

Effects of Berry Curvature on Thermoelectric Transport



Archisman Panigrahi

UG 4th Year

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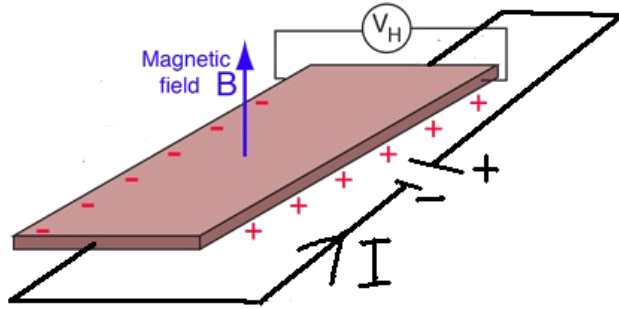
Why is this interesting?

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

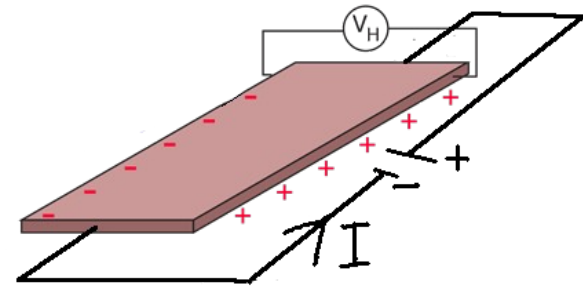
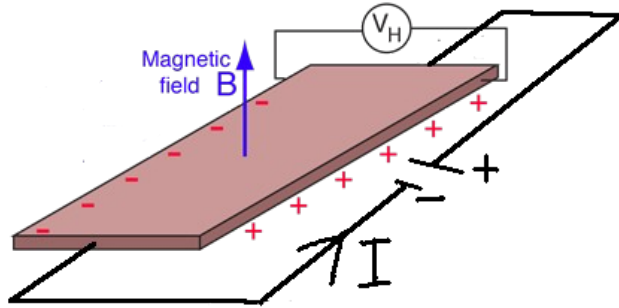
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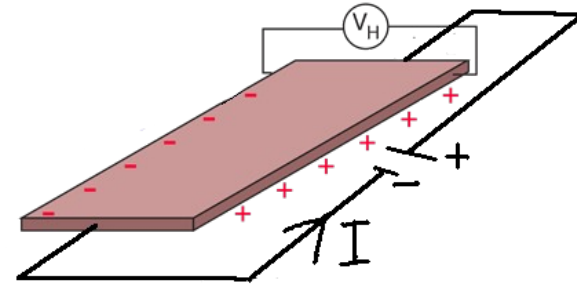
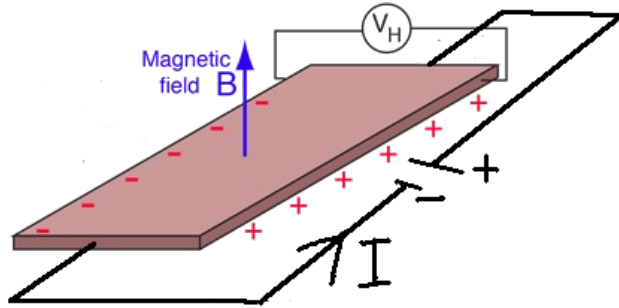
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Anomalous Hall Effect

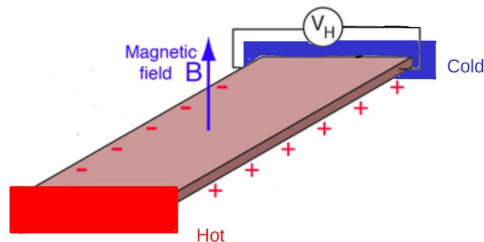
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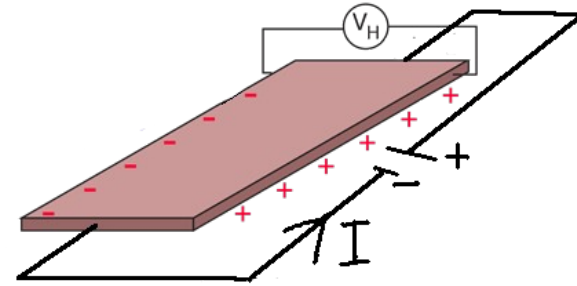
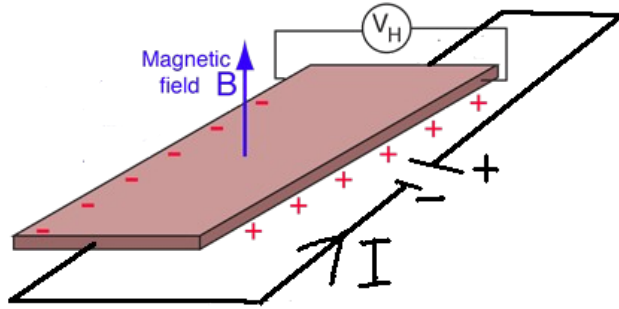
- Nernst Effect: Hall like response for a temperature gradient



Electrically insulating temperature reservoirs

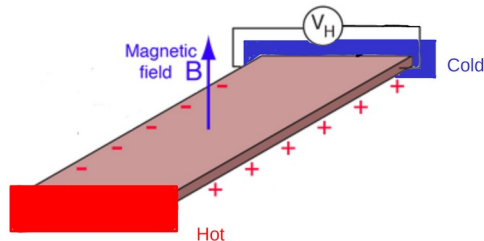
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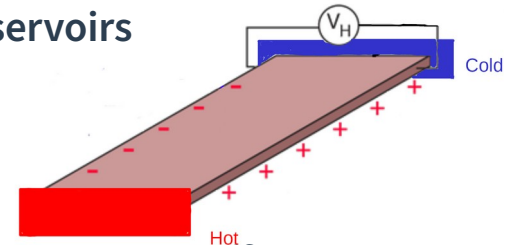


Anomalous Hall Effect

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Electrically insulating temperature reservoirs



