Effects of Berry Curvature on Thermoelectric Transport

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UG 4th Year

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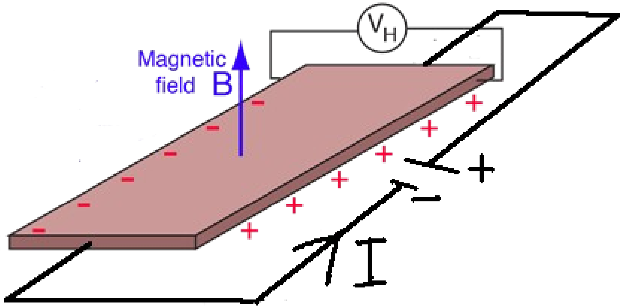
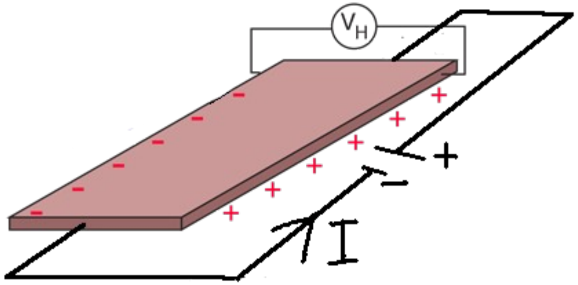
- There can be a transverse Hall voltage without a magnetic field





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

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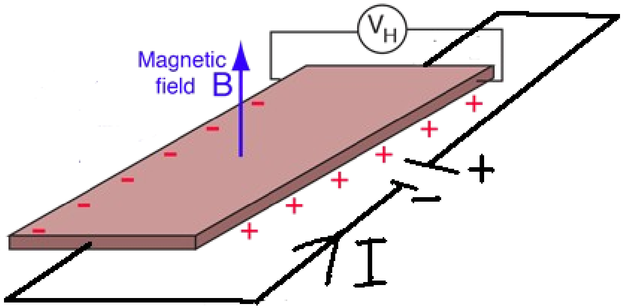

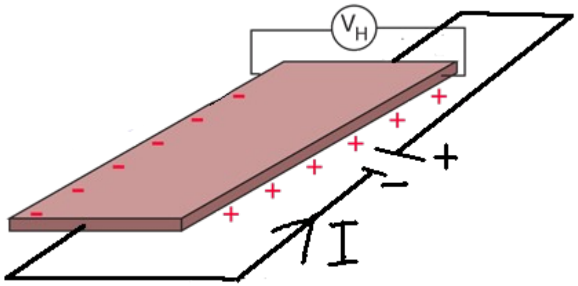

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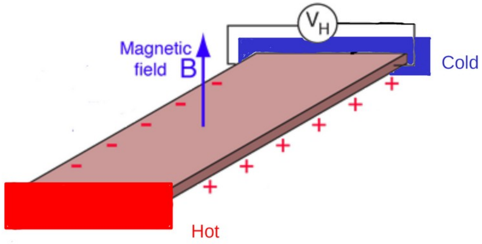
Anomalous Hall Effect

- Nernst Effect: Hall like response for a temperature gradient



Electrically insulating temperature reservoirs

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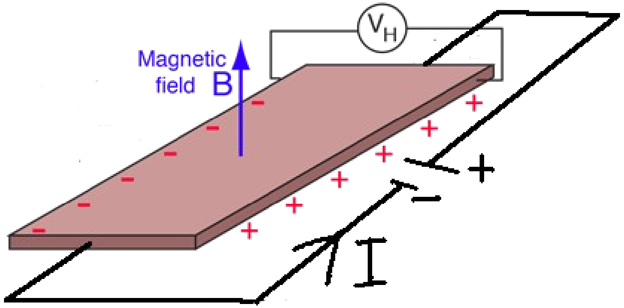

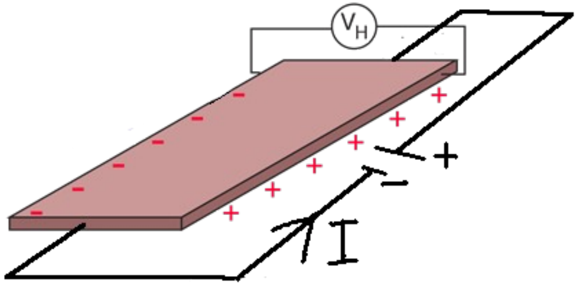

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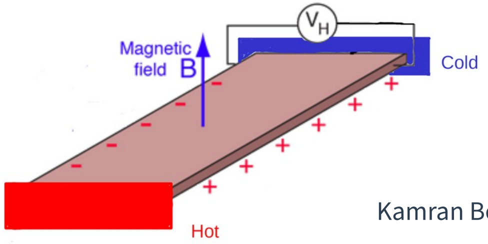
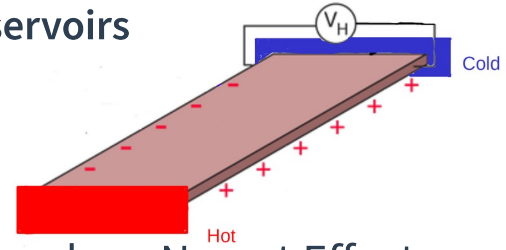


Electrically insulating temperature reservoirs

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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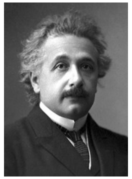

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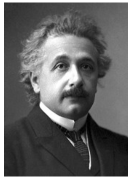

