

Effects of Berry Curvature on Thermoelectric Transport



Archisman Panigrahi

UG 4th Year

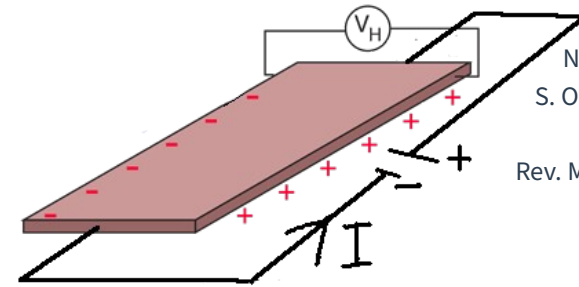
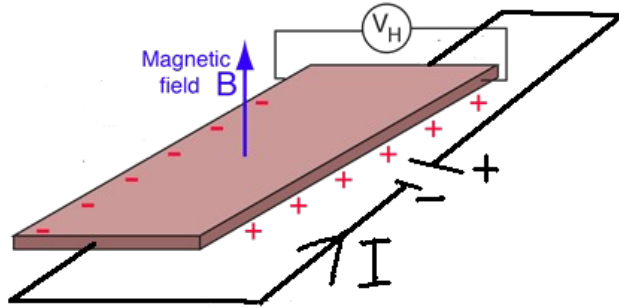
24th June 2021

Supervisor: Prof. Subroto Mukerjee, Dept. of Physics, IISc

Why is this interesting?

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- There can be a transverse Hall voltage without a magnetic field

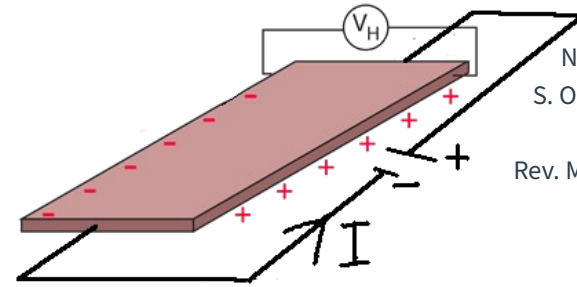
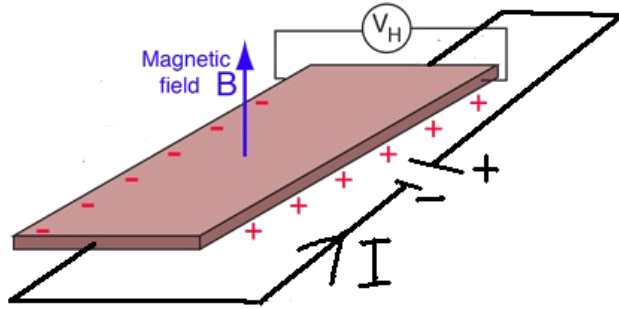


N. Nagaosa, J. Sinova,
S. Onoda, A. H. MacDonald,
and N. P. Ong
Rev. Mod. Phys. **82**, 1539 (2010)

Anomalous Hall Effect

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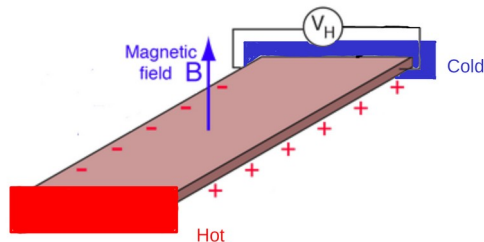
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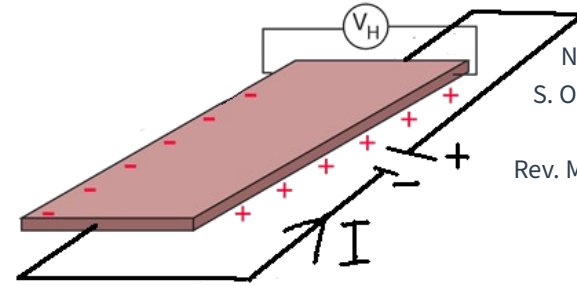
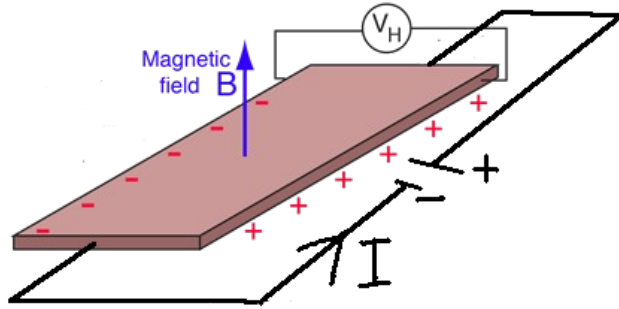
- Nernst Effect: Hall like response for a temperature gradient



Electrically insulating temperature reservoirs

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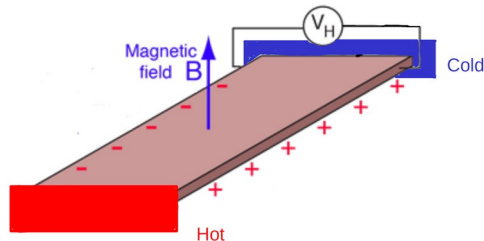
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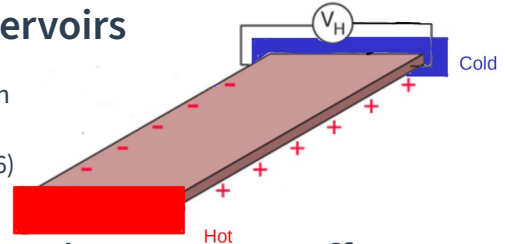
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Electrically insulating temperature reservoirs

Kamran Behnia and Hervé Aubin

Rep. Prog. Phys. **79** 046502 (2016)



Anomalous Nernst Effect

Thermoelectric transport: Einstein and Onsager relations

- Local current densities

$$\hat{\vec{j}}_e = \overleftrightarrow{L}_{11} \cdot \left(\vec{E} + \nabla \frac{\mu}{e} \right) + \overleftrightarrow{L}_{12} \cdot (-\nabla T)$$

$$\hat{\vec{j}}_Q = \overleftrightarrow{L}_{21} \cdot \left(\vec{E} + \nabla \frac{\mu}{e} \right) + \overleftrightarrow{L}_{22} \cdot (-\nabla T)$$

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(experimental)



