Effects of Berry Curvature on Thermoelectric Transport

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UG 4th Year

24th June 2021

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

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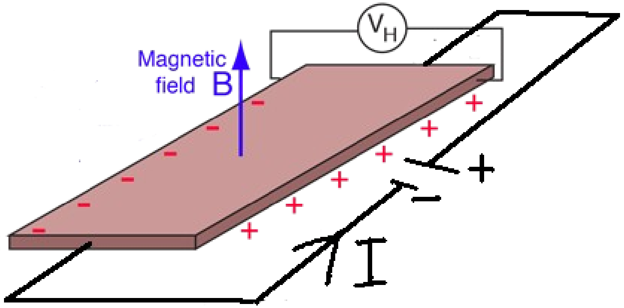

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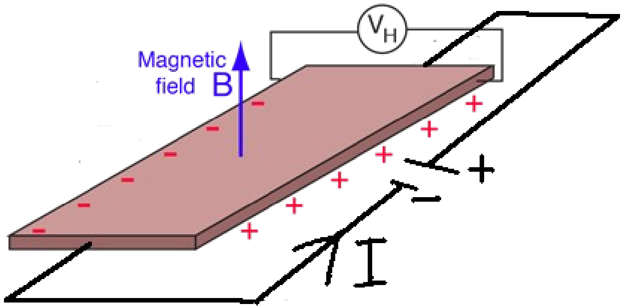

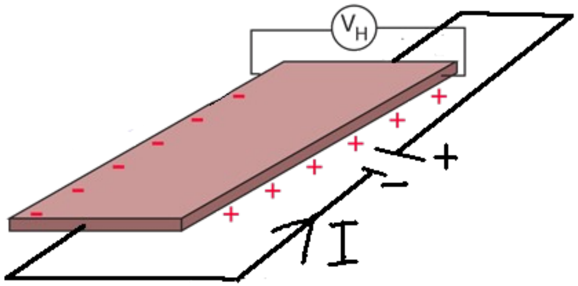

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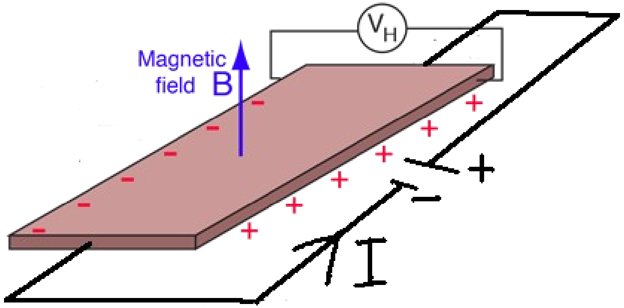

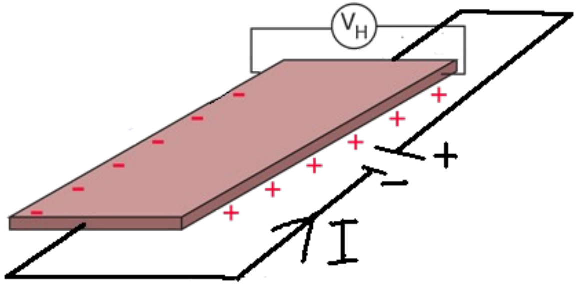

Anomalous Hall Effect

- Nernst Effect: Hall like response for a temperature gradient

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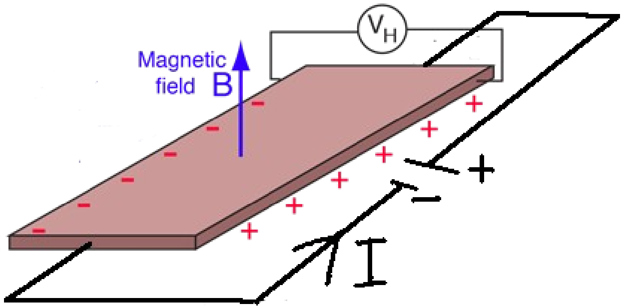

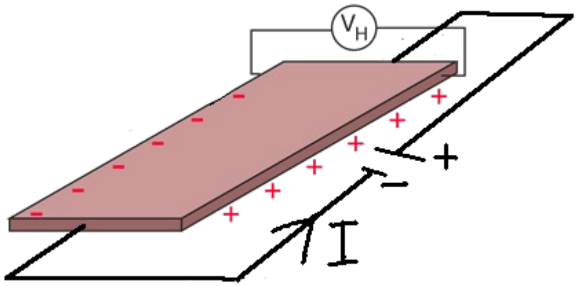

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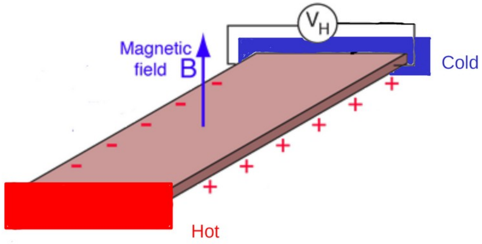