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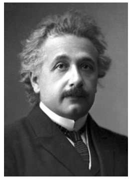

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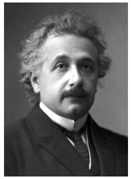

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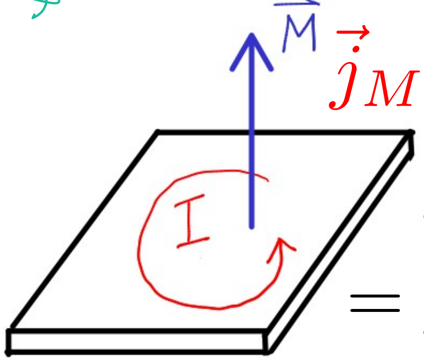

$$\vec{j}_M = \nabla \times \vec{M}$$

$$\vec{j}_{\mathrm{transport}} = \vec{j}_{\mathrm{total}} - \vec{j}_M$$

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 $H(\boldsymbol{\lambda}(t))$

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

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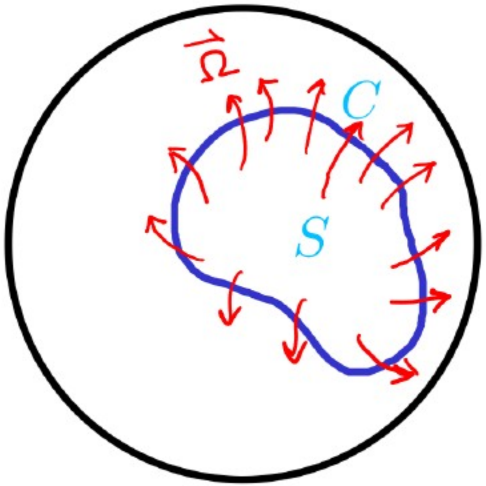

Space of $\lambda_1, \lambda_2, \ldots$

$$\gamma = i \oint_C \left\langle \varepsilon(\vec{\lambda}) \middle| \nabla_{\vec{\lambda}} \middle| \varepsilon(\vec{\lambda}) \right\rangle \cdot d\vec{\lambda}$$

$$= \oint_C \vec{A}(\vec{\lambda}) \cdot d\vec{\lambda}$$

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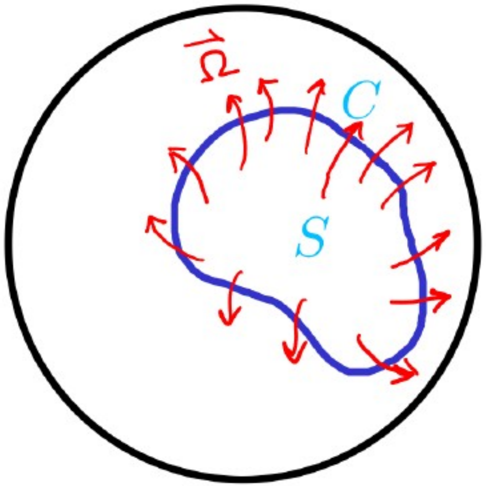

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$$= \oint_C \vec{A}(\vec{\lambda}) \cdot d\vec{\lambda} \quad = \int_S \vec{\Omega} \cdot d\vec{a}$$

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

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

Berry Curvature in reciprocal space

- **Bloch wavefunctions in periodic potential**

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Effective Schrödinger equation

$$\left[\frac{\hbar^2}{2m}(\vec{k} - i\nabla)^2 + V(\vec{r})\right] u_{n,\vec{k}}(\vec{r}) = \varepsilon_{n,\vec{k}} u_{n,\vec{k}}(\vec{r})$$

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- Crystal momentum changes with electromagneic field

$$\hbar \left\langle \dot{\vec{k}} \right\rangle = -e\left(\vec{E} + \langle \dot{\vec{r}} \rangle \times \vec{B}\right)$$

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

- Time evolution

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

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

Effects of Berry curvature

Ming-Che Chang and Qian Niu PRL **75**, 1348 (1995),
Daniel C. Ralph. arXiv: 2001.04797

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Decoupled

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(2D)

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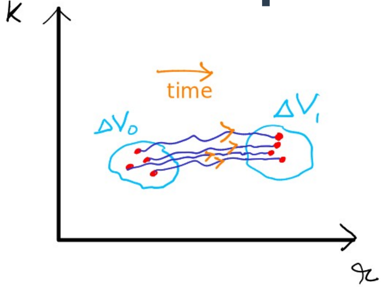
- Phase space density is modified



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

is a constant of motion

Phase space volume element

(2D)

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

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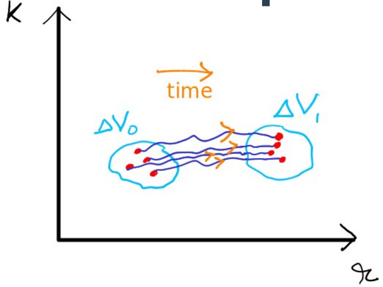

$$\Delta V\left(1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}\right)$$

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(2D)

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

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When do we get a non-zero Berry Curvature?