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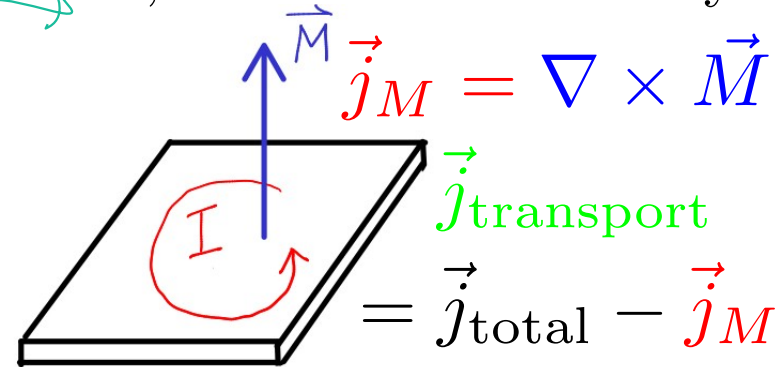
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N. R. Cooper, B. I. Halperin, and I. M. Ruzin. PRB **55** 2344 (1997)

Geometric phase and Berry Curvature

M. V. Berry. Proceedings of the Royal Society A. **392** 1802 (1984)

- Time dependent Hamiltonian $H(\boldsymbol{\lambda}(t))$

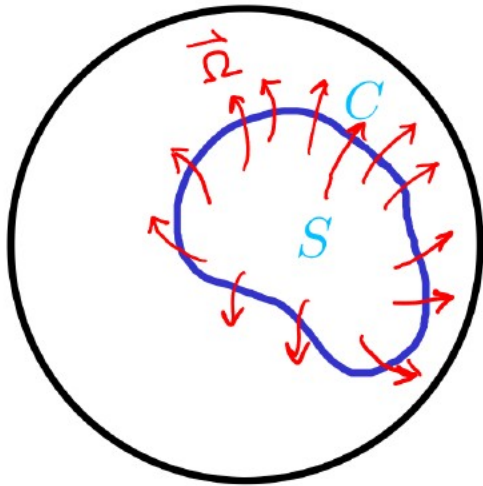
$$|\varepsilon(\boldsymbol{\lambda}(t))\rangle = e^{i\gamma(t)} e^{-\frac{i}{\hbar} \int_0^t \varepsilon(\boldsymbol{\lambda}(t')) dt'} |\varepsilon(\boldsymbol{\lambda}(0))\rangle$$

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Space of $\lambda_1, \lambda_2, \dots$

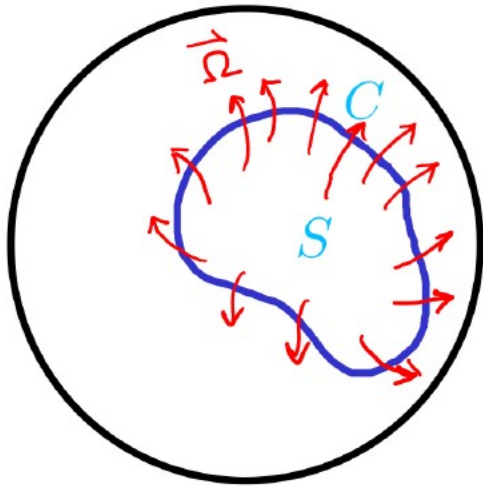
$$\begin{aligned}\gamma &= i \oint_C \langle \varepsilon(\vec{\lambda}) | \nabla_{\vec{\lambda}} | \varepsilon(\vec{\lambda}) \rangle \cdot d\vec{\lambda} \\ &= \oint_C \vec{A}(\vec{\lambda}) \cdot d\vec{\lambda}\end{aligned}$$

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Stokes' theorem: $\vec{\Omega} = \nabla \times \vec{A}$

Like magnetic field, but in parameter space

Berry Curvature in reciprocal space

- Bloch wavefunctions in periodic potential

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

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Effective Schrödinger equation

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$$\gamma_{\vec{k}}(\Delta t) = \vec{A}(\vec{k}) \cdot \Delta \vec{k}$$

- Time evolution

$$u_{n,\vec{k}} \rightarrow e^{i\gamma_{\vec{k}}(\Delta t)} e^{-i\frac{\varepsilon_{\vec{k}}\Delta t}{\hbar}} u_{n,\vec{k}+\Delta\vec{k}}$$

$$\vec{A}(\vec{k}) = i \left\langle u_{n,\vec{k}} \left| \nabla_{\vec{k}} \right| u_{n,\vec{k}} \right\rangle$$

Effects of Berry curvature

Ming-Che Chang and Qian Niu PRL **75**, 1348 (1995),
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(2D)

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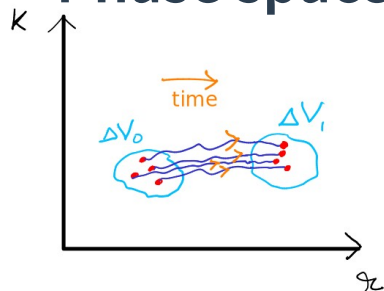
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- Phase space density is modified

Anomalous velocity



$$\Delta V \left(1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega} \right)$$

is a constant of motion

Phase space volume element

Di Xiao, Junren Shi, and Qian Niu. PRL 95, 137204 (2005)

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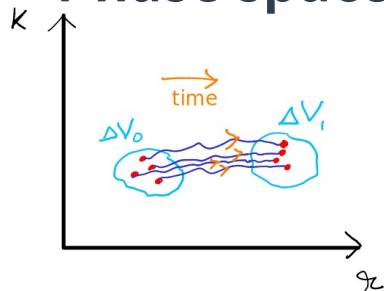
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$$\langle \mathcal{O} \rangle = 2 \int \frac{d\vec{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega}(\vec{k}) \right) \langle \mathcal{O} \rangle_{\vec{k}} \tilde{g}_{\vec{k}}$$

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When do we get a non-zero Berry Curvature?

- If inversion symmetry holds

$$\dot{\vec{r}} = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon_{\vec{k}} - \dot{\vec{k}} \times \boldsymbol{\Omega}(\vec{k})$$

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- If time reversal symmetry holds

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- When both hold simultaneously, Berry curvature is identically zero.