Anomalous Nernst Effect

Thermoelectric transport: Einstein and Onsager relations

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

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

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σ , electric conductivity

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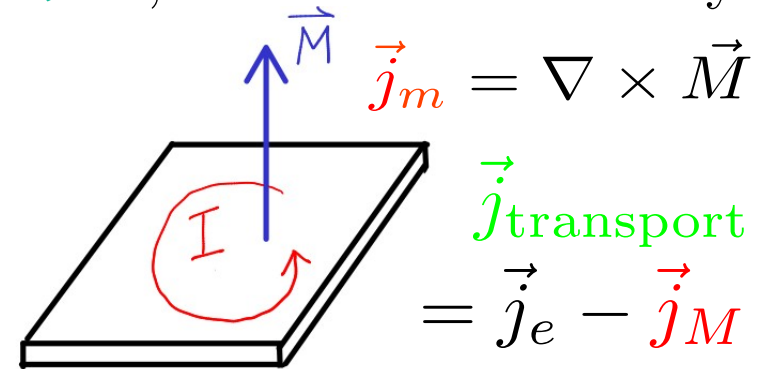
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N. R. Cooper, B. I. Halperin, and I. M. Ruzin. PRB **55** 2344 (1997)

Geometric phase and Berry Curvature

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

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

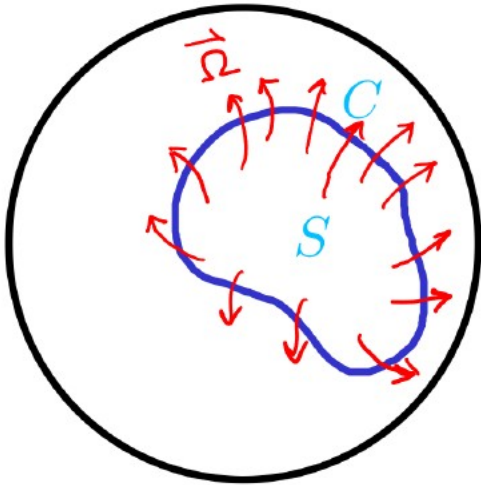
$$|\varepsilon(\boldsymbol{\lambda}(t))\rangle = e^{i\gamma(t)} e^{-\frac{i}{\hbar} \int_0^t \varepsilon(\boldsymbol{\lambda}(t')) dt'} |\varepsilon(\boldsymbol{\lambda}(0))\rangle$$

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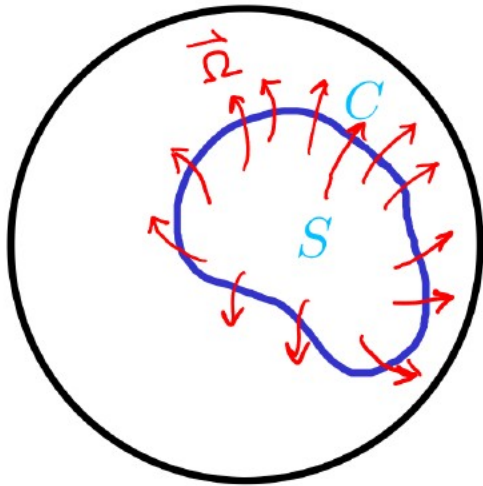
Space of $\lambda_1, \lambda_2, \dots$

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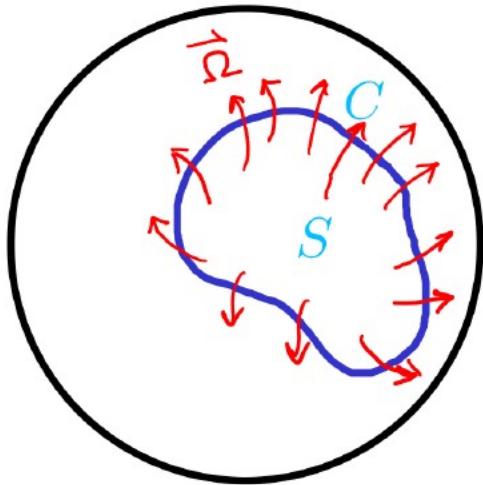
$$\begin{aligned} \gamma &= i \oint_C \langle \varepsilon(\vec{\lambda}) | \nabla_{\vec{\lambda}} | \varepsilon(\vec{\lambda}) \rangle \cdot d\vec{\lambda} \\ &= \oint_C \vec{A}(\vec{\lambda}) \cdot d\vec{\lambda} \end{aligned}$$

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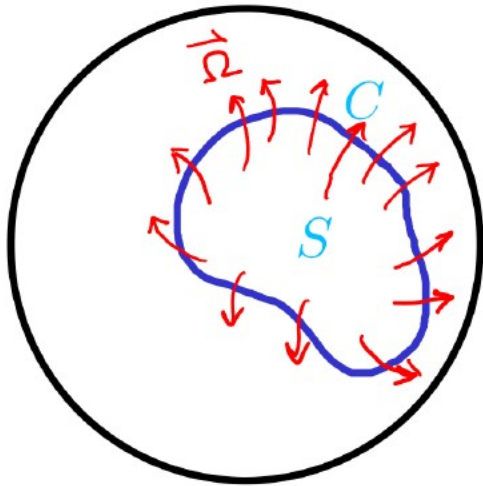
Stokes' theorem: $\vec{\Omega} = \nabla \times \vec{A}$

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Like magnetic field, but in parameter space

Berry Curvature in reciprocal space

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

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Effective Schrodinger equation

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Crystal momentum changes with electromagnetic field

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

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- Time evolution

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

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Effects of Berry curvature

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

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Anomalous velocity

Decoupled

$$\dot{\vec{r}} = \frac{\frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k} + \frac{e}{\hbar} (\vec{E} \times \boldsymbol{\Omega}) + \frac{e}{\hbar^2} (\boldsymbol{\Omega} \cdot \frac{\partial \varepsilon}{\partial k}) \vec{B}}{1 + \frac{e}{\hbar} \vec{B} \cdot \boldsymbol{\Omega}}$$
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(2D)

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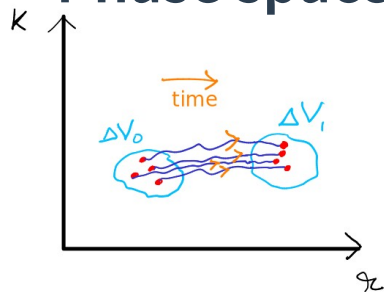
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- Phase space density is modified



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

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

Anomalous velocity

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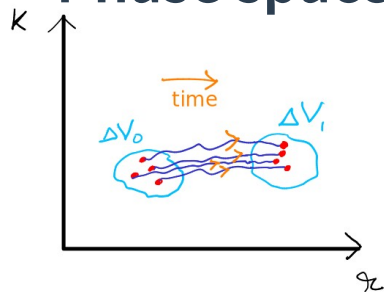
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Anomalous velocity

$$\langle \mathcal{O} \rangle (\vec{B} = 0) = 2 \int \frac{d\vec{k}}{(2\pi)^d} \langle \mathcal{O} \rangle_{\vec{k}} \tilde{g}_{\vec{k}} \quad (2D)$$

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



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

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When do we get a non-zero Berry Curvature?

