Geometric Phase Effect in Systems Driven by a Parametric Force

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Outline

- A brief review of quantum charge pump
- Dynamics under a parametric force
- Berry-phase modified density of states
- Equilibrium properties:
  - Electron density and Fermi sea volume
- Transport properties:
  - Inverse spin Hall effect

Pumping in Insulating States

- Thouless (1983)
  - Ideal: filled bands in 1D periodic potential
  - Pumped charge in a cycle is a Chern number

$$C = \frac{i}{2\pi}\sum_{\lambda} f_\lambda \int_0^T dt \int_0^{2\pi/L} dk \left[\left\langle \frac{\partial \psi_{\lambda k}}{\partial t} \middle| \frac{\partial \psi_{\lambda k}}{\partial k} \right\rangle - \left\langle \frac{\partial \psi_{\lambda k}}{\partial k} \middle| \frac{\partial \psi_{\lambda k}}{\partial t} \right\rangle \right]$$

- Niu & Thouless (1984)

  – General: disorder and many-body interaction.

  – Quantization is as robust as the quantum Hall effect

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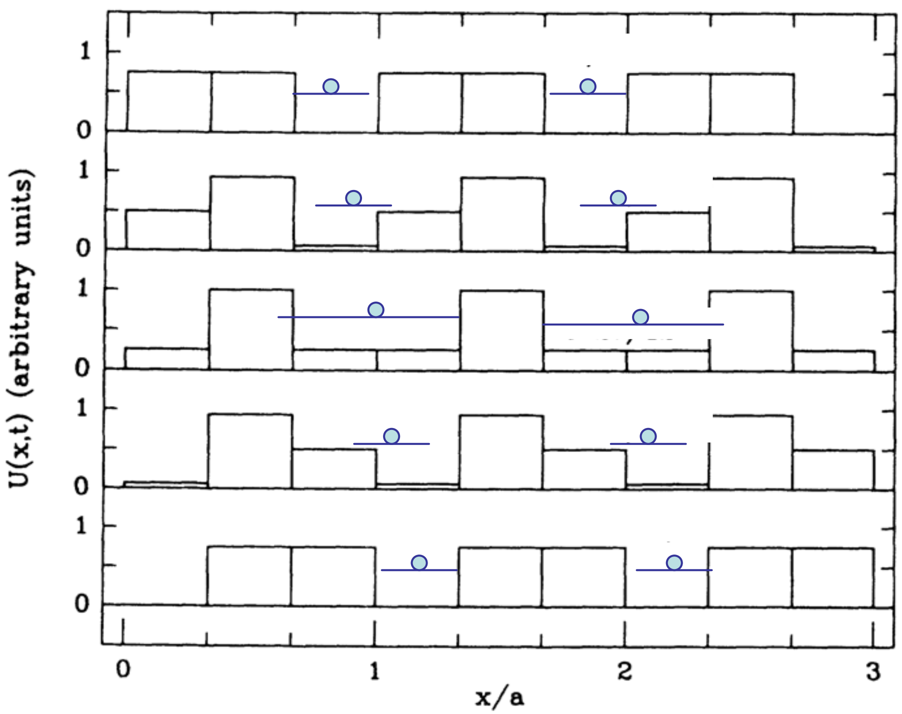
Towards a Quantum Pump of Electric Charges