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Boltzmann Transport framework

Classical charge and energy currents

$$\vec{j}_e = -nev, \vec{j}_\epsilon = n\epsilon v$$

Boltzmann Transport framework

Locally averaged
Current density

$$\left\langle \hat{\vec{j}}_e \right\rangle =$$

Classical charge and energy currents
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Semiclassical framework

Boltzmann Transport framework

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$$(-e\dot{\vec{r}})_{\vec{k}} \tilde{g}_{\vec{k}}$$

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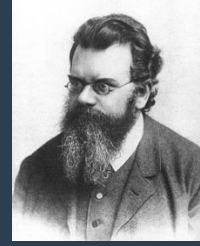
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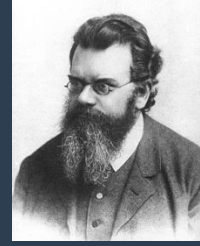
$$\left\langle \hat{\vec{j}}_Q \right\rangle = 2 \int \frac{d\vec{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega}(\vec{k}) \right) (\epsilon_{\vec{k}} - \mu) \dot{\vec{r}}_{\vec{k}} \tilde{g}_{\vec{k}}$$

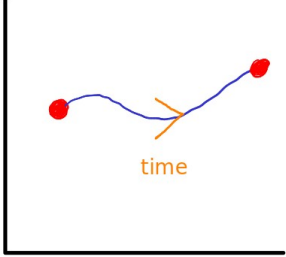
Boltzmann Transport Equation



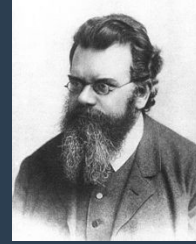
- In equilibrium, \tilde{g}_k is the Fermi distribution. $f_{\vec{k}} = \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} + 1}$
- The external fields are small, and it deviates slightly from the Fermi distribution

Boltzmann Transport Equation



- In equilibrium, \tilde{g}_k is the Fermi distribution. $f_{\vec{k}} = \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} + 1}$
- The external fields are small, and it deviates slightly from ^K the Fermi distribution $\tilde{g}_k = f_k + g_k$ A graph showing a blue curve representing the deviation of the distribution from equilibrium. The curve starts at a red dot on the left, dips, and then rises to another red dot on the right. An orange arrow labeled 'time' points to the right along the x-axis.
- The system tries to attain equilibrium, with a relaxation time $\tau \sim 10^{-14} s$ ⁹⁷
- We assume that the more the distribution deviates, the faster it would try to return to equilibrium, *relaxation time approximation*. $D_t \tilde{g}_k = -\frac{\tilde{g}_k - f_k}{\tau_k}$
$$D_t \equiv \frac{\partial}{\partial t} + \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}} + \dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}}$$

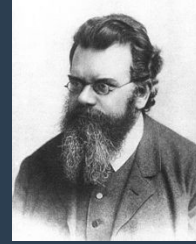
Boltzmann Transport Equation



- In steady-state, and homogeneous fields, the equation becomes,

$$\underbrace{\frac{g_k}{\tau_k} - \frac{\frac{e}{\hbar^2} \frac{\partial \varepsilon}{\partial \vec{k}} \times \vec{B}}{1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega}} \cdot \frac{\partial}{\partial \vec{k}} g_k}_{\text{treated as a perturbation}} = \frac{\partial f}{\partial \varepsilon} \frac{1}{1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \vec{k}} \cdot \left[e \vec{E} + \nabla \mu + \nabla T \frac{\varepsilon - \mu}{T} \right]$$

Boltzmann Transport Equation

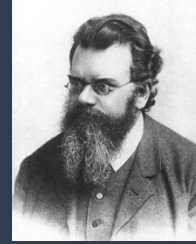


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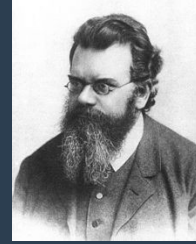
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Dimension analysis: this term $\omega_c \tau \times$
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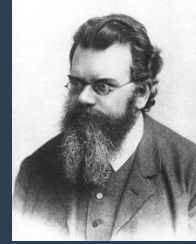
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- If $m^* \sim m, \tau \sim 10^{-14} s$ then the critical field is ~ 570 T

Boltzmann Transport Equation



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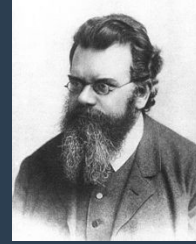
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Why even consider this term, then??

Boltzmann Transport Equation

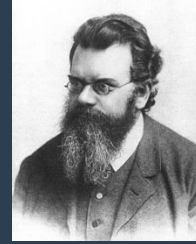


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New result (2D)

Boltzmann Transport Equation



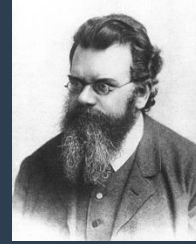
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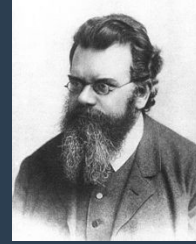
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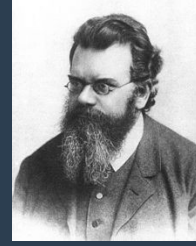
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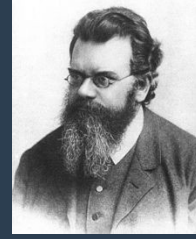
Einstein and Onsager
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1. Dantas, R.M.A., Peña-Benitez, F., Roy, B. et al. J. High Energ. Phys. **2018**, 69 (2018).

2. Ki-Seok Kim, Heon-Jung Kim, and M. Sasaki Phys. Rev. B **89**, 195137 (2014)

3. O. Pal, B. Dey, T. K. Ghosh arXiv:2102.03779 [cond-mat.mes-hall]

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Which all terms contribute

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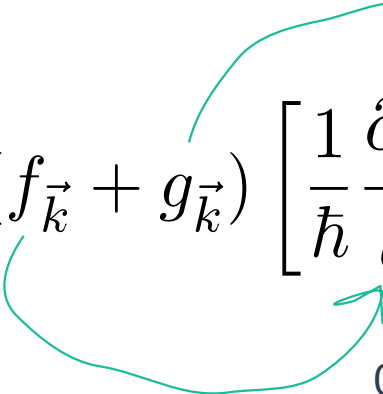
0, as it should be without any external field