Electrically insulating temperature reservoirs

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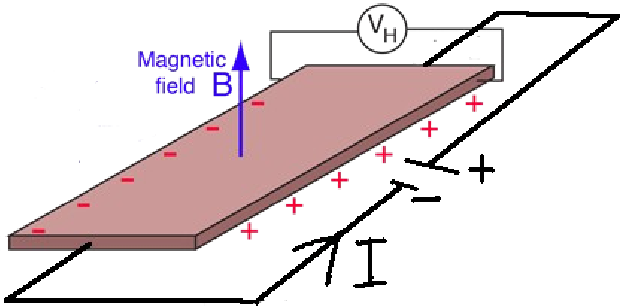

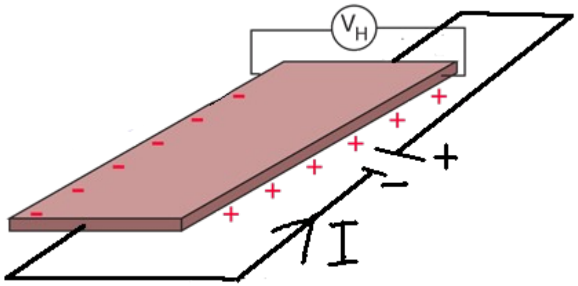

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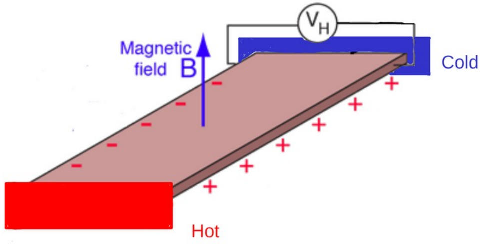

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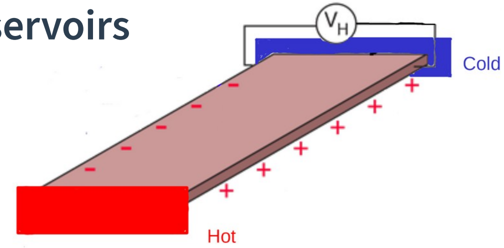

Thermoelectric transport: Einstein and Onsager relations

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

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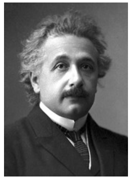

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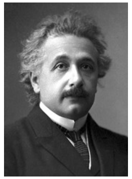

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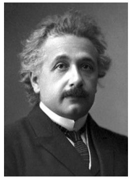

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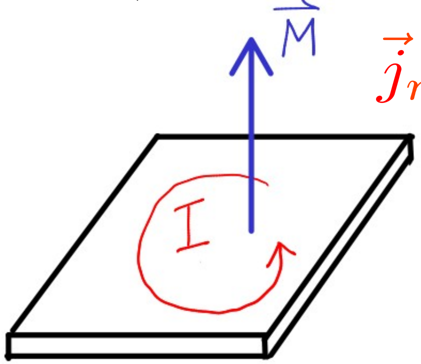

$\vec{j}_m = \nabla \times \vec{M}$

$\vec{j}_{\text{transport}} = \vec{j}_e - \vec{j}_M$

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

Geometric phase and Berry Curvature

- 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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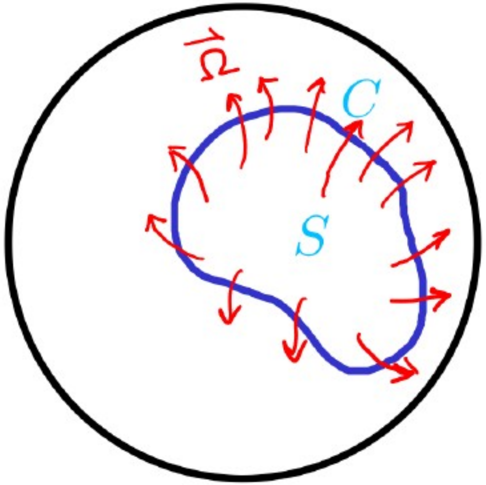