Q. Niu



- **Pump *n* electrons per cycle**
  – by gating a quantum wire

- **Extreme precision for a charge current standard**

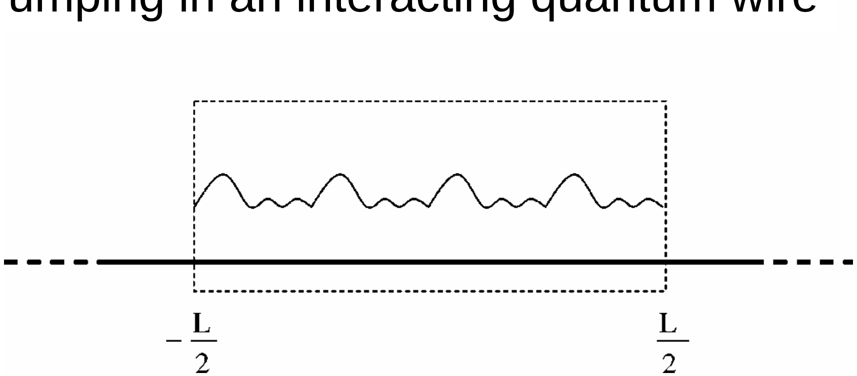
•20 ppm achieved by

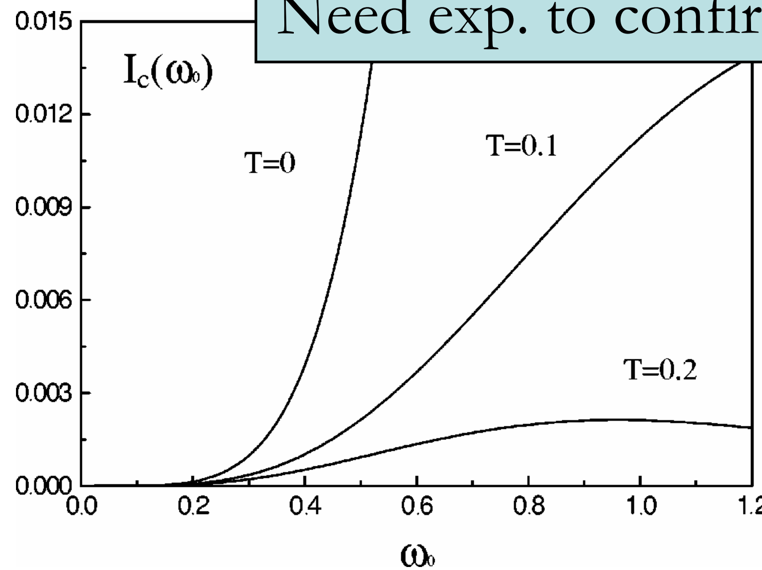
J. Cunningham, V. I. Talyanskii, J. M. Shilton, M. Pepper, M. Y. Simmons, and D. A. Ritchie, PRB (1999)

Pumping in Metallic States

- P. W. Brouwer, PRB (1998)
- M. Switkes, C. M. Marcus, K. Campman, and A. C. Gossard, Science (1999)
  L. DiCarlo, C. M. Marcus, and J. S. Harris, PRL (2003).
- Our own work: Citro, Andrei & Niu, PRB (2003)

Pumping in an interacting quantum wire





Need exp. to confirm

Parametric Force

- Analogy with adiabatic pump:
  - position dependent parameters

    vs. time dependent parameters
- Examples of parameters and forces:
  - Scalar potential – Electrical force
  - Vector potential – Lorentz force
  - Lattice positions – Deformation force
  - Zeeman field – Spin force
  - Temperature – Statistical force
- Scope and focus:
  - Equilibrium and transport properties
  - Geometric phase effects

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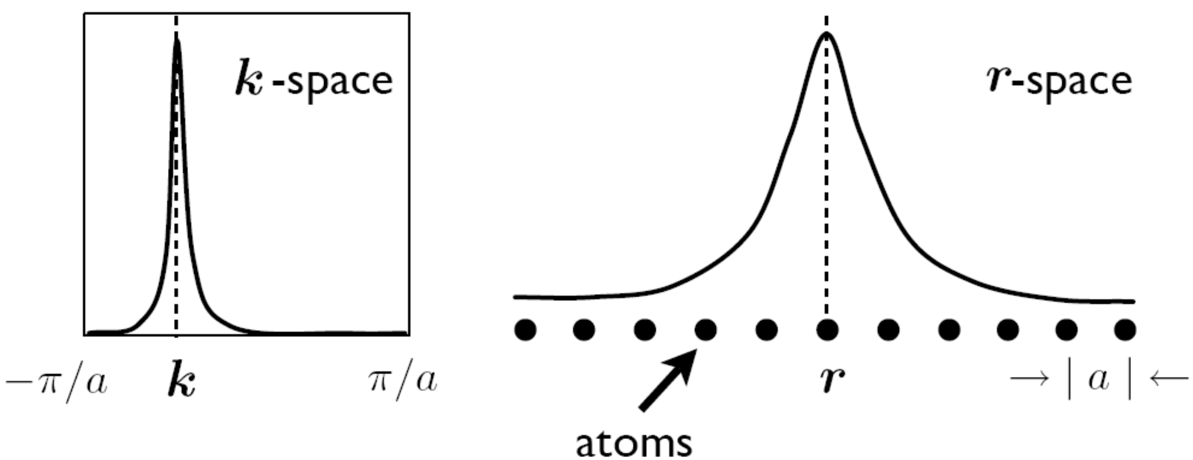
Semiclassical Approach