- If inversion symmetry holds

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

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

- 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

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

Boltzmann Transport framework

Classical charge and energy currents
 $\vec{j}_e = -nev, \vec{j}_\epsilon = n\epsilon v$
Semiclassical framework

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

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

Boltzmann Transport framework

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Heat current: From 1st law of thermodynamics, $dQ = dE - \mu dN$

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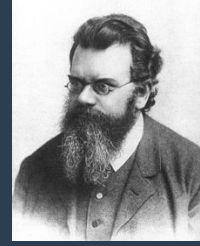
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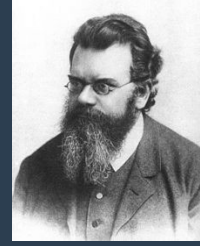
$$\langle \hat{\vec{j}}_Q \rangle = 2 \int \frac{d\vec{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \vec{B} \cdot \vec{\Omega}(\vec{k}) \right) (\epsilon_{\vec{k}} - \mu) \dot{\vec{r}}_{\vec{k}} \tilde{g}_{\vec{k}}$$

Boltzmann Transport Equation



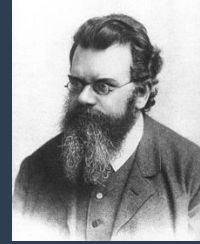
- In equilibrium, \tilde{g}_k is the Fermi distribution. $f_{\vec{k}} = \frac{1}{e^{\beta(\varepsilon_{\vec{k}} - \mu)} + 1}$
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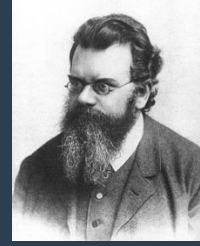
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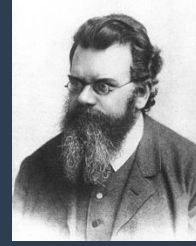
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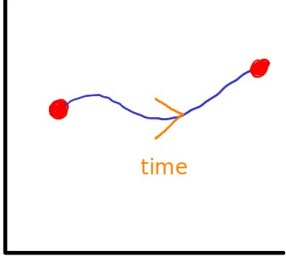
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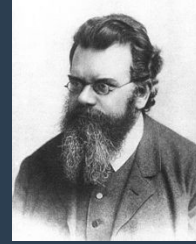
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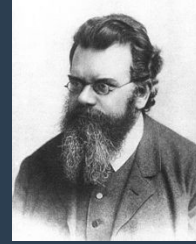
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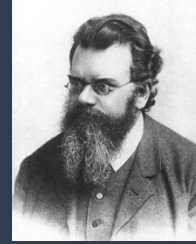


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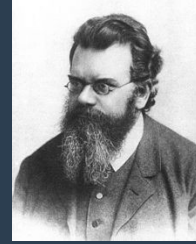
Dimension analysis: this term = $\omega_c \tau \times$
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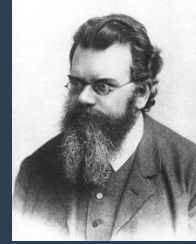
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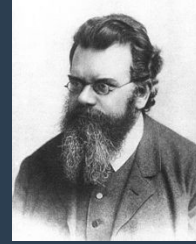
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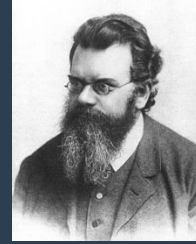
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Why even consider this term, then??

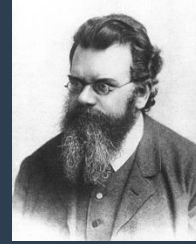
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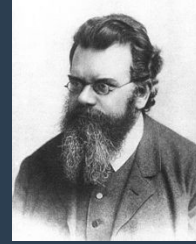


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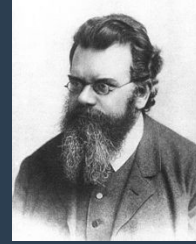
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Verified that it reduces to results obtained from Drude model

In free electron limit

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

Einstein and Onsager Relations are satisfied

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

Which all terms contribute

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

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0, as it should be without any external field

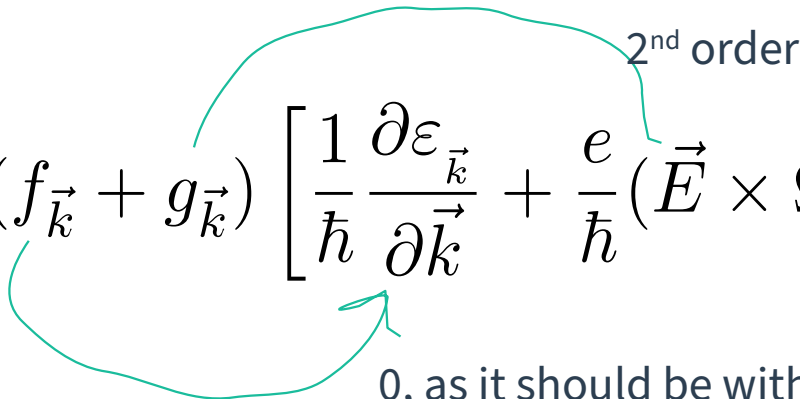
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Chern number, integer

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Independent of scattering!!