Space of $\lambda_1, \lambda_2, \ldots$

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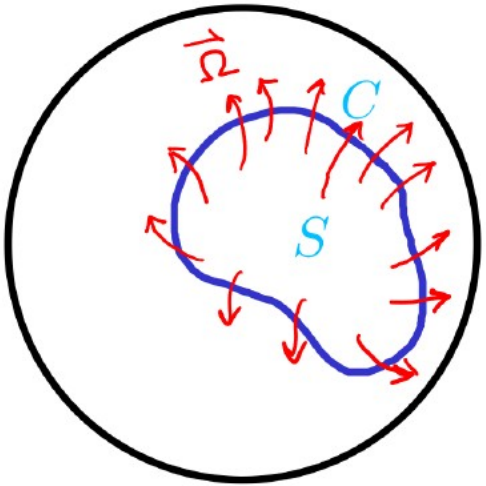

$$\gamma = i\oint_C \left\langle \varepsilon(\vec{\lambda}) \middle| \nabla_{\vec{\lambda}} \middle| \varepsilon(\vec{\lambda}) \right\rangle \cdot d\vec{\lambda}$$

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

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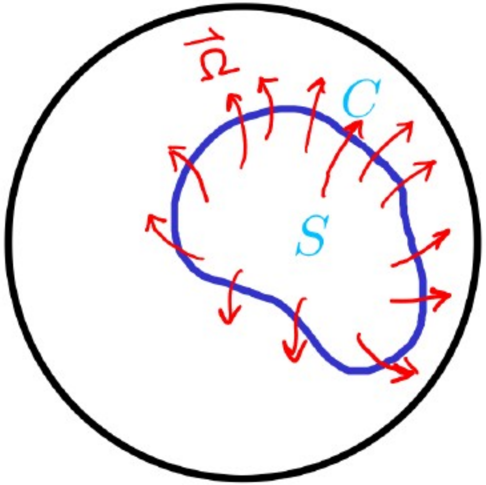

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Stokes' theorem: $\vec{\Omega} = \nabla \times \vec{A}$

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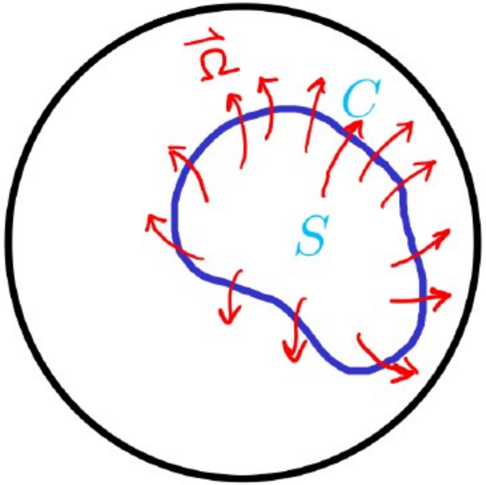

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Like magnetic field, but in parameter space

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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Effective Schrodinger equation

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

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- Time evolution

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

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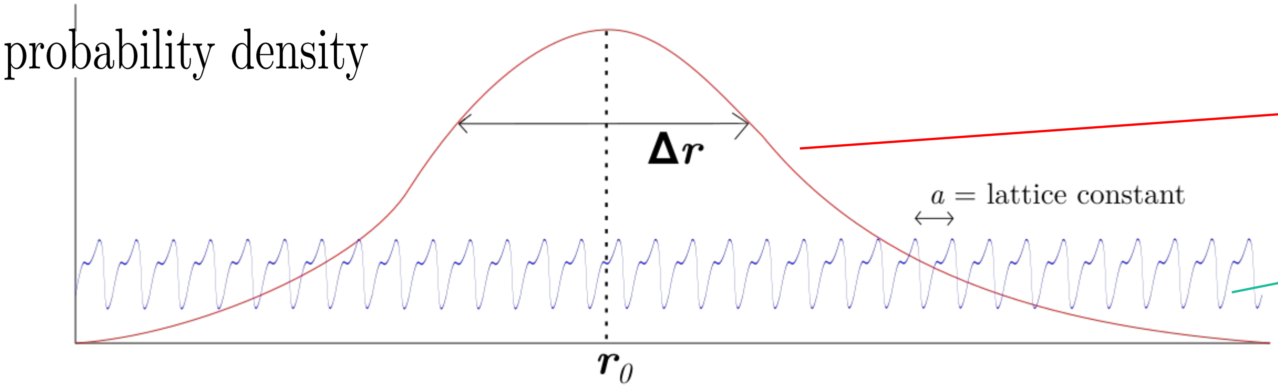
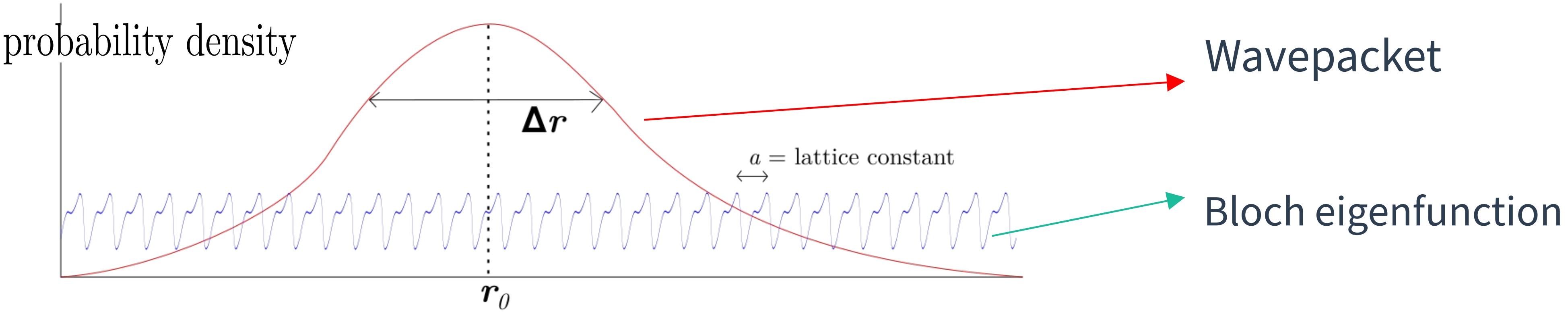
Construction of Bloch wavepacket, and its evolution