Hamiltonian $H(\hat{\boldsymbol{r}}, \hat{\boldsymbol{k}}; \beta(\hat{\boldsymbol{r}}, t))$

Fast and periodic

Slowly varying parameters

Classical particle described by a wave packet centered at k and r.



Equations of Motion

Sundaram & Niu, PRB (1999)

$$\dot{\boldsymbol{x}} = \frac{\partial \varepsilon}{\partial \boldsymbol{k}} - (\overleftrightarrow{\Omega}_{\boldsymbol{kx}} \cdot \dot{\boldsymbol{x}} + \overleftrightarrow{\Omega}_{\boldsymbol{kk}} \cdot \dot{\boldsymbol{k}}) + \boldsymbol{\Omega}_{t\boldsymbol{k}}$$

$$\dot{\boldsymbol{k}} = -\frac{\partial \varepsilon}{\partial \boldsymbol{x}} + (\overleftrightarrow{\Omega}_{\boldsymbol{xx}} \cdot \dot{\boldsymbol{x}} + \overleftrightarrow{\Omega}_{\boldsymbol{xk}} \cdot \dot{\boldsymbol{q}}) - \boldsymbol{\Omega}_{t\boldsymbol{x}}$$

Local basis

Berry curvatures:

$$(\overleftrightarrow{\Omega}_{\boldsymbol{kk}})_{\alpha\beta} \equiv \Omega_{k_\alpha k_\beta} \equiv i\left[\left\langle \frac{\partial u}{\partial k_\alpha} \middle| \frac{\partial u}{\partial k_\beta} \right\rangle - \left\langle \frac{\partial u}{\partial k_\beta} \middle| \frac{\partial u}{\partial k_\alpha} \right\rangle\right]$$

$$(\boldsymbol{\Omega}_{t\boldsymbol{x}})_\alpha \equiv \Omega_{t x_\alpha} \equiv i\left[\left\langle \frac{\partial u}{\partial t} \middle| \frac{\partial u}{\partial x_\alpha} \right\rangle - \left\langle \frac{\partial u}{\partial x_\alpha} \middle| \frac{\partial u}{\partial t} \right\rangle\right]$$

Adiabatic Pumping and Polarization

Adiabatic pumping: $\beta(\boldsymbol{x}, t) = \beta(t)$

Equation of motion: $\dot{k} = 0\,, \qquad \dot{x} = \frac{\partial \varepsilon}{\partial k} + \Omega_{tk}$

Current: $j = -e \int_0^{2\pi/a} \frac{dk}{2\pi} \Omega_{tk}$

Charge pumping
(A complete cycle in T)

$$Q = -e \int_0^T dt \int_0^{2\pi/a} \frac{dk}{2\pi} i \Big[\Big\langle \frac{\partial u}{\partial t} \Big| \frac{\partial u}{\partial k} \Big\rangle - \Big\langle \frac{\partial u}{\partial k} \Big| \frac{\partial u}{\partial t} \Big\rangle \Big]$$

Thouless, PRB (1983)

Polarization
$\lambda = \lambda(t)$

$$\Delta P = -e \int_0^1 d\lambda \int_0^{2\pi/a} \frac{dk}{2\pi} i \Big[\Big\langle \frac{\partial u}{\partial \lambda} \Big| \frac{\partial u}{\partial k} \Big\rangle - \Big\langle \frac{\partial u}{\partial k} \Big| \frac{\partial u}{\partial \lambda} \Big\rangle \Big]$$

King-Smith & Vanderbilt, PRB (1983)