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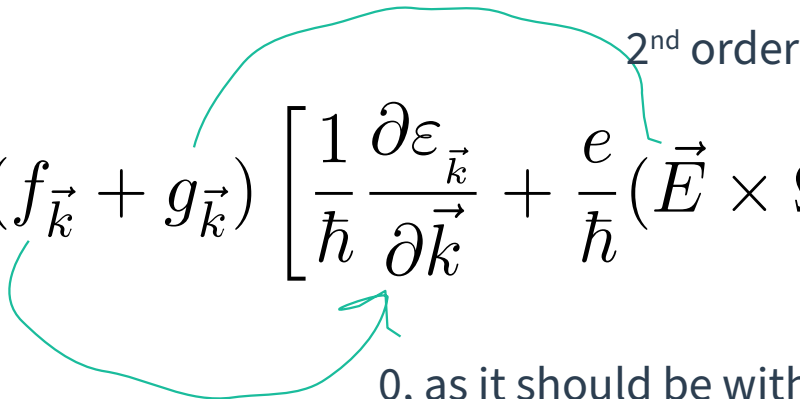
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Chern number, integer
Independent of scattering!!

Which all terms contribute

- For a filled band, $\sigma_{xy} = -\sigma_{yx} = \frac{2e^2}{h} \mathcal{C}$ quantized!!

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- There is an issue here

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Issue

- Apparently, a temp gradient or a chemical potential gradient cannot give rise to anomalous Hall effect
- No term like $\nabla\mu \times \vec{\Omega}$ and $\nabla T \times \vec{\Omega}$

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(Nernst)

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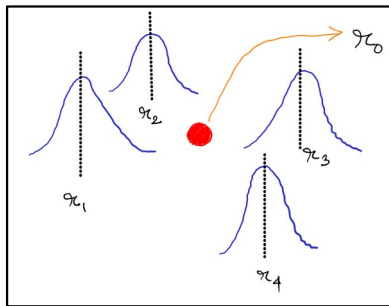
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- **What we missed:**

- The wavepackets are not localized



(Nernst)



Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu. PRL **97**, 026603 (2006)

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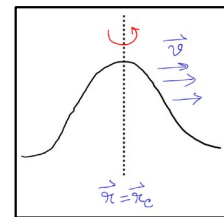
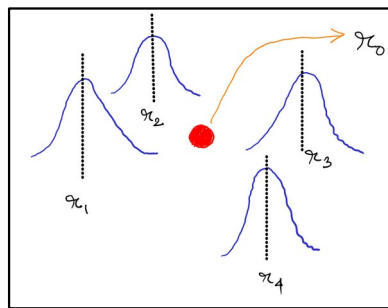
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What we missed:

- The wavepackets are not localized
- Circulating magnetization currents



(Nernst)

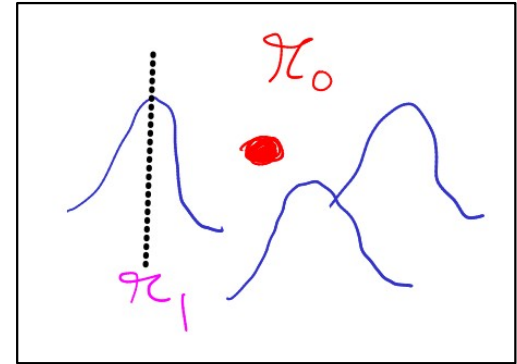


Orbital magnetic moment

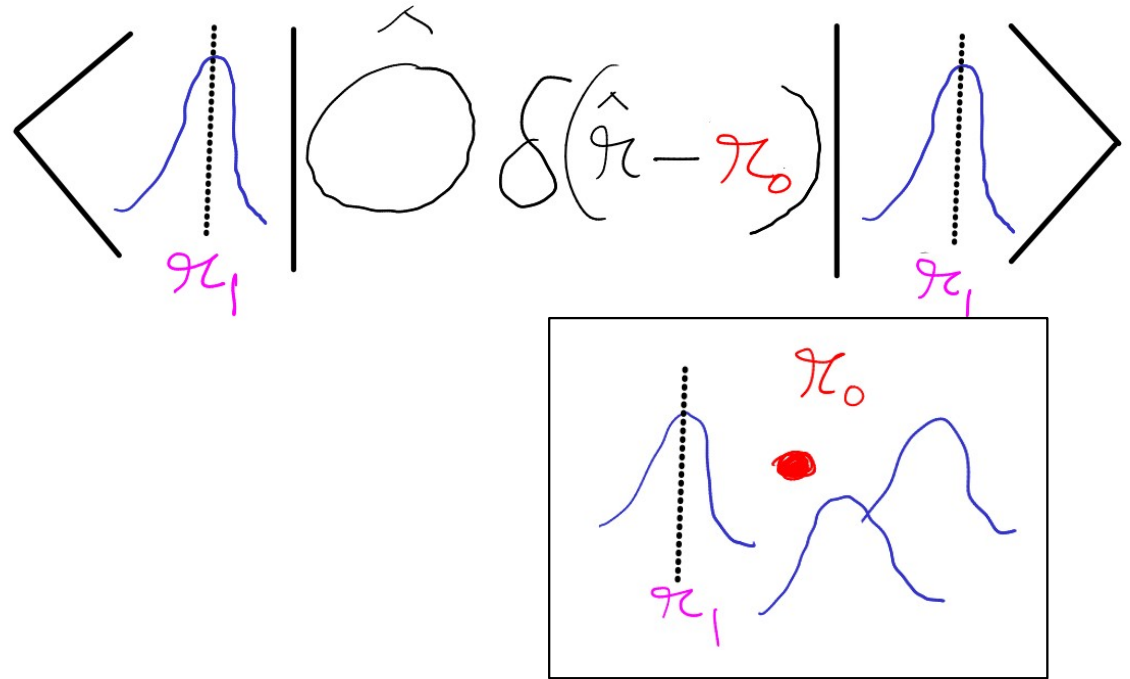
$$\vec{m}_k = -\frac{e}{2m} \langle \psi_{k,r_0} | (\hat{\vec{r}} - \vec{r}_0) \times \hat{\vec{p}} | \psi_{k,r_0} \rangle$$

Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu. PRL **97**, 026603 (2006)