Wavepacket

Bloch eigenfunction

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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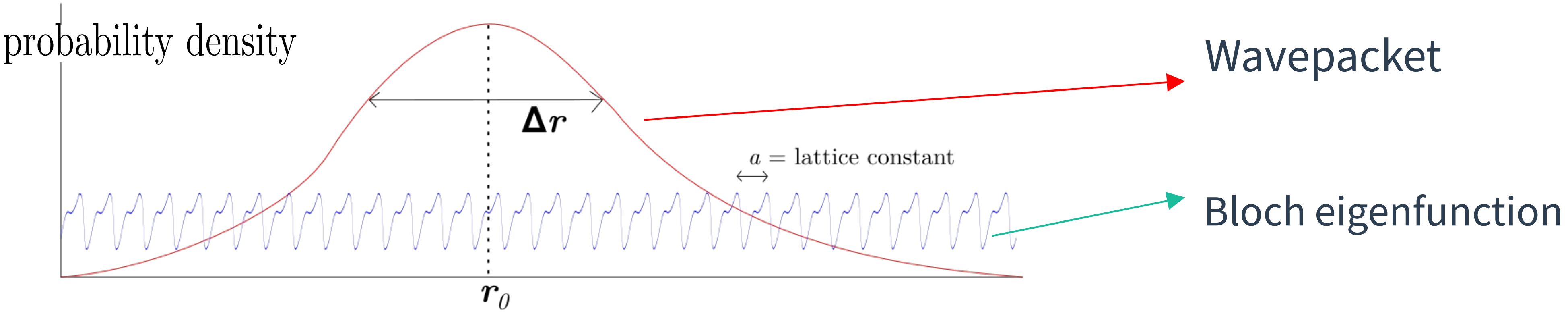

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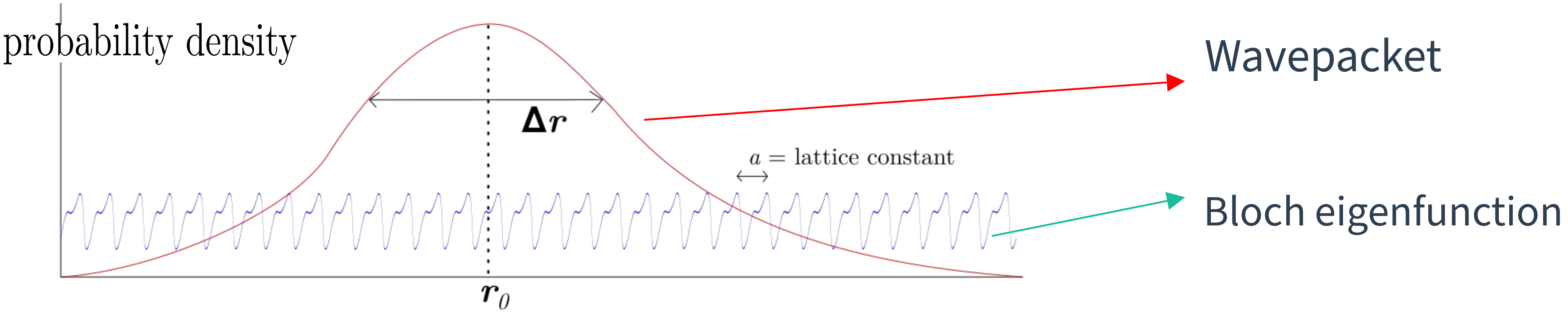