Dynamics under Parametric Force

For simplicity, assume 1D & time-independent

$$\beta(x,t) = \beta(x)$$

Equation of motion

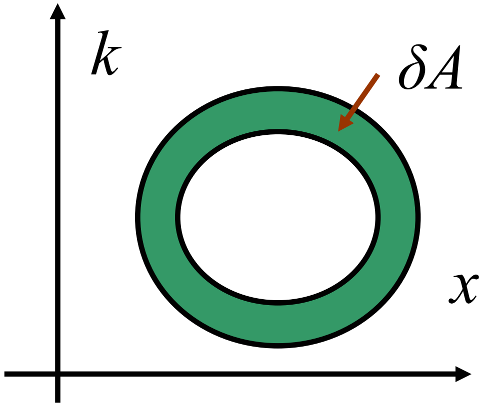
$$\dot{x} = \frac{\partial \varepsilon}{\partial k} - \Omega_{kx}\dot{x} \;, \qquad \dot{k} = -\frac{\partial \varepsilon}{\partial x} + \Omega_{xk}\dot{k}$$

Conservation of energy

$$\varepsilon = \varepsilon_0 + \Delta\varepsilon \;, \qquad \Delta\varepsilon = -\Im\Big[\Big\langle \frac{\partial u}{\partial x}\Big|(\varepsilon - H)\Big|\frac{\partial u}{\partial k}\Big\rangle\Big]$$

Wilkinson-Rammal
term

Semiclassical Quantization



Semi. Quantization $\oint k\, dx = 2\pi(n + \frac{1}{2} - \frac{\gamma_B}{2\pi})$

Berry phase

$$\gamma_B = \int dx dk\, \Omega_{kx}$$

$$\delta A = \frac{2\pi}{1 + \bar{\Omega}_{kx}}$$

Phase-space volume of a quantum state

Average Berry curvature over δA

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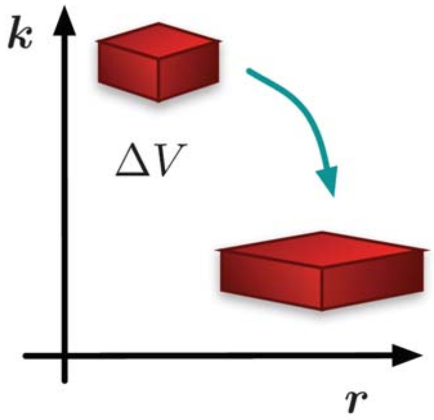
Evolution of Phase-Space Volume



Phase-space volume $\Delta V = \Delta \boldsymbol{r} \Delta \boldsymbol{k}$

Conservation of phase-space volume

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

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

Liouville theorem breaks down! (unless the volume is redefined)

$$\Delta V = \frac{\text{const.}}{\sqrt{\det |\overleftrightarrow{\boldsymbol{\Omega}} - \overleftrightarrow{\mathbf{J}}|}}$$

$$\overleftrightarrow{\Omega} = \begin{pmatrix} \overleftrightarrow{\Omega}^{rr} & \overleftrightarrow{\Omega}^{rk} \\ \overleftrightarrow{\Omega}^{kr} & \overleftrightarrow{\Omega}^{kk} \end{pmatrix} \quad \overleftrightarrow{\mathbf{J}} = \begin{pmatrix} 0 & \overleftrightarrow{\mathrm{I}} \\ -\overleftrightarrow{\mathrm{I}} & 0 \end{pmatrix}$$

Berry-Phase Modified Density of States

Density of states $D = \frac{1}{(2\pi)^d}$ ⇒ $D = \frac{1}{(2\pi)^d}\sqrt{\det|\overleftrightarrow{\mathbf{\Omega}} - \overleftrightarrow{\mathbf{J}}|}$

Special cases

$$D = (2\boldsymbol{\pi})^{-d}\det(\overleftrightarrow{\mathrm{I}} - \overleftrightarrow{\Omega}^{\boldsymbol{rk}}) \qquad \text{if} \quad \boldsymbol{B} = 0, \overleftrightarrow{\boldsymbol{\Omega}}^{\boldsymbol{rk}} \neq 0$$

$$D = (2\pi)^{-d}(1 + \frac{e}{\hbar}\boldsymbol{\Omega_k}\cdot\boldsymbol{B}) \qquad \text{if} \quad \boldsymbol{B} \neq 0, \overleftrightarrow{\boldsymbol{\Omega}}^{\boldsymbol{rk}} = 0$$