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

- If inversion symmetry holds

$$\vec{\Omega}(\vec{k}) = \vec{\Omega}(-\vec{k})$$

- If time reversal symmetry holds

$$\vec{\Omega}(\vec{k}) = -\vec{\Omega}(-\vec{k})$$

- 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

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Semiclassical framework

Locally averaged

Current density

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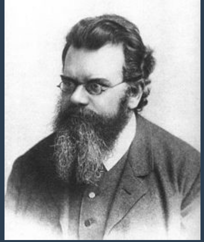
$$\left\langle \hat{\vec{\dot{j}}}_Q \right\rangle = 2 \int \frac{d\vec{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}\left(\vec{k}\right)\right) (\varepsilon_{\vec{k}} - \mu)\dot{\vec{r}}_{\vec{k}} \tilde{g}_{\vec{k}}$$

Boltzmann Transport Equation



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

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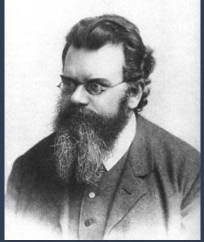

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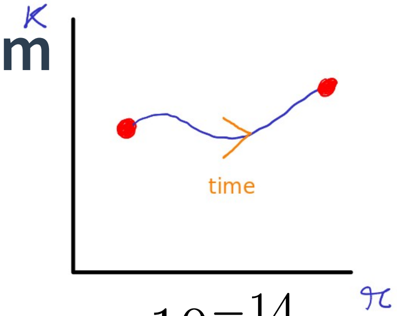
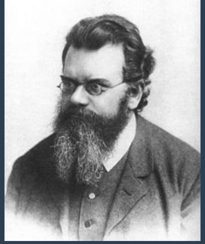


- The system tries to attain equilibrium, with a relaxation time $\tau \sim 10^{-14} s$
- We assume that the more the distribution deviates, the faster it would try to return to equilibrium, *relaxation time approximation.* $D_t \tilde{g}_k = -\dfrac{\tilde{g}_k - f_k}{\tau_k}$

$$D_t \equiv \frac{\partial}{\partial t} + \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}} + \dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}}$$

Boltzmann Transport Equation



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

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

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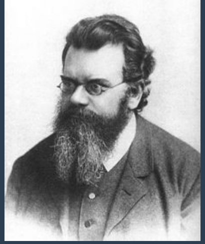

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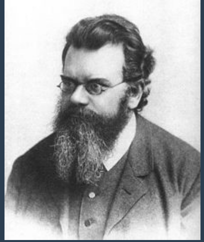
- Why is the perturbation theory valid?

Boltzmann Transport Equation



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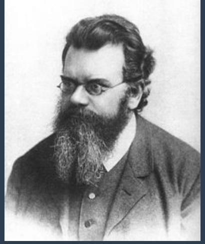
  Dimension analysis: this term $\omega_c \tau \times$ the first $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency

  $$B \ll B_{critical} = \frac{m^*}{e\tau}$$

- This is small compared to the first term when

Boltzmann Transport Equation



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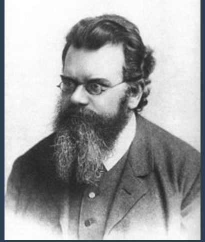
- If $m^* \sim m, \tau \sim 10^{-14} s$ then the critical field is ~ 570 T

Boltzmann Transport Equation



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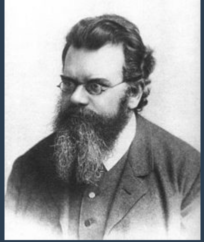
Why even consider this term, then??

Boltzmann Transport Equation



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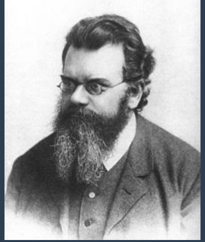
New result (2D)

Boltzmann Transport Equation



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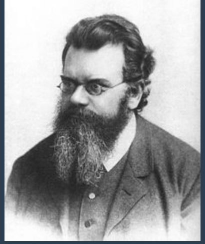
Boltzmann Transport Equation



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$$\begin{aligned} g_k = {} & \frac{\partial f}{\partial\varepsilon}\frac{1}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\tau_k}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}}\cdot\vec{S} \\ & + \frac{\frac{e\tau_k}{\hbar^2}}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\partial\varepsilon}{\partial\vec{k}}\cdot\vec{B}\times\left[\frac{\partial}{\partial\vec{k}}\left[\frac{\frac{\partial f}{\partial\varepsilon}\tau_k}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\right]\frac{\vec{S}}{\hbar}\cdot\frac{\partial\varepsilon}{\partial\vec{k}} + \frac{\frac{\partial f}{\partial\varepsilon}\tau_k}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\left[\left(\frac{1}{\hbar}\vec{S}\cdot\frac{\partial}{\partial\vec{k}}\right)\frac{\partial\varepsilon}{\partial\vec{k}}\right]\right] \end{aligned}$$

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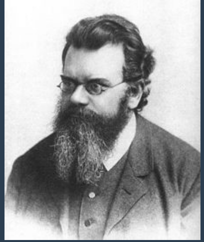
Boltzmann Transport Equation



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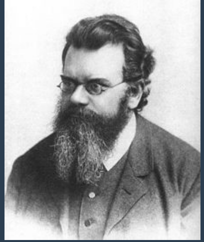
$$g_k = \frac{\partial f}{\partial\varepsilon}\frac{1}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\tau_k}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}}\cdot\vec{S} \longrightarrow \text{Regular Ohmic transport}$$

New result (2D)