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- But we have an issue here

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

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(Nernst)

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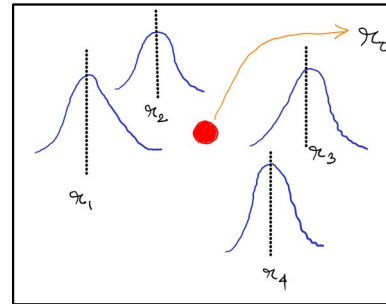
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- **What we missed:**

- The wavepackets are not localized



(Nernst)



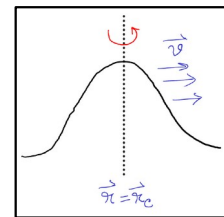
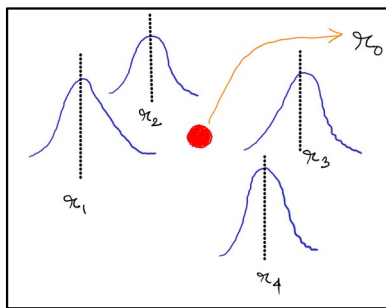
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What we missed:

- The wavepackets are not localized
- Circulating magnetization currents



Orbital magnetic moment

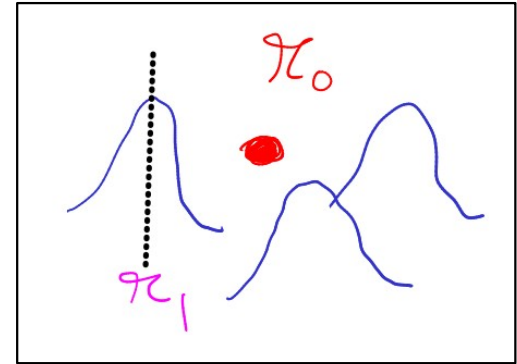
$$\vec{m}_k = -\frac{e}{2m} \langle \psi_{k,r_0} | (\vec{r} - \vec{r}_0) \times \hat{p} | \psi_{k,r_0} \rangle$$



(Nernst)

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

Wavepackets are not localized

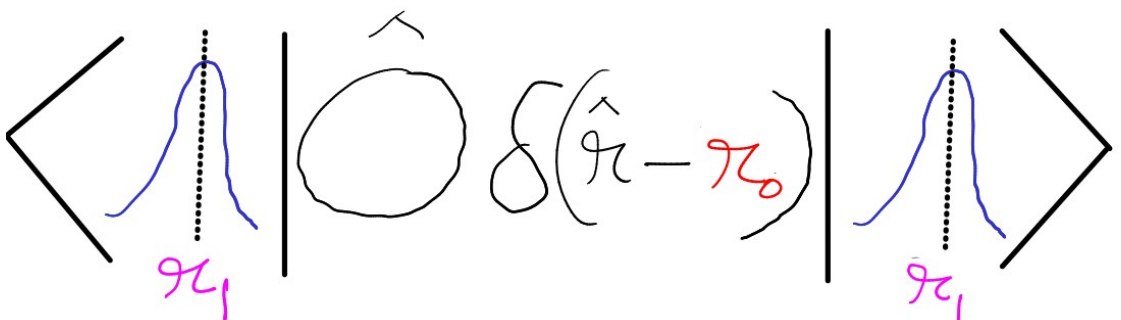


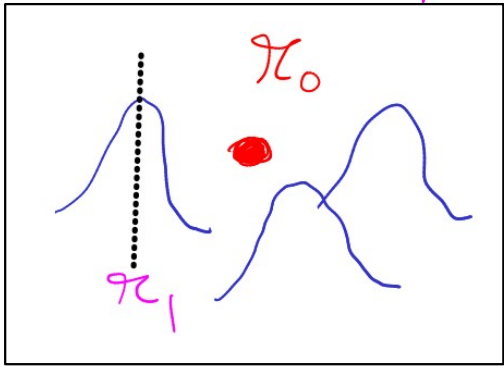
Wavepackets are not localized

The diagram illustrates a quantum measurement process. The top part shows a bra-ket expression: $\langle \psi_1 | \hat{O} \delta(\hat{H} - E_0) | \psi_1 \rangle$. The wavepacket $|\psi_1\rangle$ is represented by a blue curve with a vertical dotted line at E_1 . The operator \hat{O} is a circle with a dot. The energy E_0 is written in red. Below this, a box shows the wavepacket $|\psi_1\rangle$ (blue curve) and a red dot representing the energy E_0 . The wavepacket is centered at E_1 , which is lower than E_0 , demonstrating that the wavepacket is not localized at the energy E_0 .

Wavepackets are not localized

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

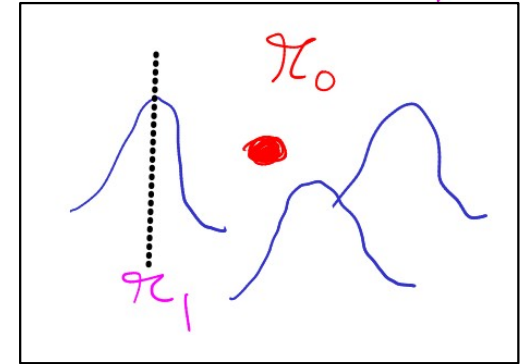




Wavepackets are not localized

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

- 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 $\hat{O} = \frac{-e\hat{p}}{m}$

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

- Similarly, for heat current

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

Effects of orbital magnetization

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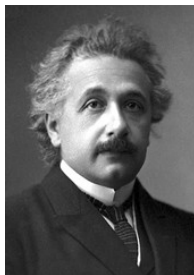
$$\vec{M}^e = - \left. \frac{\partial G}{\partial \vec{B}} \right|_{\vec{B}=0} = \frac{1}{\beta} \int \frac{2d\vec{k}}{(2\pi)^d} \frac{e}{\hbar} \vec{\Omega}(\vec{k}) \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) + \int \frac{2d\vec{k}}{(2\pi)^d} f \vec{m}_{\vec{k}}$$

Phase space density correction is important

Transport current

Now we are ready to calculate the transport electric current

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



How about Onsager relation?

- We can 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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 \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 \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) \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 \left(\varepsilon_0(\vec{k})_k - \mu \right) + k_B T \log \left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)} \right) \right] \\
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Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu.
PRL **97**, 026603 (2006)

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Possible resolution for the Einstein relation to hold

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

$$\approx \int \frac{2d\vec{k}}{(2\pi)^d} \frac{e\vec{\Omega}}{\hbar} \mu f_k \underbrace{=}_{2D} \frac{2e\mu}{h} \left(\sum_{fully\ filled} \mathcal{C}_n + \int_{partially\ filled} \frac{\Omega_z}{2\pi} \right)$$

- Interpretation ?? Along the lines of Raffaele Resta 2010 J. Phys.: Condens. Matter 22 123201
- Zero for trivial states, and bound energy current is due to topological states, as a response to change in chemical potential

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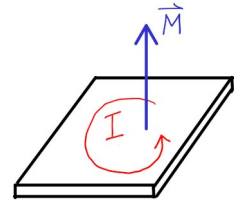
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change in chemical potential $\frac{\Delta I_0^E}{\Delta \mu} = \frac{\mu}{e} \left(2 \frac{e^2}{h} \right) \# \text{Topological states}$