Wavepackets are not strictly localized



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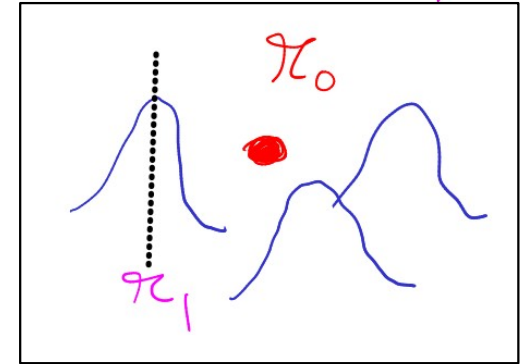
$$\langle \hat{O} \rangle (\mathcal{H}_0) = \int \int \langle \text{wavepacket} | \hat{O} \delta(\hat{\mathcal{H}} - \mathcal{H}_0) | \text{wavepacket} \rangle$$

The diagram illustrates the concept that wavepackets are not strictly localized. The main equation shows the expectation value of an operator \hat{O} in a state \mathcal{H}_0 as a double integral over energy and position. The integrand involves the expectation value of \hat{O} in a state defined by a delta function of the Hamiltonian minus \mathcal{H}_0 , sandwiched between two wavepacket states. The wavepackets are represented by blue curves with vertical dashed lines indicating their centers, labeled \mathcal{H}_1 . An inset shows two wavepackets, one centered at \mathcal{H}_1 and another at \mathcal{H}_0 , with a red dot marking the \mathcal{H}_0 position.

Wavepackets are not strictly localized

$$\langle \hat{O} \rangle (\mathcal{H}_0) = \int \int \langle \mathcal{H}_1 | \hat{O} \delta(\hat{\mathcal{H}} - \mathcal{H}_0) | \mathcal{H}_1 \rangle$$

- To be technically correct, we should use the operator $\frac{\hat{O}\delta(\hat{r} - \vec{r}_0) + \delta(\hat{r} - \vec{r}_0)\hat{O}}{2}$ in case \hat{O} does not commute with \hat{r}



- To calculate electric current, we use $\hat{O} = \frac{-e\hat{p}}{m}$

$$\langle \hat{j}_e \rangle \Big|_{\vec{B}=0} = -e \int \frac{2d\vec{k}}{(2\pi)^d} g_{\vec{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}} + f_{\vec{k}} \frac{e}{\hbar} (\vec{E} \times \vec{\Omega}(\vec{k})) + \nabla \times \int \frac{2d\vec{k}}{(2\pi)^d} f_{\vec{k}} \vec{m}_{\vec{k}}$$

This result can be found in existing scientific literature
without any derivation, I was able to derive it

- Similarly, for energy current

$$\langle \hat{j}_E \rangle = \int \frac{2d\vec{k}}{(2\pi)^d} \varepsilon_0(\vec{k}) \left[g_{\vec{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}} + \frac{e}{\hbar} f_{\vec{k}} (\vec{E} \times \vec{\Omega}(\vec{k})) \right] - \vec{E} \times \int \frac{2d\vec{k}}{(2\pi)^d} f_{\vec{k}} \vec{m}_{\vec{k}}$$

Effects of orbital magnetization

- New energy eigenvalues

$$\varepsilon_{\vec{k}} = \varepsilon_0(\vec{k}) - \vec{m}_{\vec{k}} \cdot \vec{B}$$

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$$G = -\frac{1}{\beta} \sum_{\vec{k}} \log \left(1 + e^{-\beta(\varepsilon_{\vec{k}} - \vec{m}_{\vec{k}} \cdot \vec{B} - \mu)} \right)$$
$$= -\frac{1}{\beta} \int \frac{d\vec{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega} \right) \log \left(1 + e^{-\beta(\varepsilon_{\vec{k}} - \vec{m}_{\vec{k}} \cdot \vec{B} - \mu)} \right)$$

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$$\vec{M}^e = - \left. \frac{\partial G}{\partial \vec{B}} \right|_{\vec{B}=0} = \frac{1}{\beta} \int \frac{2d\vec{k}}{(2\pi)^d} \frac{e}{\hbar} \vec{\Omega}(\vec{k}) \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) + \int \frac{2d\vec{k}}{(2\pi)^d} f \vec{m}_{\vec{k}}$$

Phase space density correction is important

Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu. PRL **97**, 026603 (2006)

Transport current

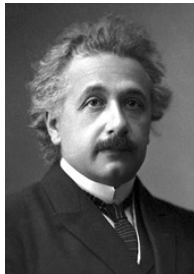
Now we are ready to calculate the transport electric current

$$\begin{aligned}
 \vec{j}_{\text{transport}}^e &= \langle \hat{\vec{j}}_e \rangle - \nabla \times \vec{M}^e \\
 &= \int \frac{2d\vec{k}}{(2\pi)^d} (-e) g_{\vec{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}} - f_{\vec{k}} \frac{e^2}{\hbar} \left(\left[\vec{E} + \frac{\nabla \mu}{e} \right] \times \vec{\Omega}(\vec{k}) \right) \\
 &\quad - \frac{\nabla T}{T} \times \int \frac{2d\vec{k}}{(2\pi)^d} \frac{e}{\hbar} \vec{\Omega}(\vec{k}) \left[f_{\vec{k}}(\varepsilon_0(\vec{k}) - \mu) + k_B T \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) \right]
 \end{aligned}$$

Regular Ohmic, Hall, Nernst

Anomalous Hall

Anomalous Nernst



Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu. PRL **97**, 026603 (2006)

How about Onsager relation?

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$$\begin{aligned}\vec{j}_{\text{transport}}^Q &= \vec{j}_{\text{transport}}^E - \mu \vec{j}_{\text{transport}}^N = \vec{j}_{\text{transport}}^E - \frac{\mu}{-e} \vec{j}_{\text{transport}}^e \\ &= \int \frac{2d\vec{k}}{(2\pi)^d} (\varepsilon_0(\vec{k}) - \mu) \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}} g_k \\ &\quad + \vec{E} \times \int \frac{2d\vec{k}}{(2\pi)^d} \left[(\varepsilon_0(\vec{k}) - \mu) \frac{e}{\hbar} \vec{\Omega} f_k + k_B T \frac{e\vec{\Omega}}{\hbar} \log(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)}) \right]\end{aligned}$$

Regular
response

Anomalous



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PRL **97**, 026603 (2006)