Physical quantity

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

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

Xiao, Shi & Niu, PRL (2005)

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Equilibrium Properties: electron density

Example I: Lattice deformation

$V(x) \to V(x+s(x))$, where $s(x)$ is the displacement field

Berry curvature

$$\Omega_{kx} = \frac{\partial s}{\partial x}\left(m\frac{\partial^2 \varepsilon}{\partial k^2} - 1\right)$$

Electron density

(zero temperature)

$$n = \int_{-k_F}^{k_F} \frac{dk}{2\pi}(1 + \Omega_{kx})$$

Either n or k_F has to change under lattice deformation

Change to Fermi sea size

Charge neutrality requires
(consider background charge)

$$\frac{\delta n}{n_0} = -\frac{\partial s}{\partial x}$$

Change of Fermi vector

$$k_F = k_{F0} + \delta k_F$$

$$\delta k_F = -m \frac{\partial s}{\partial x} \frac{\partial \varepsilon}{\partial k}\Big|_{k_{F0}}$$

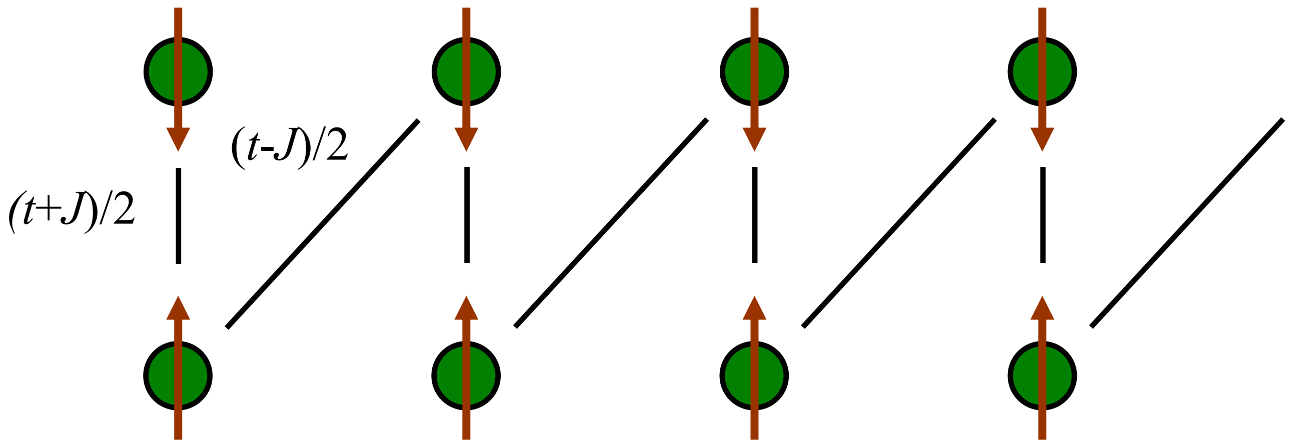
For a filled band,

$$n = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi}(1 + \Omega_{kx}) = n_0(1 - \frac{\partial s}{\partial x})$$

Charge neutrality condition is automatically satisfied.

Equilibrium Properties: electron density

Example II: Antiferromagnetic Spin Chain (Quasi 1D Ferroelectric)