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

Edge and bulk



Berry curvature and Chern numbers of some microscopic models

- In a two band system with Hamiltonian $H = d_x \sigma_x + d_y \sigma_y + d_z \sigma_z$

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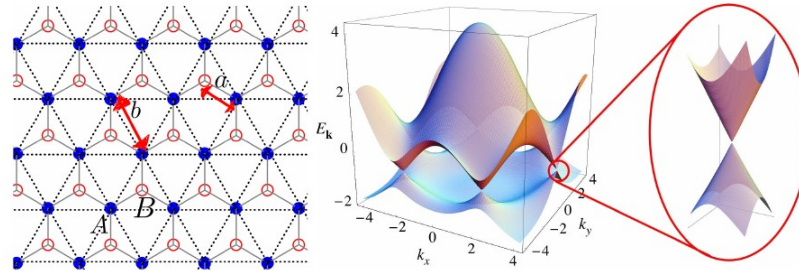
$$\Omega_z = i \int d\vec{r} \nabla_{\vec{k}_x} u_{\vec{k}}^* \times \nabla_{\vec{k}_y} u_{\vec{k}} = \frac{1}{2} \hat{d} \cdot \left(\frac{\partial \hat{d}}{\partial k_x} \times \frac{\partial \hat{d}}{\partial k_y} \right)$$

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- Monolayer graphene

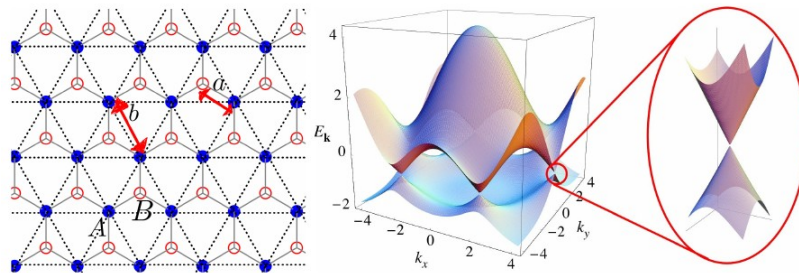


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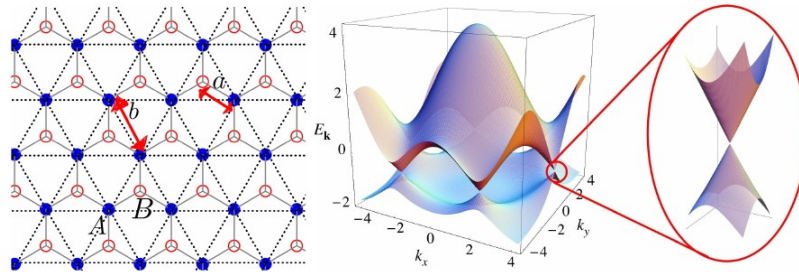
Non-zero Berry curvature when there is a finite band gap : growing on BN substrate

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Non-zero Berry curvature when there is a finite band gap : growing on BN substrate

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

Valley Polarization

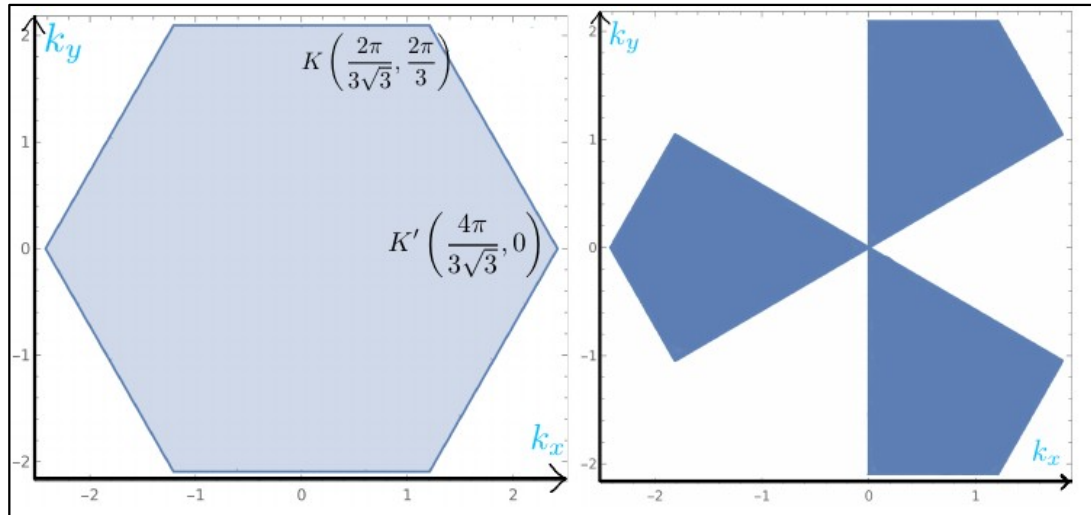
- Electrons can be made to selectively occupy valleys with circularly polarized light