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 &\quad + \vec{E} \times \int \frac{2d\vec{k}}{(2\pi)^d} \left[(\varepsilon_0(\vec{k}) - \mu) \frac{e}{\hbar} \vec{\Omega} f_k + k_B T \frac{e \vec{\Omega}}{\hbar} \log(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)}) \right] \\
 &\quad + \int \frac{2d\vec{k}}{(2\pi)^d} (-\mu) \frac{1}{\hbar} \nabla \mu \times \vec{\Omega} f_k \\
 &\quad - \frac{\mu}{\hbar} \int \frac{2d\vec{k}}{(2\pi)^d} \frac{\nabla T}{T} \times \vec{\Omega} \left[f_k (\varepsilon_0(\vec{k})_k - \mu) + k_B T \log(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)}) \right] \\
 &\quad - \nabla \mu \times \frac{\partial \vec{M}_0^E}{\partial \mu} - \nabla T \times \frac{\partial \vec{M}_0^E}{\partial T}
 \end{aligned}$$

Regular
response

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Possible resolution for the Einstein relation to hold

$$-\frac{\partial \vec{M}_0^E}{\partial \mu} = \int \frac{2d\vec{k}}{(2\pi)^d} \frac{\vec{\Omega}}{\hbar} \left[\varepsilon_0(\vec{k}) f_k + k_B T \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) \right]$$

New result, not found in existing
scientific literature

Possible resolution for the Einstein relation to hold

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$$\approx \int \frac{2d\vec{k}}{(2\pi)^d} \frac{\vec{\Omega}}{\hbar} \mu f_k$$

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, can be finite even at zero temperature

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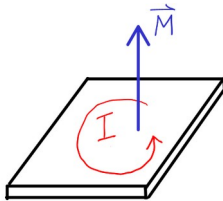
, can be finite even at zero temperature

~ sum of Chern numbers of filled bands

$$I_0^E = \left| \vec{M}_0^E \times \hat{n} \right|$$

In 2D

$$\frac{\Delta I_0^E}{\Delta \mu} = \left(2 \frac{\mu}{h} \right) (\# \text{Topological states} \oslash - \# \text{Topological states} \oslash)$$



Possible resolution for the Einstein relation to hold

$$-\frac{\partial \vec{M}_0^E}{\partial \mu} = \int \frac{2d\vec{k}}{(2\pi)^d} \frac{\vec{\Omega}}{\hbar} \left[\underset{-\mu}{\varepsilon_0(\vec{k})} f_k + \underset{+\mu}{k_B T \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right)} \right]$$

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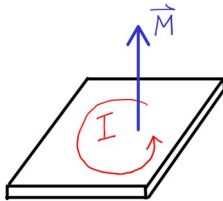
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~ sum of Chern numbers of filled bands

Raffaele Resta 2010 J. Phys.: Condens. Matter **22** 123201 : Showed a similar relation for circulating electric current

- Contribution is zero for trivial states, and each topological state contributes $\frac{\mu}{h} = \frac{\mu}{e^2} \left(\frac{e^2}{h} \right)$ to the bound energy current in 2D

$$\frac{\Delta I_0^E}{\Delta \mu} = \left(2 \frac{\mu}{h} \right) (\# \text{Topological states} \ominus - \# \text{Topological states} \oslash)$$



Some materialistic examples: Valley Polarization

Monolayer graphene and Transition Metal Dichalcogenides

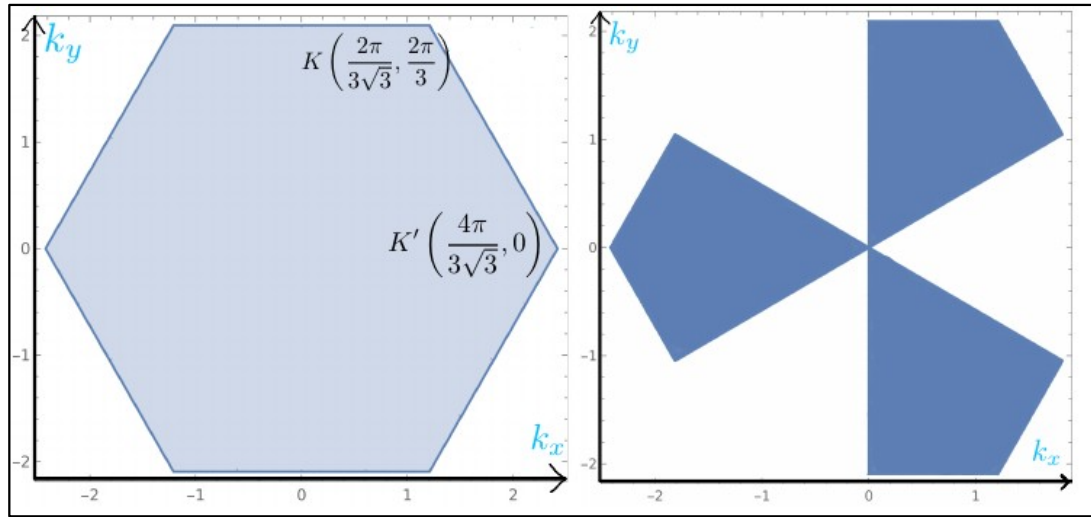
$$\vec{\Omega} = 0 \text{ without band gap} \quad \text{Time Reversal Symmetry } \vec{\Omega}(\vec{k}) = -\vec{\Omega}(-\vec{k}), \mathcal{C} = 0$$