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$$\psi(\vec{r}, {\color{red} t=\Delta t}) = \qquad {\color{red}\left(e^{i(\vec{k}+\Delta\vec{k})\cdot\vec{r}} e^{i\vec{A}\cdot\Delta\vec{k}} e^{-i\frac{\varepsilon_{\vec{k}}\Delta t}{\hbar}} u_{n,\vec{k}+\Delta\vec{k}} \right)}$$

Effects of Berry curvature

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

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- The semiclassical equation of velocity is modified

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

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Anomalous velocity

Decoupled

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

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Anomalous velocity

(2D)

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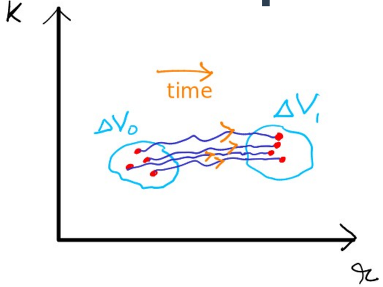
Anomalous velocity

- Phase space density is modified



(2D)

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

is a constant of motion

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

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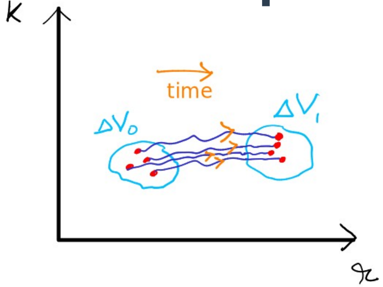

$$\Delta V\left(1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}\right)$$

is a constant of motion

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

(2D)

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

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

When do we get a non-zero Berry Curvature?

- 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.

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

Boltzmann Transport framework

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Boltzmann Transport framework

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

Boltzmann Transport framework

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$$\left\langle \hat{\vec{j}}_Q \right\rangle_k = \left\langle \hat{\vec{j}}_E \right\rangle_k - \mu \left\langle \hat{\vec{j}}_N \right\rangle_k$$

Boltzmann Transport framework

Classical charge and energy currents

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

Semiclassical framework

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

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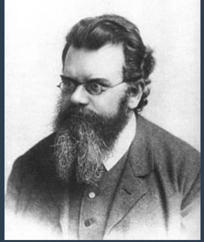
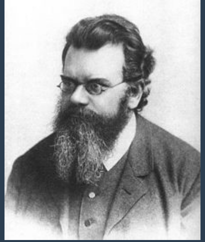
Boltzmann Transport Equation



- 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

Boltzmann Transport Equation



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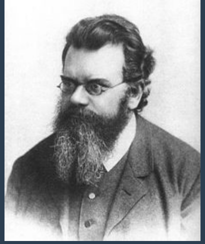

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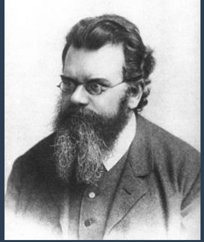

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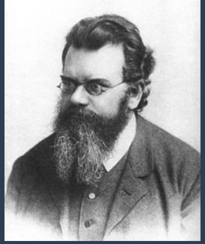

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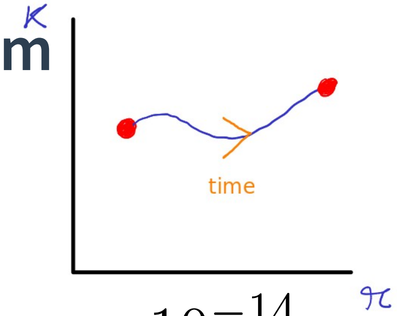

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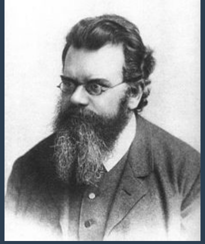
$$D_t \equiv \frac{\partial}{\partial t} + \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}} + \dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}}$$

Boltzmann Transport Equation



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

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

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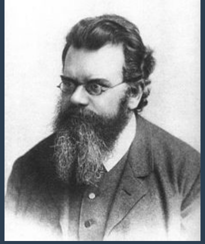

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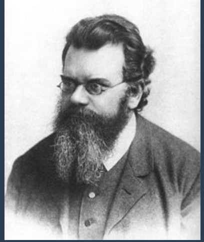
Boltzmann Transport Equation