Regular Hall, Nernst

$$+\frac{\frac{e\tau_k}{\hbar^2}}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\partial\varepsilon}{\partial\vec{k}}\cdot\vec{B}\times\left[\frac{\partial}{\partial\vec{k}}\left[\frac{\frac{\partial f}{\partial\varepsilon}\tau_k}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\right]\frac{\vec{S}}{\hbar}\cdot\frac{\partial\varepsilon}{\partial\vec{k}}+\frac{\frac{\partial f}{\partial\varepsilon}\tau_k}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\left[\left(\frac{1}{\hbar}\vec{S}\cdot\frac{\partial}{\partial\vec{k}}\right)\frac{\partial\varepsilon}{\partial\vec{k}}\right]\right]$$

Boltzmann Transport Equation



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Einstein and Onsager Relations are satisfied

- **The solution, with** $\vec{S} = e\vec{E}+\nabla\mu+\frac{\varepsilon-\mu}{T}\nabla T$

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Regular Ohmic transport

New result (2D)

Regular Hall, Nernst

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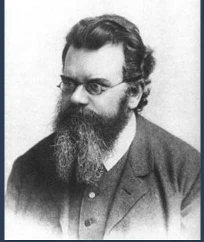

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1. Dantas, R.M.A., Peña-Benitez, F., Roy, B. et al. J. High Energ. Phys. **2018**, 69 (2018).
2. Ki-Seok Kim, Heon-Jung Kim, and M. Sasaki Phys. Rev. B **89**, 195137 (2014)
3. O. Pal, B. Dey, T. K. Ghosh arXiv:2102.03779 [cond-mat.mes-hall]

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→ Regular Ohmic transport

New result (2D)

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Which all terms contribute

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

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0, as it should be without any external field

Which all terms contribute

2nd order

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$$\left\langle \hat{\vec{j}}_e \right\rangle_{anomalous} = -2 \frac{e^2}{h} \vec{E} \times \int_{\text{filled}} \frac{d^2 \vec{k}}{2\pi} \vec{\Omega}_z(\vec{k})$$

Which all terms contribute

2nd order

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

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For a filled band,

Chern number, integer

Which all terms contribute

2nd order

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For a filled band,

Chern number, integer

Independent of scattering!!

Which all terms contribute

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

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

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Independent of scattering!!

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- For a <u>filled band</u>, $\sigma_{xy} = -\sigma_{yx} = \dfrac{2e^2}{h}\mathcal{C}$ quantized!!
- This is not the (usual) quantum Hall effect

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

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Independent of scattering!!

Which all terms contribute

- For a <u>filled band</u>, $\sigma_{xy} = -\sigma_{yx} = \frac{2e^2}{h}\mathcal{C}$ quantized!!
- This is not the (usual) quantum Hall effect
- There is an issue here

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

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Independent of scattering!!

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 $\nabla T \times \vec{\Omega}$

Issue

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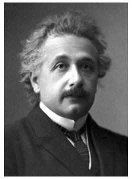

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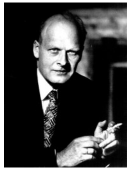

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(Nernst)

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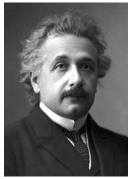
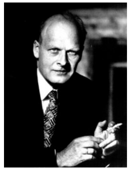
  

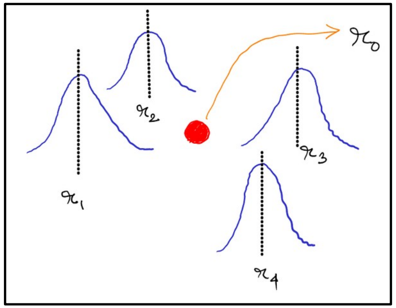
☹ ☹ ☹

(Nernst)

- No term like $\nabla\mu \times \vec{\Omega}$ and $\nabla T \times \vec{\Omega}$

- **What we missed:**

- The wavepackets are not localized



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

Issue

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- **What we missed:**
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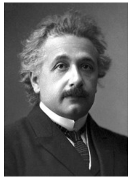
- Circulating magnetization currents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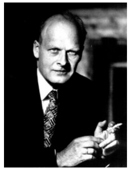
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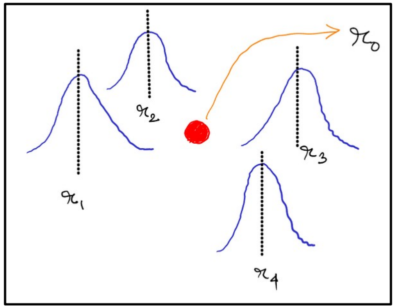
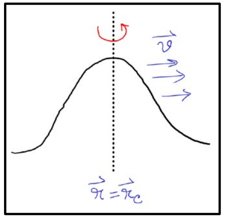