Some materialistic examples: Valley Polarization

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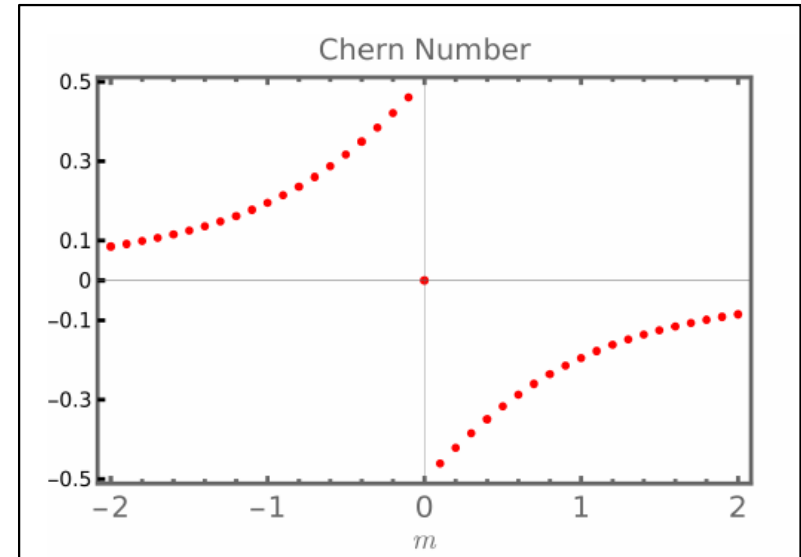
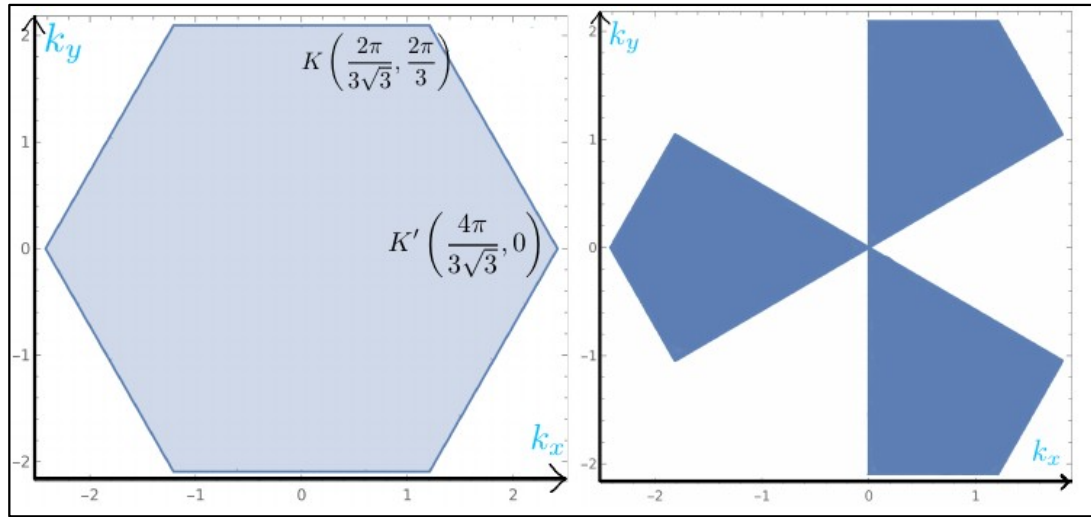
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Time Reversal Symmetry $\vec{\Omega}(\vec{k}) = -\vec{\Omega}(-\vec{k}), \mathcal{C} = 0$










- Electrons can be made to selectively occupy valleys with circularly polarized light

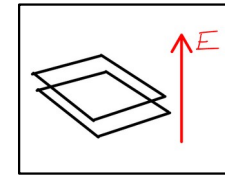
1. A. Friedlan and M. M. Dignam PRB **103**, 075414 (2021) (theory)

2. McIver, J.W., Schulte, B., Stein, F.U. et al. Nat. Phys. 16, 38–41 (2020) (experimental work)








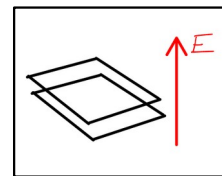
Results for valley Chern number in continuum limit

			\overline{n}	C	
	$E = K$			→	Monolayer graphene
	$E = \sqrt{K^2 + \Delta^2}$	$\neq 0$	$\pm \frac{1}{2}$	→	Monolayer graphene with broken sublattice symmetry (Boron Nitride, TMD)
	$E = K^2$			→	Bilayer graphene
	$E = \sqrt{K^4 + \Delta^2}$	$\neq 0$	± 1	→	Biased Bilayer graphene
	$E = \frac{\Delta}{\sqrt{k^2 + \alpha^2 k^4 n}}$	$\neq 0$	$-\frac{1}{2}, n > \frac{1}{2}$ $+\frac{1}{2}, n < \frac{1}{2}$	→	



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	$E = \frac{\Delta}{\sqrt{k^2 + \alpha^2 k^4 n}}$	$\neq 0$	$-\frac{1}{2}, n > \frac{1}{2}$ $+\frac{1}{2}, n < \frac{1}{2}$	\longrightarrow	$H(\vec{k}) = k_x \sigma_x + k_y \sigma_y + \alpha(k_x^2 + k_y^2)^n \sigma_z$ $n \neq \frac{1}{2}$



New results

- The condition on the energy magnetization for Einstein relation to hold for anomalous Heat current, and found an interpretation to that in terms of the number of circulating topological states.
- Solution of Boltzmann transport equation upto linear order in 2D, that captures the effects of Berry curvature in regular Ohmic, regular Hall and regular Nernst effects.

This is relevant in biased bilayer graphene, where there is non zero Berry curvature, but anomalous response is zero due to Time Reversal Symmetry.

Apart from that

- Filled all the missing steps in the formalism developed in several papers
- Found an explicit derivation for

$$\left\langle \hat{j}_e \right\rangle \Big|_{\vec{B}=0} = -e \int \frac{2d\vec{k}}{(2\pi)^d} g_{\vec{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_0(\vec{k})}{\partial \vec{k}} + f_{\vec{k}} \frac{e}{\hbar} (\vec{E} \times \vec{\Omega}(\vec{k})) + \nabla \times \int \frac{2d\vec{k}}{(2\pi)^d} f_{\vec{k}} \vec{m}_{\vec{k}}$$

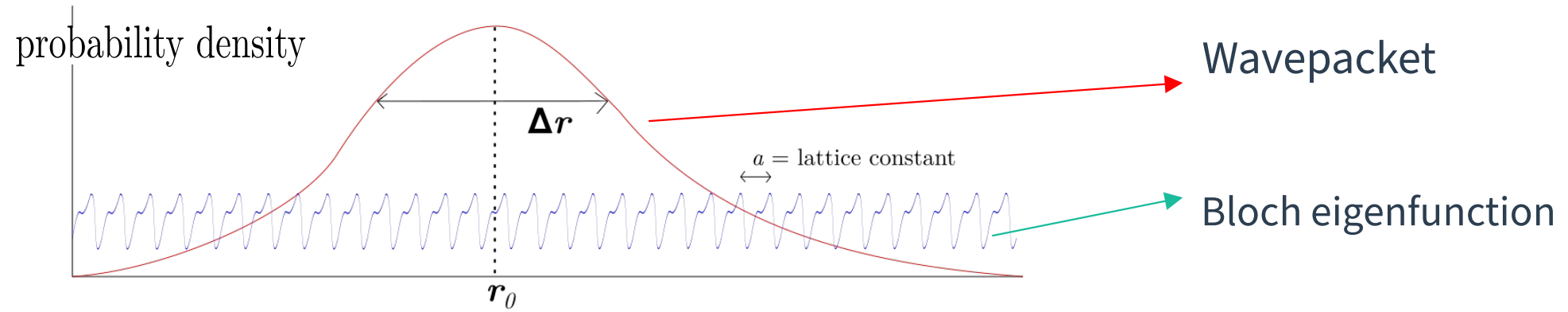
which is not available in existing literature