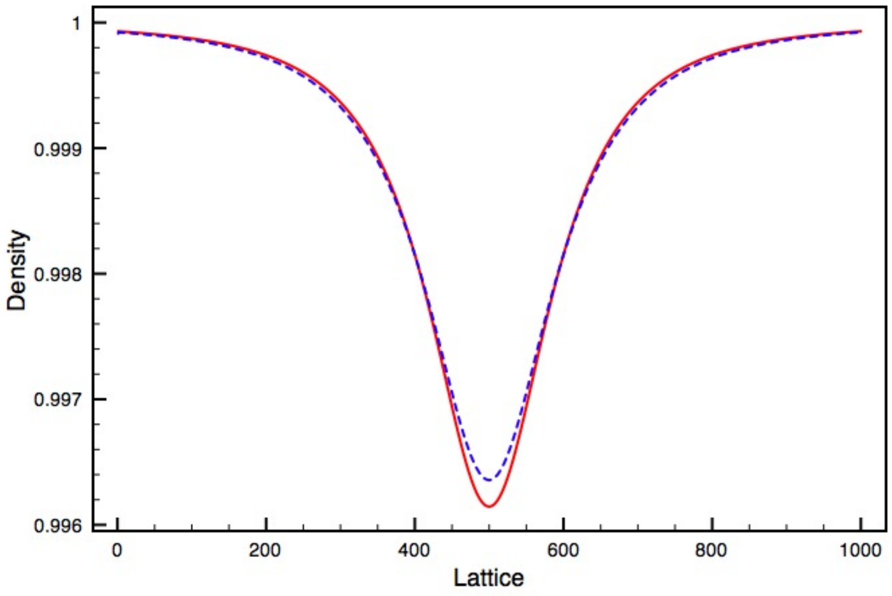
Hamiltonian $$H(k,x) = t\cos\frac{k}{2}\sigma_x + J\sin\frac{k}{2}\sigma_y + h(x)\sigma_z$$

$$\Omega_{kx} = \frac{tJ\nabla h}{2(h^2 + t^2\cos^2\frac{k}{2} + J^2\sin^2\frac{k}{2})^{3/2}}$$

position-dependent Zeeman field

Change of Electron Density

For a filled band (insulator), $t = 2, J = 1, h$: -5 ⟶5; 1000 sites



Theory (solid line)

$$n = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} \Big(1 + \frac{tJ\nabla h}{2(h^2 + t^2\cos^2\frac{k}{2} + J^2 \sin^2\frac{k}{2})^{3/2}} \Big)$$

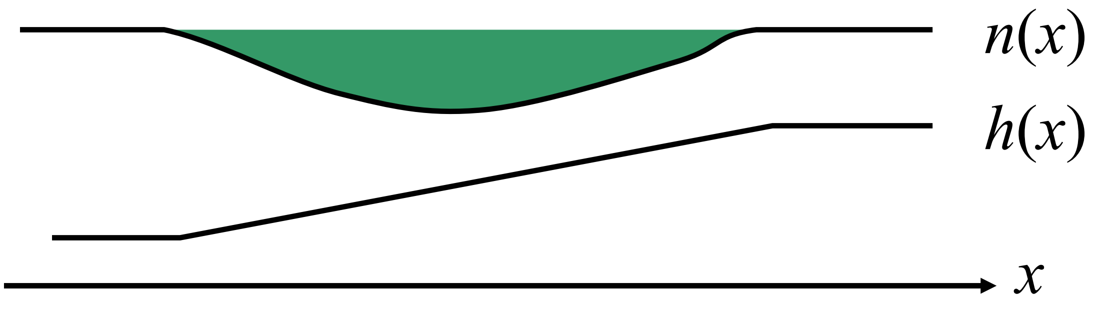
Polarization and Charge Accumulation

$$\boldsymbol{\nabla} \cdot \mathcal{P}(\boldsymbol{r}) = -\rho(\boldsymbol{r}) = \delta n(\boldsymbol{r})$$

A new derivation of polarization formula

$$\Delta\mathcal{P} = \int_{x_1}^{x_2} dx\, \delta n = -e\int_{x_1}^{x_2} dx \int_0^{2\pi/a} \frac{dk}{2\pi}\Omega_{kx}$$
$$= -e\int_{h_1}^{h_2} dh \int_0^{2\pi/a} \frac{dk}{2\pi} i\Big[\Big\langle\frac{\partial u}{\partial k}\Big|\frac{\partial u}{\partial h}\Big\rangle - \Big\langle\frac{\partial u}{\partial h}\Big|\frac{\partial u}{\partial k}\Big\rangle\Big]$$