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

Valley Polarization

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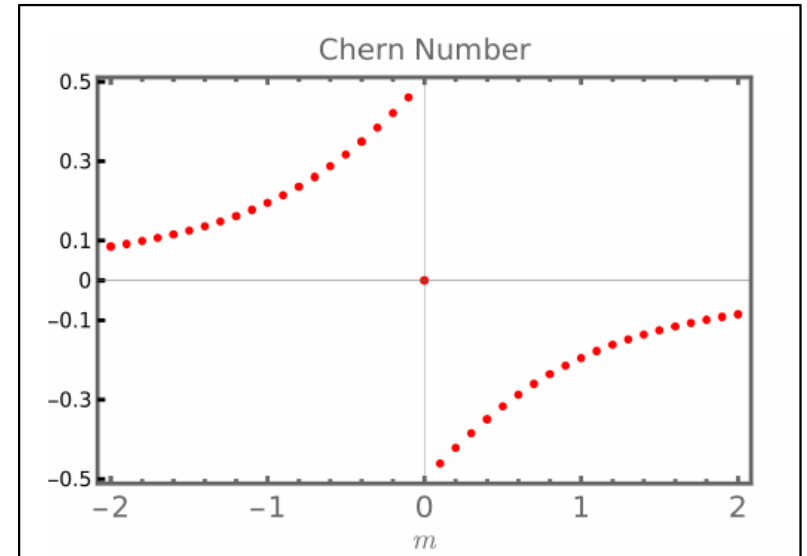
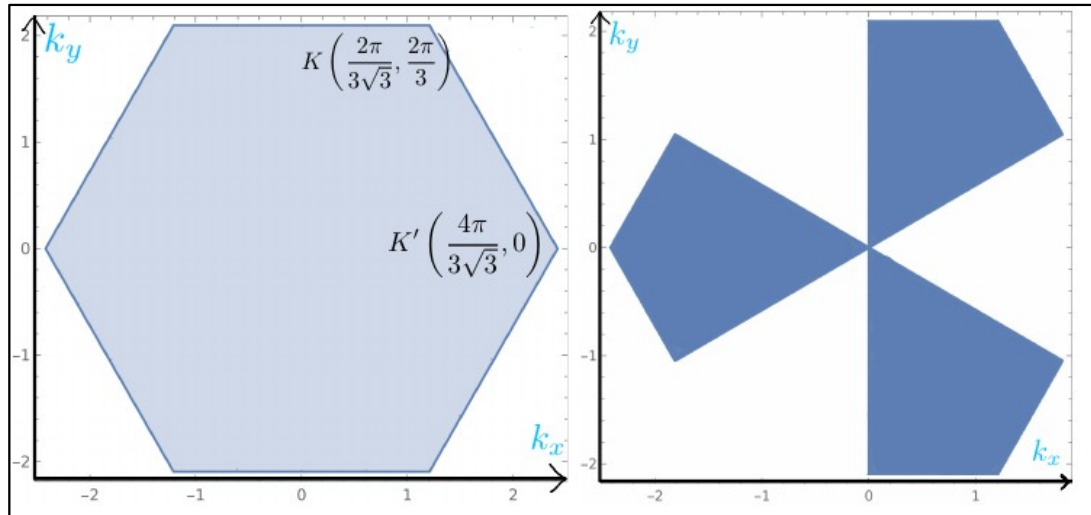
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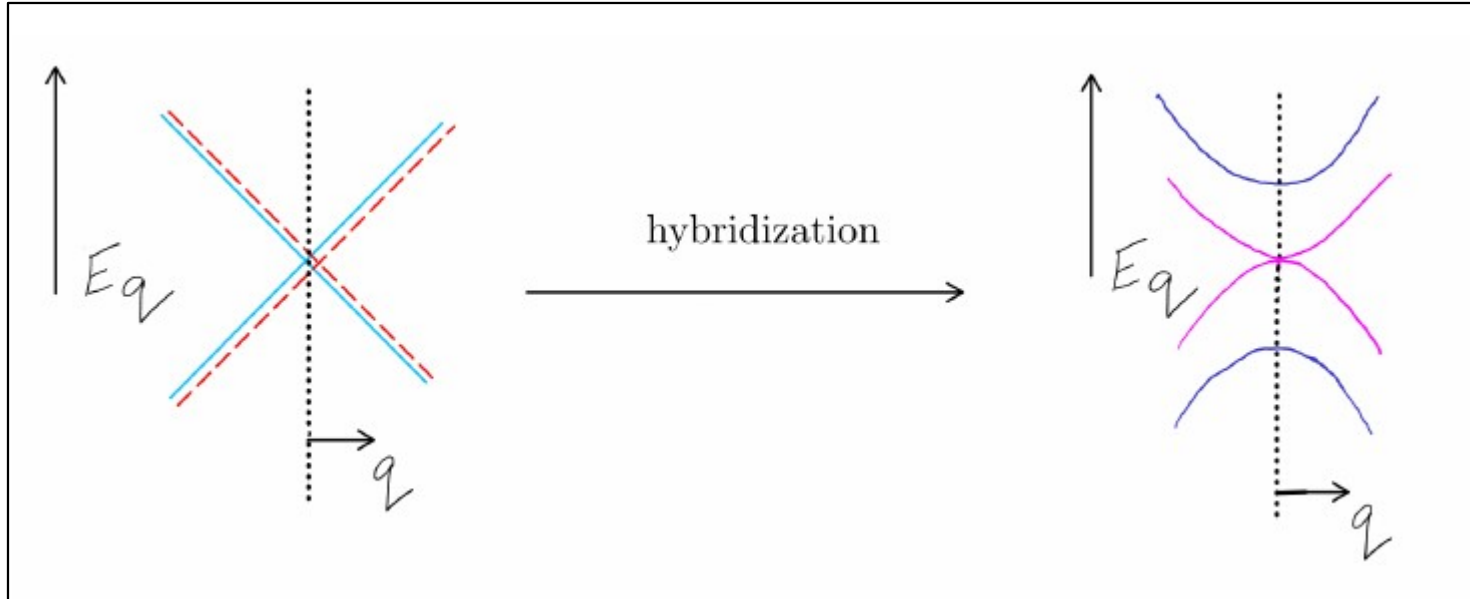
Valley Polarization

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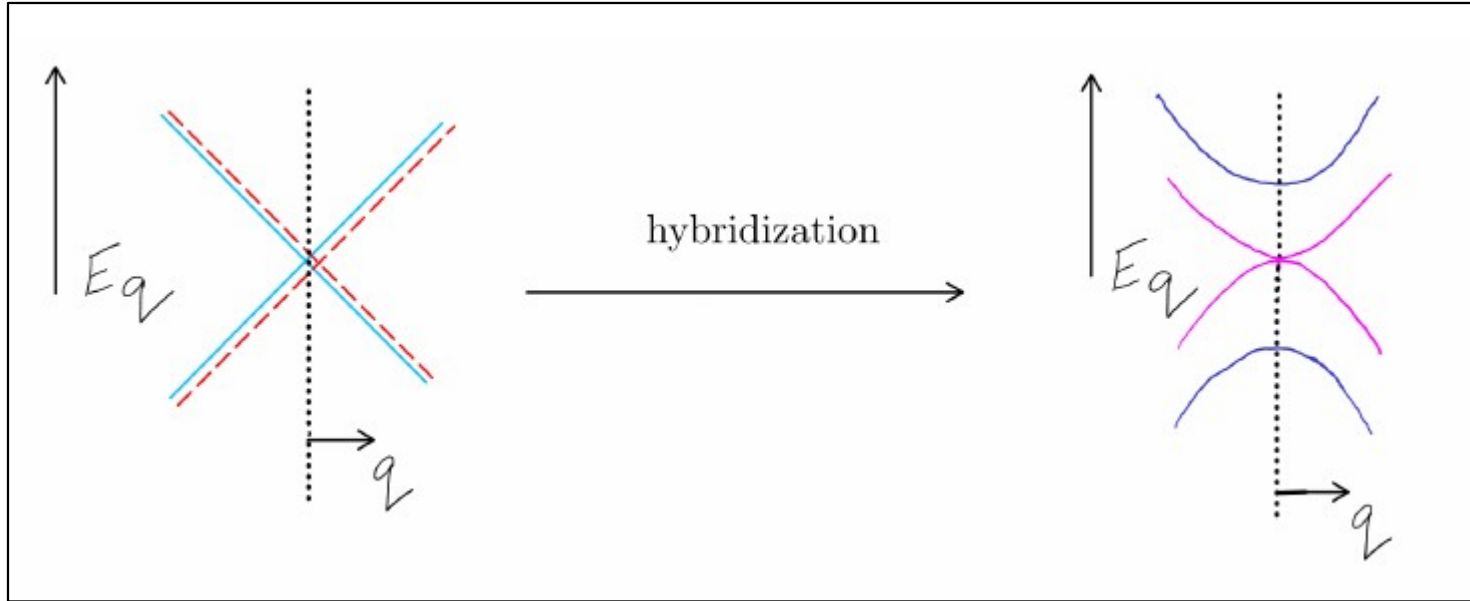
A. Friedlan and M. M. Dignam PRB **103**, 075414 (2021)