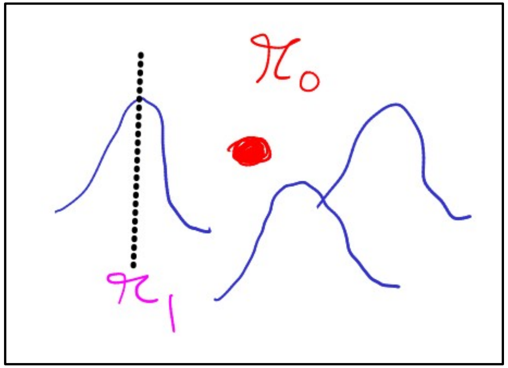


Orbital magnetic moment

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

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

Wavepackets are not strictly localized



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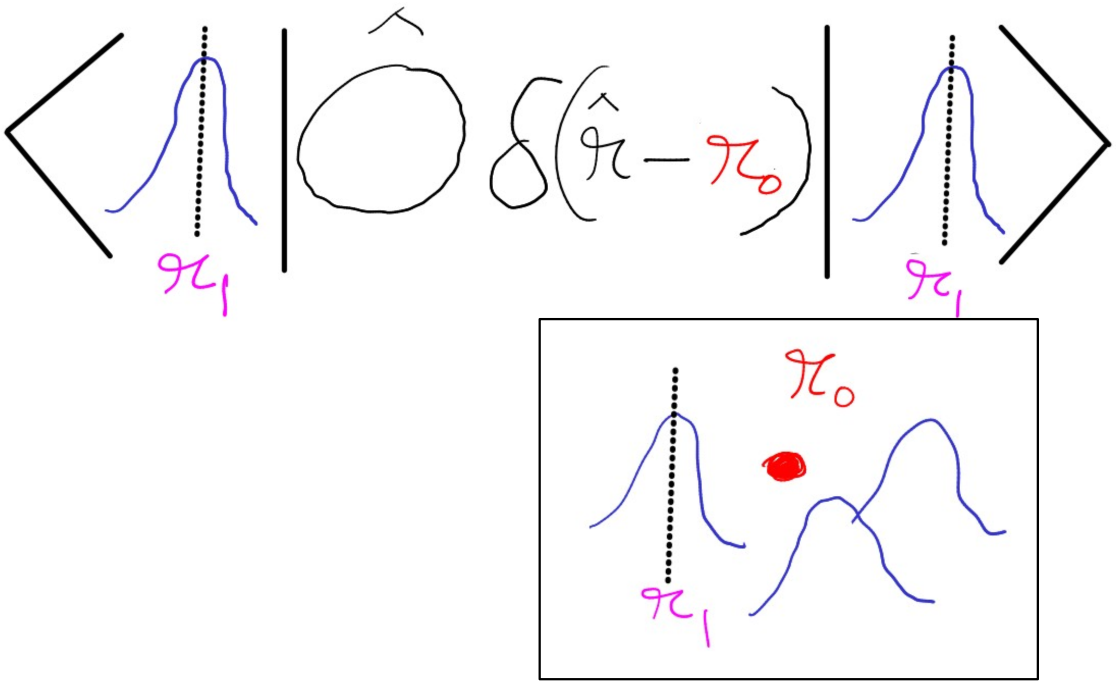
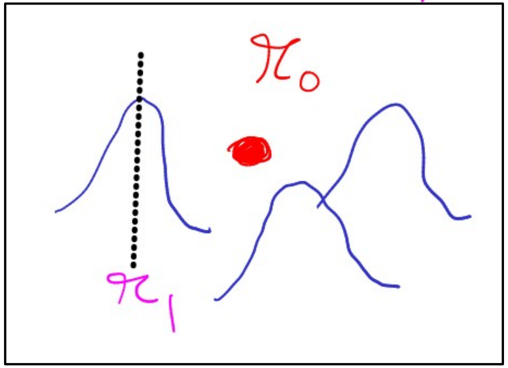


Wavepackets are not strictly localized

$$\langle \hat{O} \rangle (r_0) = \int_{r_1} \int_{k} \Big\langle {}_{r_1} \Big| \hat{O}\, \delta(\hat{r} - r_0) \Big| {}_{r_1} \Big\rangle$$



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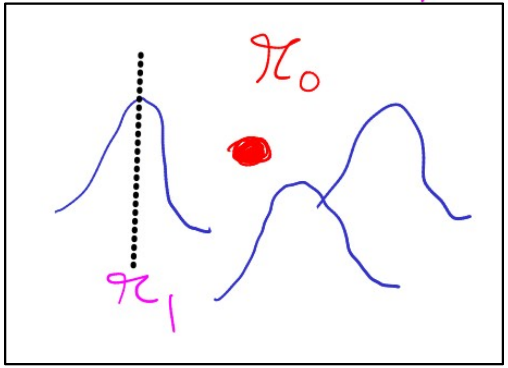

- To be technically correct, we should use the operator $\frac{\hat{O}\delta(\hat{r}-\vec{r}_0)+\delta(\hat{r}-\vec{r}_0)\hat{O}}{2}$ in case $\hat{O}$ does not commute with $\hat{r}$

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

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

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

- **Similarly, for energy current**

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

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

Effects of orbital magnetization

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

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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

$$\vec{j}^{e}_{\text{transport}} = \left\langle \hat{\vec{j}}_e \right\rangle - \nabla \times \vec{M}^e$$

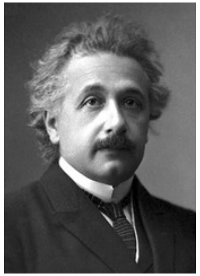
$$= \int \frac{2d\vec{k}}{(2\pi)^d}(-e)g_{\vec{k}}\frac{1}{\hbar}\frac{\partial\varepsilon_0(\vec{k})}{\partial\vec{k}} - f_{\vec{k}}\frac{e^2}{\hbar}\left(\left[\vec{E} + \frac{\nabla\mu}{e}\right] \times \vec{\Omega}(\vec{k})\right)$$

$$- \frac{\nabla T}{T} \times \int \frac{2d\vec{k}}{(2\pi)^d}\frac{e}{\hbar}\vec{\Omega}(\vec{k})\left[f_{\vec{k}}(\varepsilon_0(\vec{k}) - \mu) + k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\vec{k})-\mu)}\right)\right]$$

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?