- Studied valley Chern numbers of several microscopic models

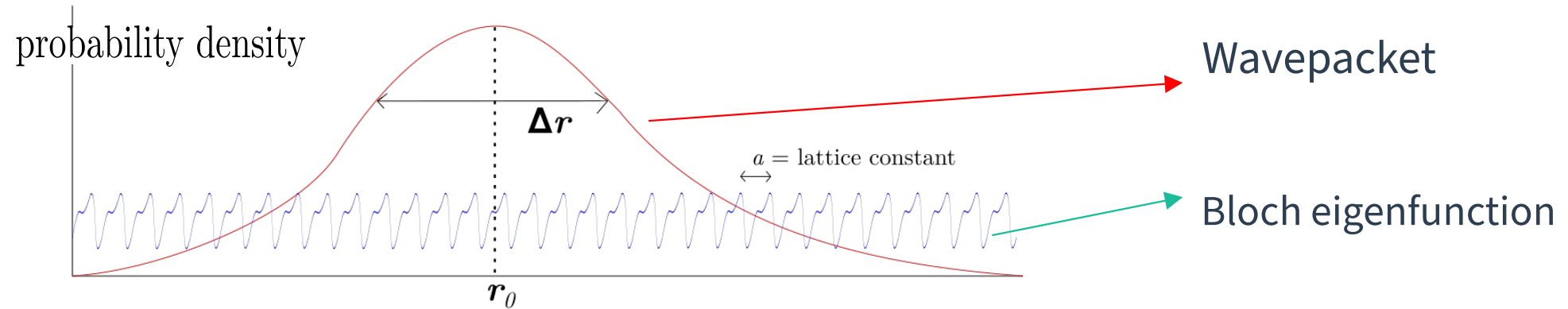


Thank you

Appendix: Construction of Bloch wavepacket, and its evolution

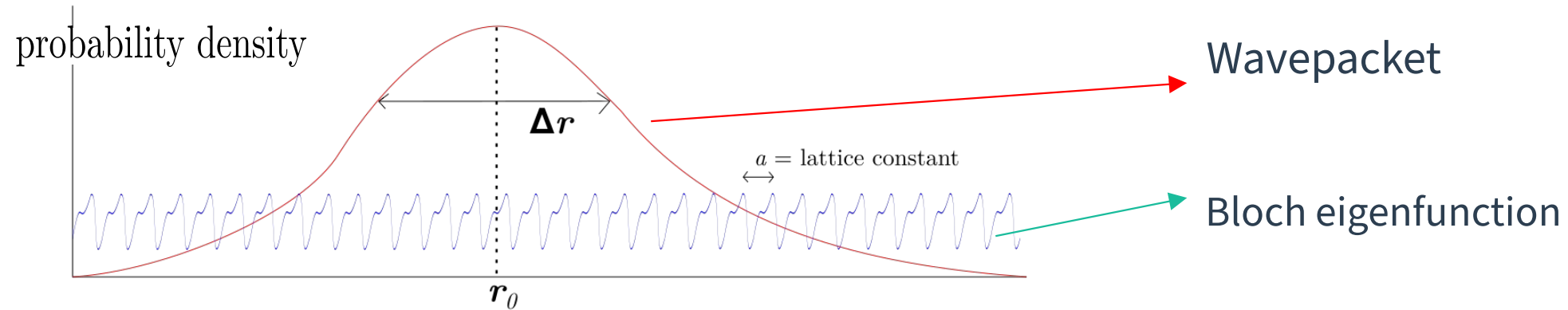


Appendix: Construction of Bloch wavepacket, and its evolution



$$\psi(\vec{r}, t = 0) \underbrace{=}_{?} \int d\vec{k} w(\vec{k} - \vec{k}_0) e^{-i\vec{k} \cdot \vec{r}_0} \left(e^{i\vec{k} \cdot \vec{r}} u_{n, \vec{k}}(\vec{r}) \right)$$

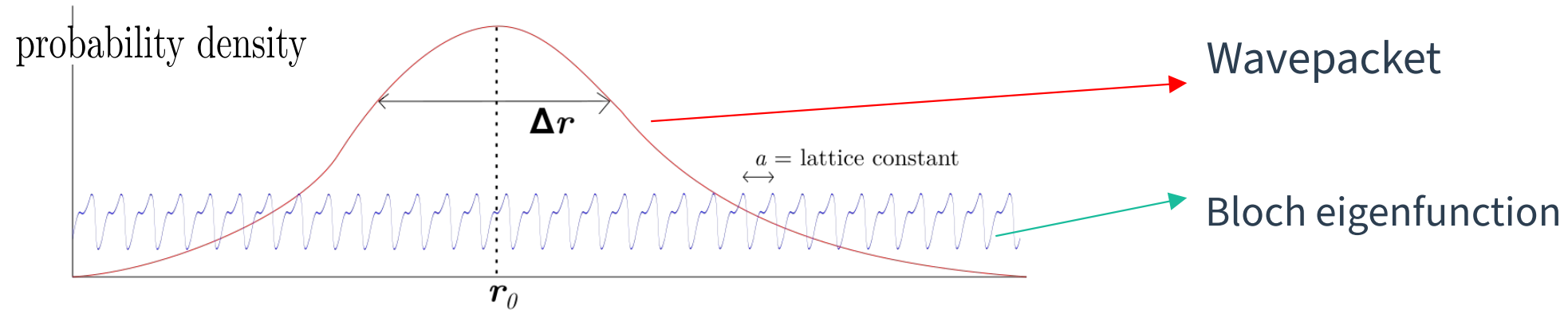
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$$\psi(\vec{r}, t = \Delta t) \left(e^{i(\vec{k} + \Delta\vec{k}) \cdot \vec{r}} e^{i\vec{A} \cdot \Delta\vec{k}} e^{-i\frac{\epsilon_{\vec{k}} \Delta t}{\hbar}} u_{n,\vec{k} + \Delta\vec{k}} \right)$$