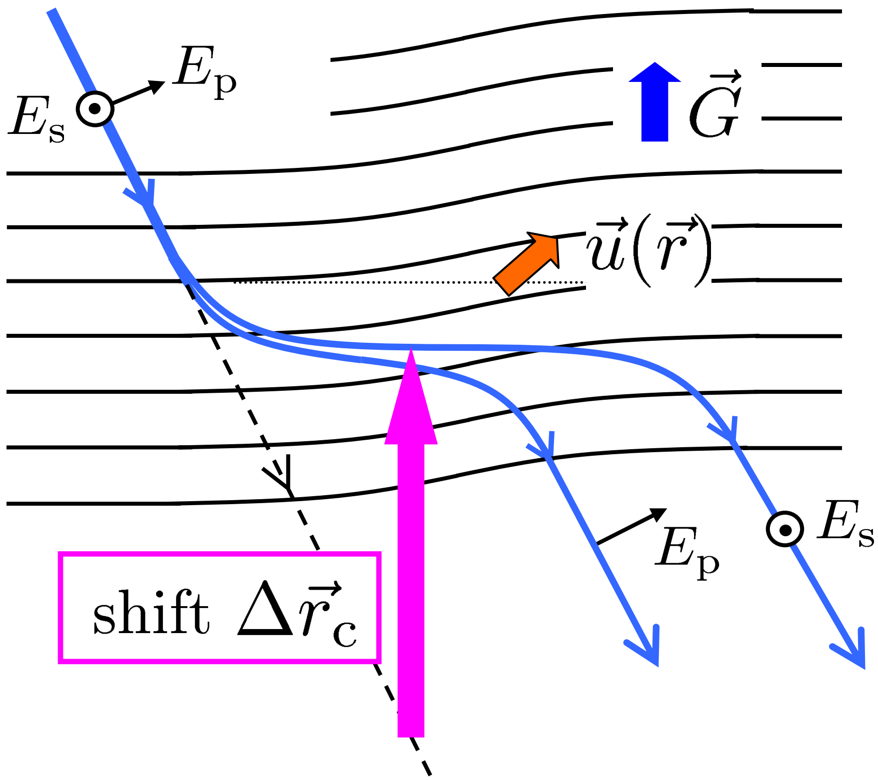
- Shift
  $|\Delta\vec{r}_{\rm c}| \sim 0.1\ \mathrm{mm}$

The deformation $|\vec{u}(\vec{r})| \sim 0.1\ \mathrm{nm}$
gives the shift $|\Delta\vec{r}_{\rm c}| \sim 0.1\ \mathrm{mm}.$

Summary

Bloch state has non-trivial structures

Equations of motion for **wavepackets** have **Berry phase** terms.



Formula

$$\vec{r}_c - \vec{r}_0 = \vec{v}_g t$$
$$\pm\vec{G}\left[\vec{G}\cdot\Big(\vec{u}(\vec{r}_c) - \vec{u}(\vec{r}_0)\Big)\right]\frac{\omega}{2\Delta\omega}\frac{1}{k^2}$$

- parallel to $\vec{G}$
- maximum when $\vec{u} \parallel \vec{G}$
- $\pm$ for lower and upper bands
- magnified by a factor $\frac{\omega}{\Delta\omega} \sim 10^{-6}$
- $|\Delta\vec{r}_c| \sim 0.1\ \mathrm{mm}$