- We can similarly define energy magnetization, $\vec{M}^E = \vec{M}_0^E + \underbrace{\phi(\vec{r})}_{\text{electric potential energy}} \vec{M}^N$

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Regular response

Anomalous

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

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

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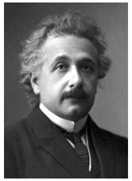
&+ \vec{E} \times \int \frac{2d\vec{k}}{(2\pi)^d}\left[(\varepsilon_0(\vec{k})-\mu)\frac{e}{\hbar}\vec{\Omega} f_k + k_B T \frac{e\vec{\Omega}}{\hbar}\log\left(1+e^{-\beta(\varepsilon_0(\vec{k})-\mu)}\right)\right] \\
&+ \int \frac{2d\vec{k}}{(2\pi)^d}(-\mu)\frac{1}{\hbar}\nabla\mu \times \vec{\Omega}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


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




Possible resolution for the Einstein relation to hold

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

New result, not found in existing scientific literature

Possible resolution for the Einstein relation to hold

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

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

$$-\mu+\mu$$

New result, not found in existing scientific literature

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

, finite even at zero temperature

~ sum of Chern numbers of filled bands

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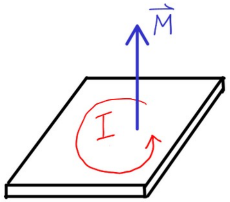
$$I_0^E = \left|\vec{M}_0^E \times \hat{n}\right|$$



In 2D

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

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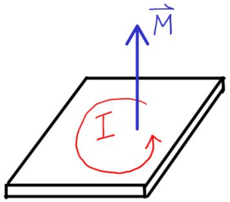

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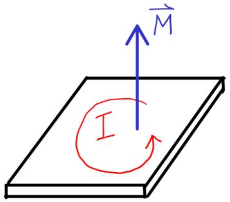
Raffaele Resta 2010 J. Phys.: Condens. Matter **22** 123201 **: Showed a similar relation for circulating electric current**

- **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**



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Some materialistic examples: Valley Polarization
Monolayer graphene and Transition Metal Dichalcogenides

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

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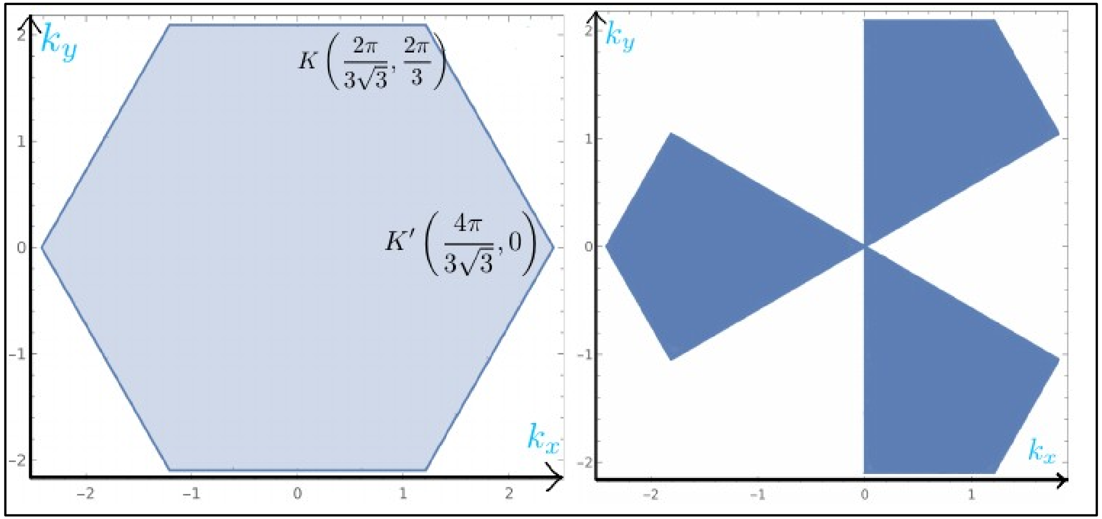