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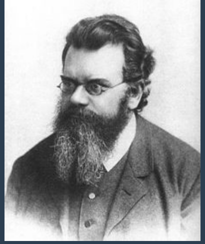

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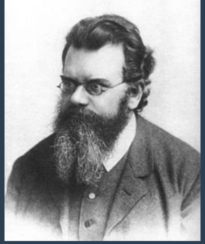
- This is less than the first term when

Boltzmann Transport Equation



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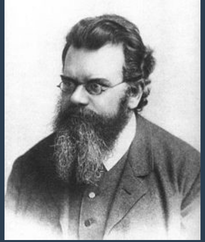
- If $m^* \sim m, \tau \sim 10^{-14} s$ then the critical field is ~ 570 T

Boltzmann Transport Equation



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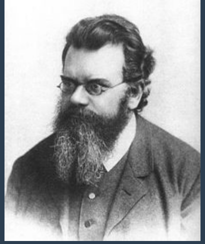
Why even consider this term, then??

Boltzmann Transport Equation



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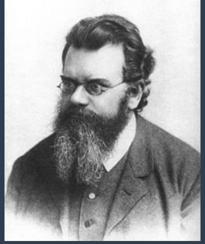

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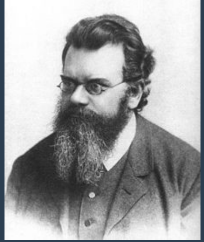
- The solution, with $\vec{S} = e\vec{E} + \nabla\mu + \frac{\varepsilon - \mu}{T}\nabla T$

Boltzmann Transport Equation



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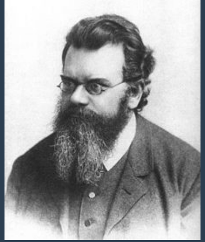
$$g_k = \frac{\partial f}{\partial \varepsilon}\frac{1}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \cdot \vec{S}$$
$$+ \frac{\frac{e\tau}{\hbar^2}}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\partial \varepsilon}{\partial \vec{k}} \cdot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

Boltzmann Transport Equation



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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

$$g_k = \frac{\partial f}{\partial \varepsilon}\frac{1}{1+\frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \cdot \vec{S}$$
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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

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

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

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

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- But we have an issue here

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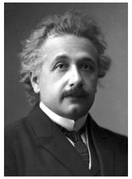
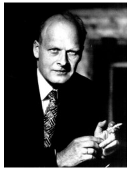
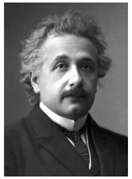
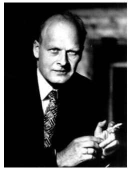




☹ ☹ ☹

(Nernst)

Issue

   (Nernst)

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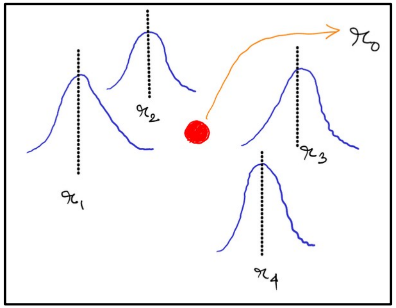
- The wavepackets are not localized



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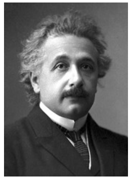 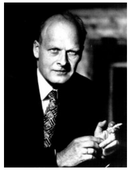 

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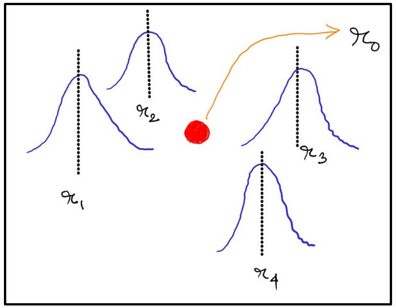
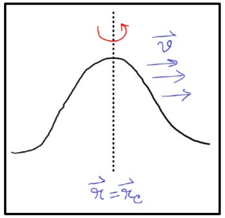
  - Circulating magnetization currents