Bilayer Graphene

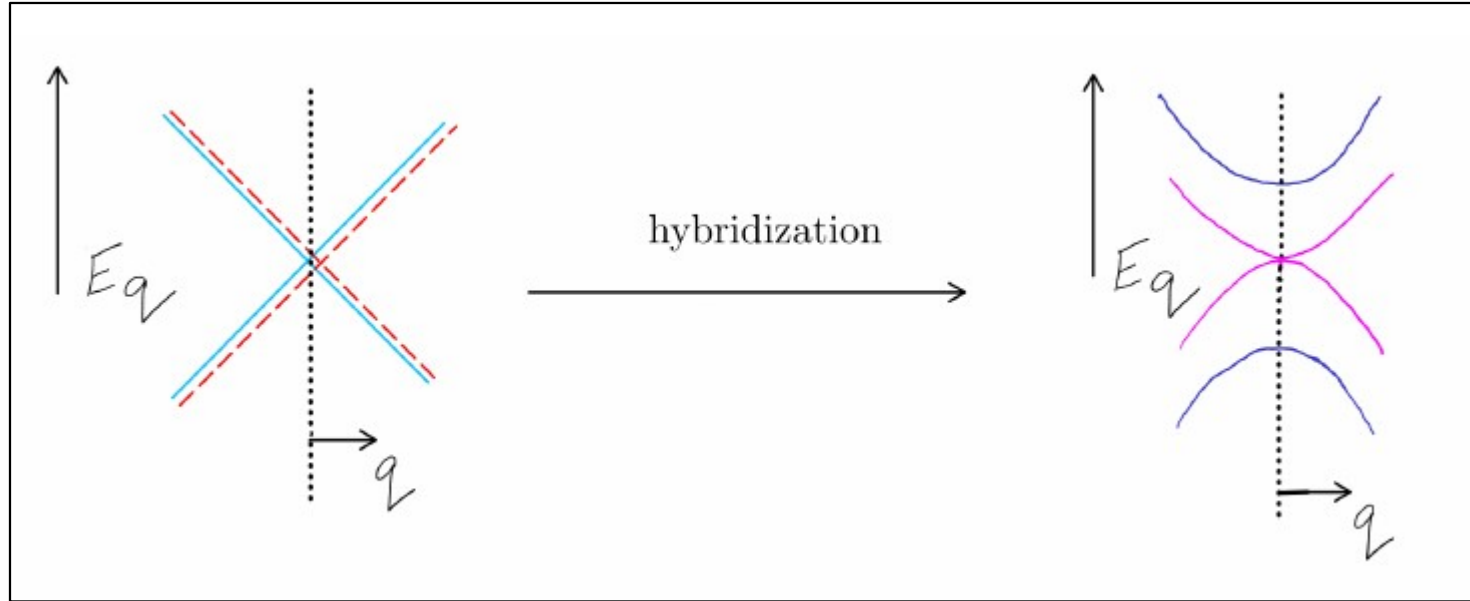


Bilayer Graphene

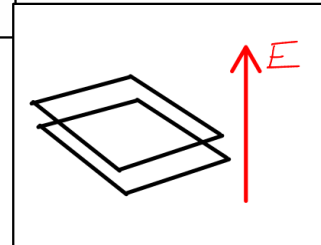


- We can generate a band gap by applying an electric field






Bilayer Graphene








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Results for valley Chern number

		$\vec{\Omega}$	\mathcal{C}
	$E = K$	0	0
	$E = \sqrt{K^2 + \hbar^2}$	$\neq 0$	$\pm \frac{1}{2}$
	$E = K^2$	0	0
	$E = \sqrt{K^4 + \Delta^2}$	$\neq 0$	± 1
	$E = \frac{\hbar}{\sqrt{k^2 + \alpha^2 k^{4n}}}$	$\neq 0$	$-\frac{1}{2}, n > \frac{1}{2}$ $+\frac{1}{2}, n < \frac{1}{2}$

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

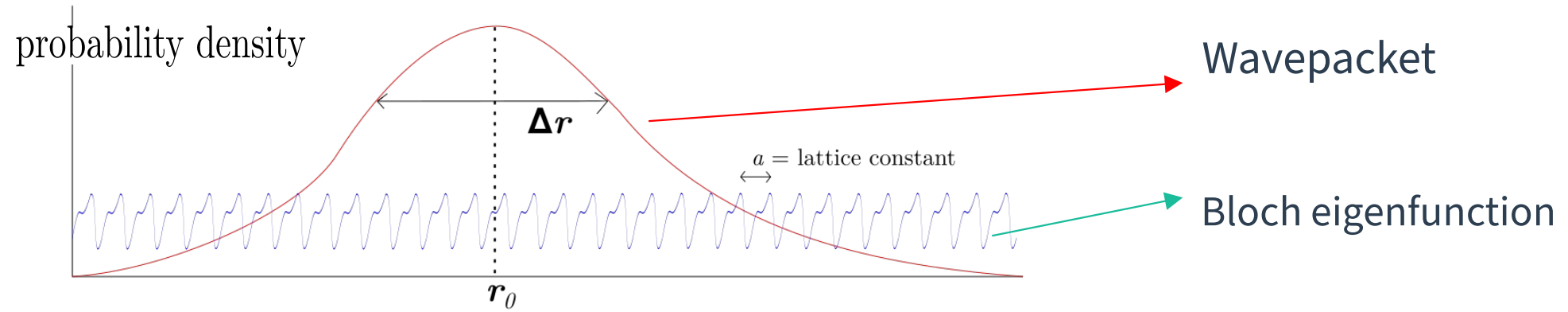
New results

- The condition on the energy magnetization for Einstein relation to hold for anomalous Heat current
- Solution of Boltzmann transport equation upto linear order, that captures the effects of Berry curvature in regular Ohmic, regular Hall and regular Nernst effects