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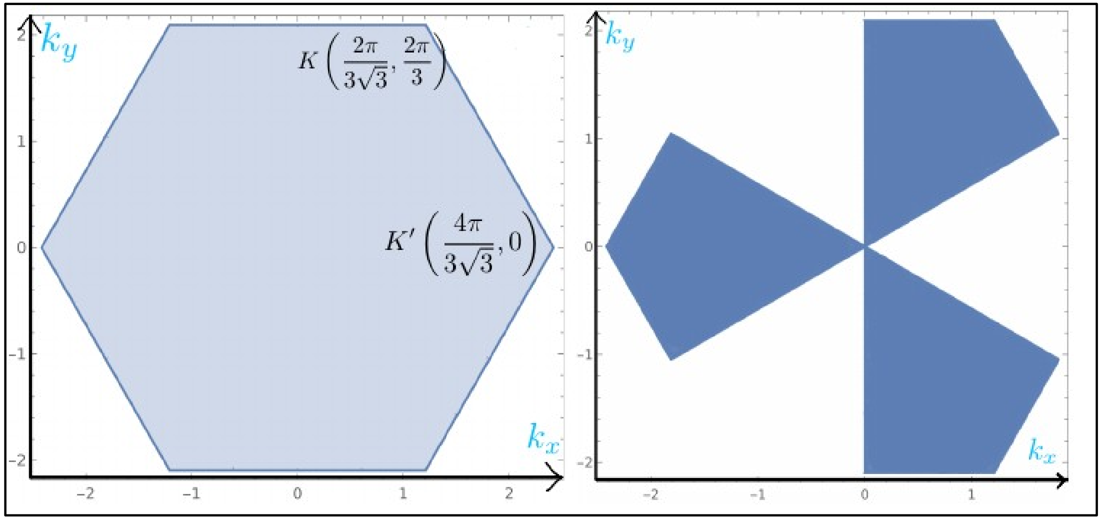
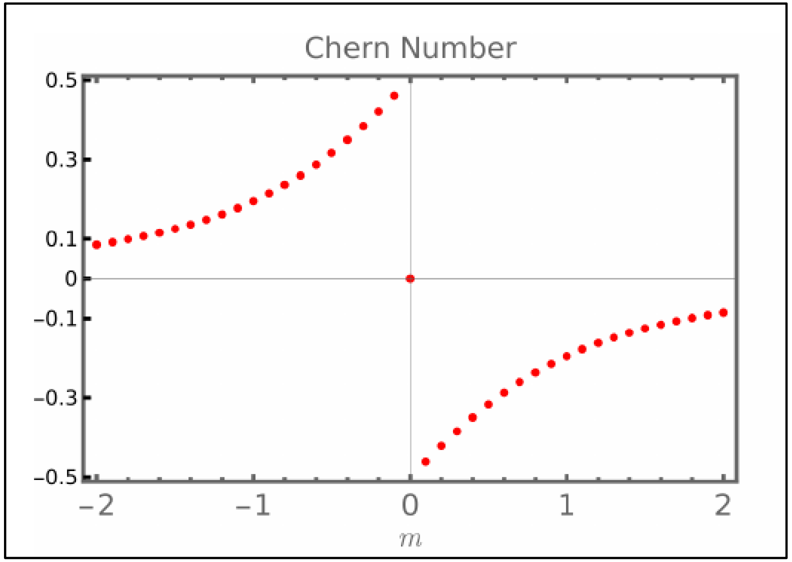
- **Electrons can be made to selectively occupy valleys with circularly polarized light**

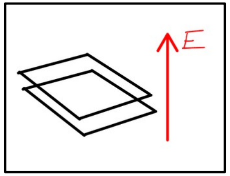
1. A. Friedlan and M. M. Dignam PRB **103**, 075414 (2021) (theory)
2. McIver, J.W., Schulte, B., Stein, FU. et al. Nat. Phys. 16, 38–41 (2020) (experimental work)





Results for valley Chern number in continuum limit

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



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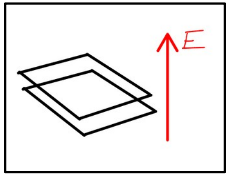
→ Monolayer graphene

→ Monolayer graphene with broken sublattice symmetry (Boron Nitride)

→ Bilayer graphene

→ Biased Bilayer graphene



→ $$H(\vec{k}) = k_x\sigma_x + k_y\sigma_y + \alpha(k_x^2+k_y^2)^n\sigma_z$$

$$n \neq \frac{1}{2}$$

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

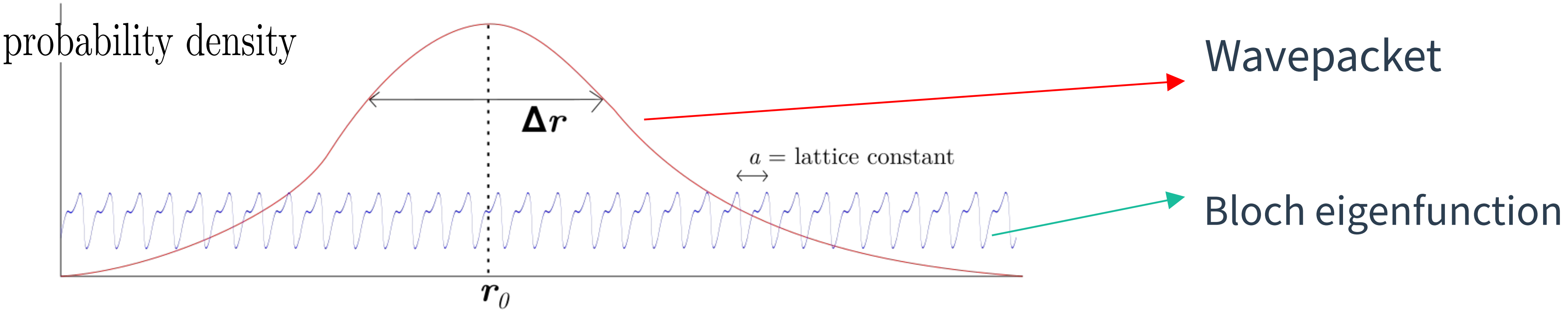
- Filled all the missing steps in the formalism developed in several papers
- Found an explicit derivation for