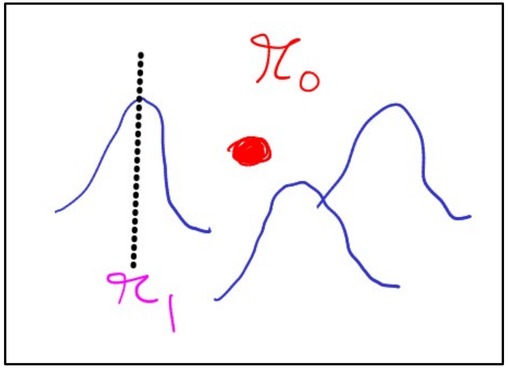


Orbital magnetic moment

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

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

Wavepackets are not localized



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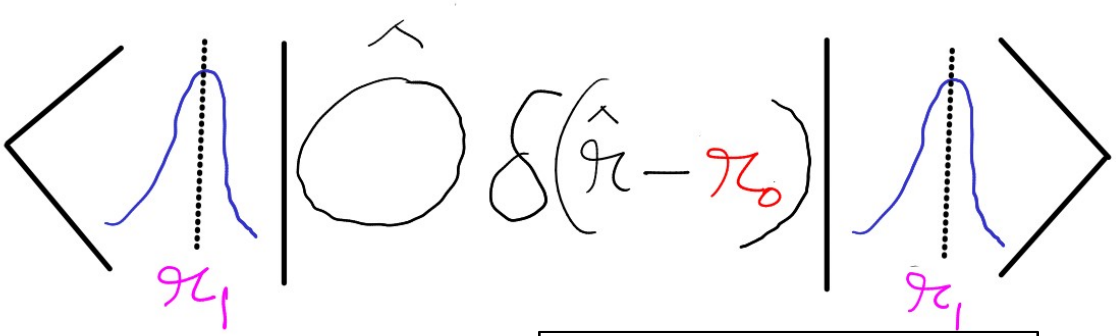
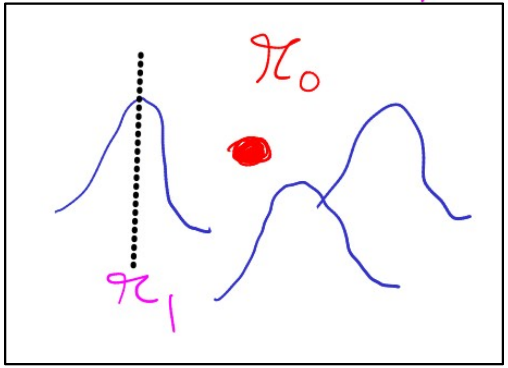
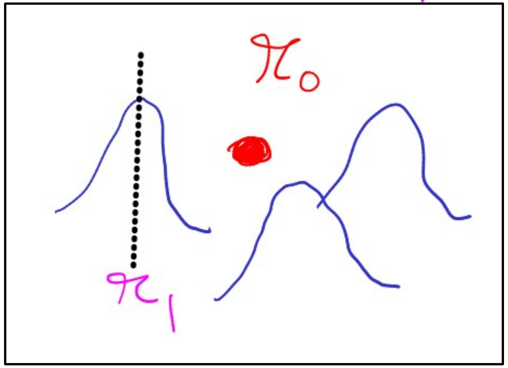




Wavepackets are not localized

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



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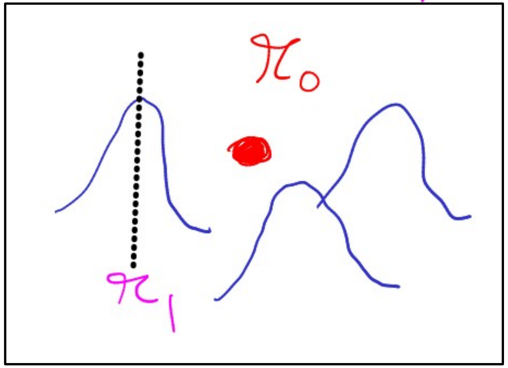

- To be technically correct, we should use the operator $\frac{\hat{O}\delta(\hat{r}-\vec{r}_0)+\delta(\hat{r}-\vec{r}_0)\hat{O}}{2}$ in case $\hat{O}$ does not commute with $\hat{r}$

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

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

- **Similarly, for heat current**

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

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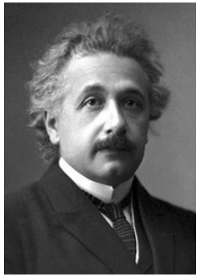
$$\vec{M}^e = -\left.\frac{\partial G}{\partial \vec{B}}\right|_{\vec{B}=0} = \frac{1}{\beta}\int \frac{2d\vec{k}}{(2\pi)^d}\frac{e}{\hbar}\vec{\Omega}(\vec{k})\log\left(1 + e^{-\beta(\varepsilon_0(\vec{k}) - \mu)}\right) + \int \frac{2d\vec{k}}{(2\pi)^d} f\vec{m}_{\vec{k}}$$

Phase space density correction is important

Transport current

Now we are ready to calculate the transport electric current

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



How about Onsager relation?