Charge pumping in space



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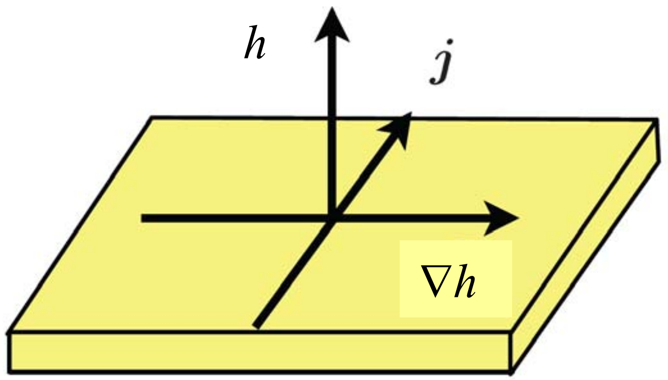
Transport: Inverse Spin Hall Effect

- Charge Hall current driven by the gradient of a Zeeman field
- Reciprocal of the spin Hall effect
- Avoids the problem of measuring spin current directly



The Model and Berry Curvatures

2D electrons in an asymmetric quantum well

$$H = \frac{k^2}{2m} + \alpha(\boldsymbol{k} \times \boldsymbol{\sigma}) \cdot \hat{z} + h(\boldsymbol{r})\sigma_z$$

Rashba spin-orbit coupling

Zeeman field

Berry curvatures

$$\Omega_{k_x,k_y} = \pm\frac{\alpha^2 h}{2\Delta^3}\,, \qquad \Omega_{k_x,h} = \mp\frac{\alpha^2 k_y}{2\Delta^3}\,, \qquad \Omega_{k_y,h} = \pm\frac{\alpha^2 k_x}{2\Delta^3}$$

$$\Delta \equiv \sqrt{\alpha^2 k^2 + h^2}.$$

Dynamics and Transport

Equations of motion under a spin force $F = \nabla_x h$

$$\hbar \dot{x} = (1 - F\Omega_{k_x,h})\partial_{k_x}\varepsilon + F\partial_{k_x}\delta\varepsilon \ ,$$
$$\hbar \dot{y} = \partial_{k_y}\varepsilon + F\partial_{k_y}\delta\varepsilon - F\Omega_{k_x,k_y}\partial_h\varepsilon - F\Omega_{k_y,h}\partial_{k_x}\varepsilon$$

Transport charge current

$$j = -e\int d\boldsymbol{k}\, D(\boldsymbol{r},\boldsymbol{k})g(\boldsymbol{r},\boldsymbol{k})\dot{\boldsymbol{r}} - e\boldsymbol{\nabla}\times\int d\boldsymbol{k}\,\boldsymbol{\Omega}_{\boldsymbol{k}}(\mu-\varepsilon)$$

Current from equation of motion

Current from orbital magnetization

Xiao, Yao, Fang & Niu, PRL (2006)

Inverse Spin-Hall Current in Metals

Charge current due to spin force F

$$j_y = -\frac{e}{\hbar}F\int^{\mu}[d\boldsymbol{k}](\Omega_{k_x,h}\partial_{k_y}\varepsilon - \Omega_{k_y,h}\partial_{k_x}\varepsilon + \partial_h\Omega_{k_x,k_y}\varepsilon - \partial_h\Omega_{k_x,k_y}\mu - \Omega_{k_x,k_y}\partial_h\mu + \partial_{k_y}\delta\varepsilon)\ ,$$

For Rashba model $\quad j_y = -\frac{e}{8\pi}F$

Spin current due to electric force E_y

$$j_x^s = \frac{e}{8\pi}E_y$$

Onsager relation is satisfied. Shi, Zhang, Xiao & Niu, PRL (2006)

Inverse Spin-Hall Current in Insulators

For a filled band,

$$j_y = \frac{e}{\hbar} F \partial_h \left(\mu \int_{BZ} [d\mathbf{k}] \Omega_{k_x,k_y}\right) = \frac{e}{h} C F \partial_h \mu$$

- No inverse spin Hall effect, if Chern number C=0, or $\partial_h \mu$=0
- No spin Hall effect in such a band by Onsager relation.
- These conclusions remain true for multiple bands, where C should be regarded as the total Chern number.
- We assumed local equilibrium under charge neutrality condition.
- Otherwise, if there are species of electrons with different chemical potentials, as in the Kane-Mele graphene model,

$$j_y = \frac{e}{h} F \sum_\alpha C_\alpha \partial_h \mu_\alpha$$

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