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

  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



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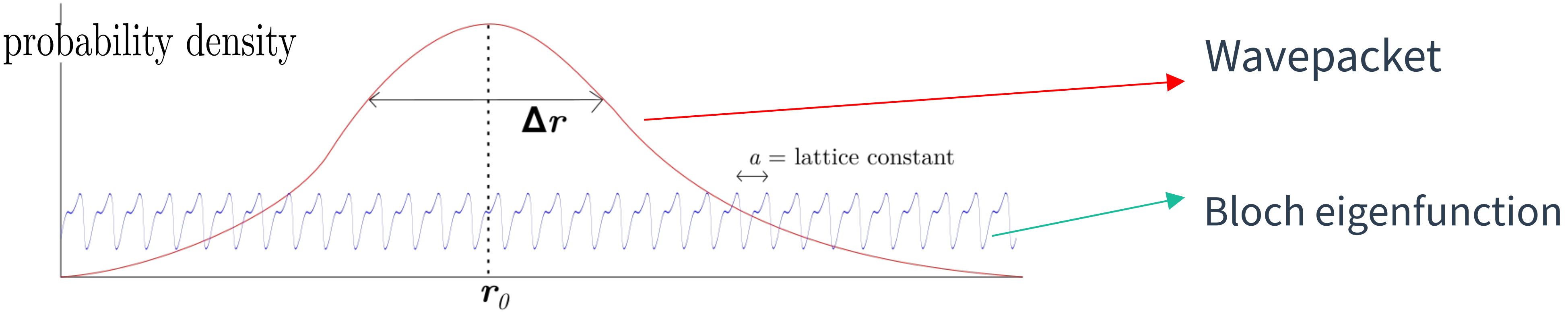
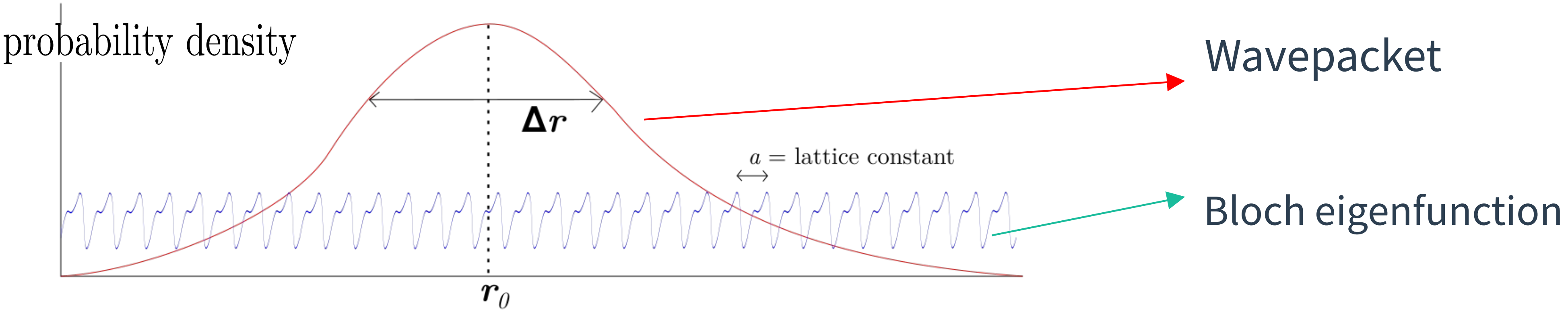


$$\psi(\vec{r}, t=0) \underbrace{=}_{?} \int d\vec{k} w(\vec{k}-\vec{k}_0) e^{-i\vec{k}\cdot\vec{r}_0} \left(e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}}(\vec{r}) \right)$$

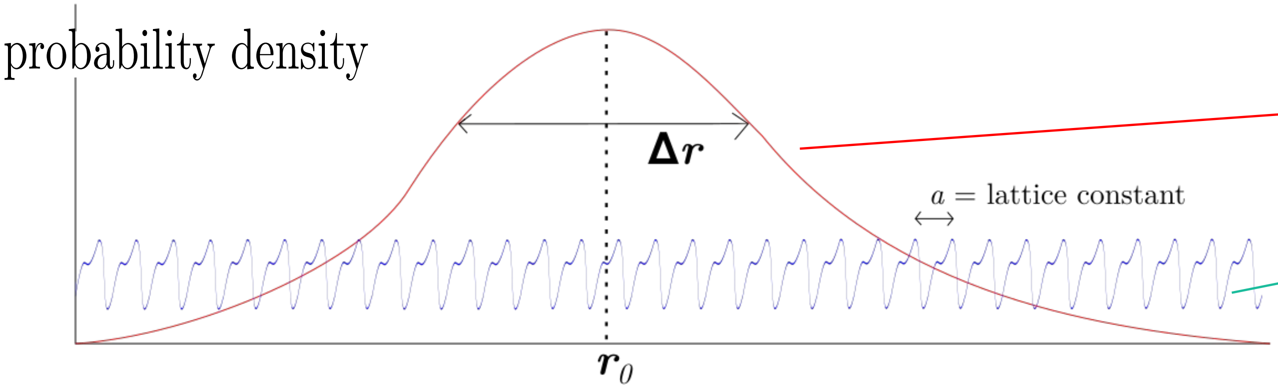
Appendix: Construction of Bloch wavepacket, and its evolution



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

$$\psi(\vec{r}, t=0) = \int d\vec{k} w(\vec{k}-\vec{k}_0) e^{i\vec{A}(\vec{k_0})\cdot(\vec{k}-\vec{k}_0)} e^{-i\vec{k}\cdot\vec{r}_0} \left(e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}}(\vec{r})\right)$$

Appendix: Construction of Bloch wavepacket, and its evolution



Wavepacket

Bloch eigenfunction

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

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

$$\psi(\vec{r}, t=\Delta t)$$

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