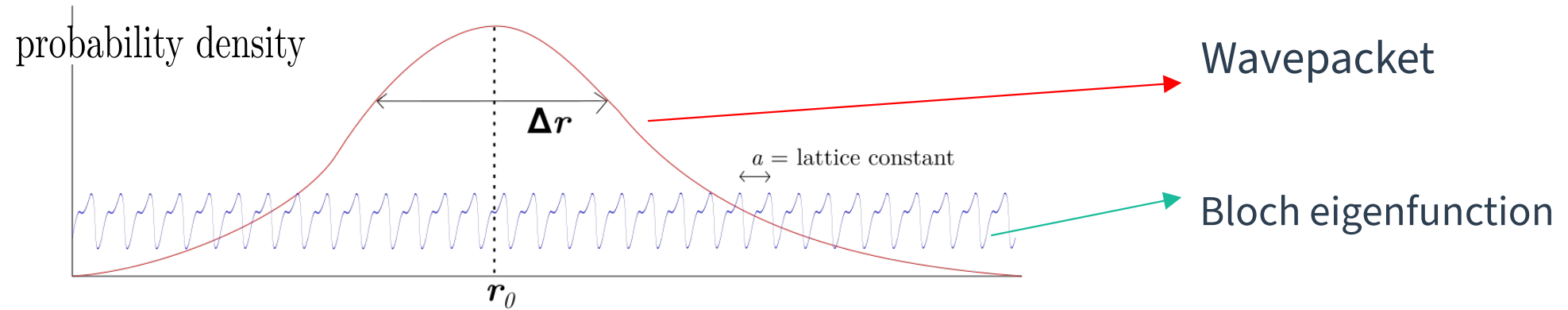


Thank you

Appendix: Construction of Bloch wavepacket, and its evolution

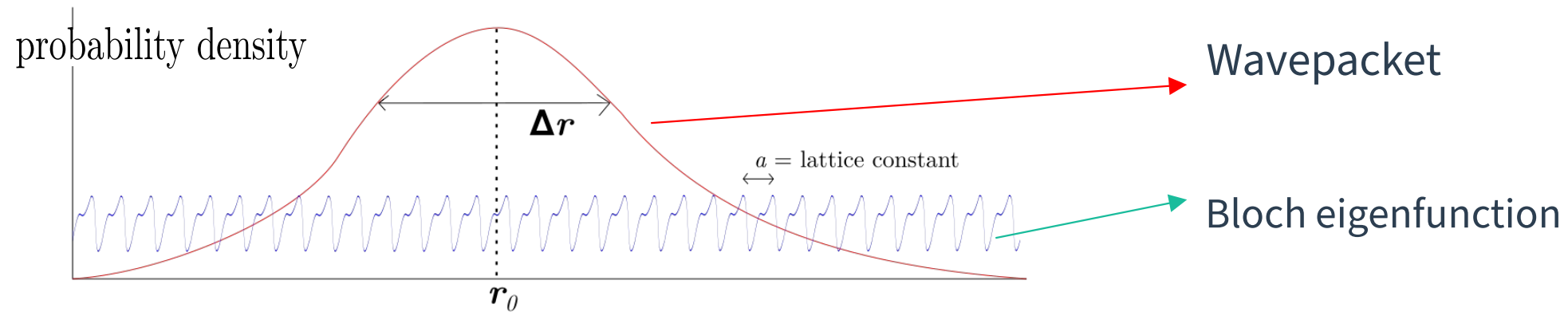


Appendix: Construction of Bloch wavepacket, and its evolution



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

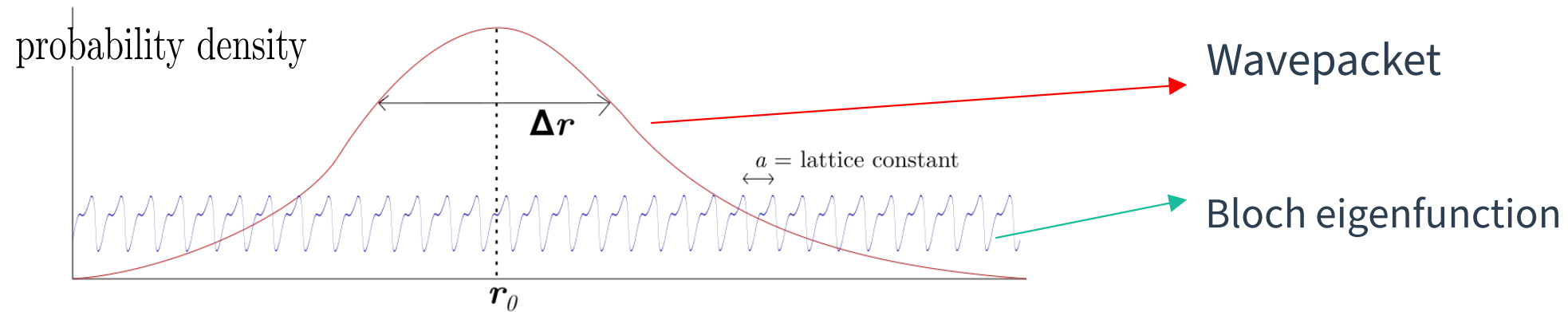
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$$\psi(\vec{r}, t = \Delta t) \left(e^{i(\vec{k} + \Delta\vec{k}) \cdot \vec{r}} e^{i\vec{A} \cdot \Delta\vec{k}} e^{-i\frac{\epsilon_{\vec{k}} \Delta t}{\hbar}} u_{n,\vec{k} + \Delta\vec{k}} \right)$$