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

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

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&= \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 \\
&+ \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] \\
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&- \nabla\mu \times \frac{\partial \vec{M}_0^E}{\partial \mu} - \nabla T \times \frac{\partial \vec{M}_0^E}{\partial T}
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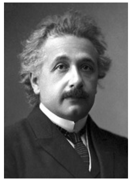


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Possible resolution for the Einstein relation to hold

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

Berry curvature and Chern numbers of some microscopic models

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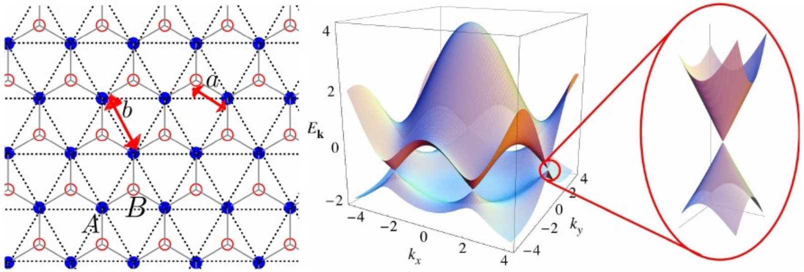
- Monolayer graphene



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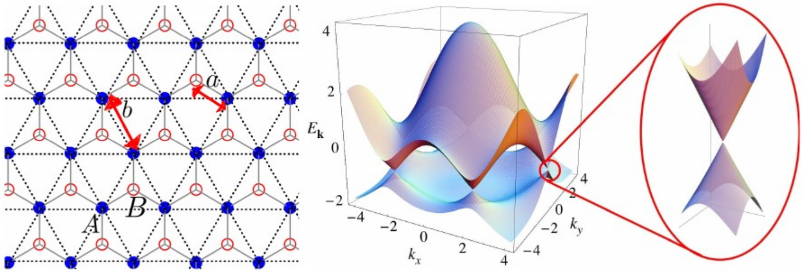

Non-zero Berry curvature when there is a finite band gap : growing on BN substrate

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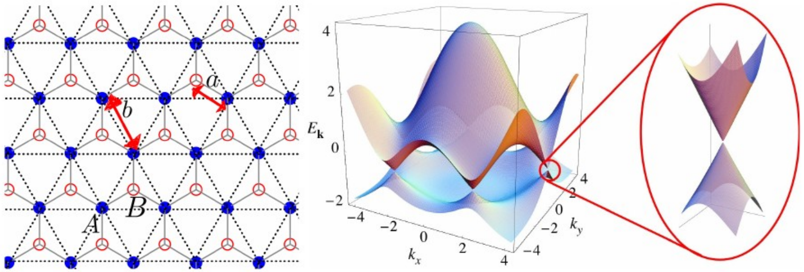

Non-zero Berry curvature when there is a finite band gap : growing on BN substrate

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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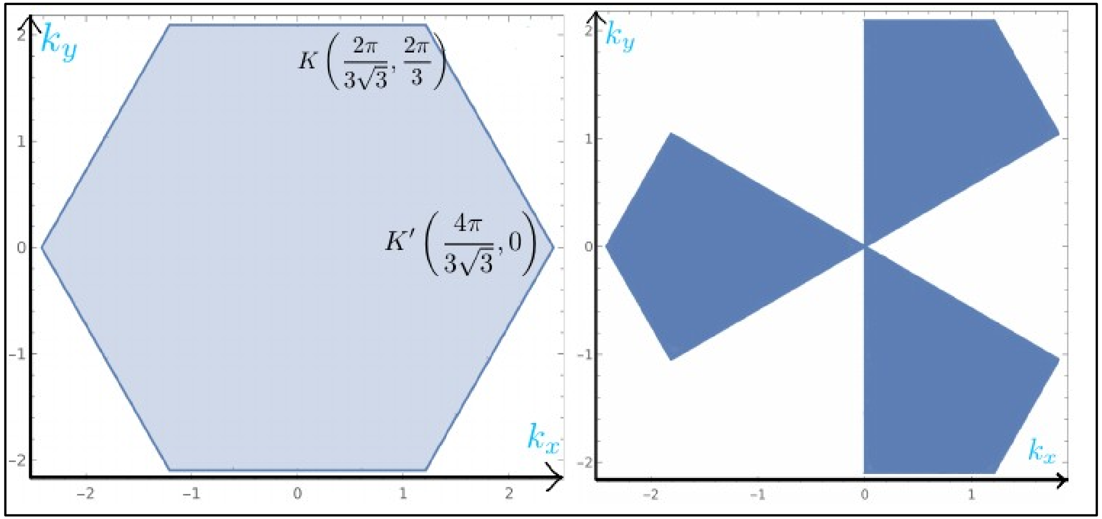

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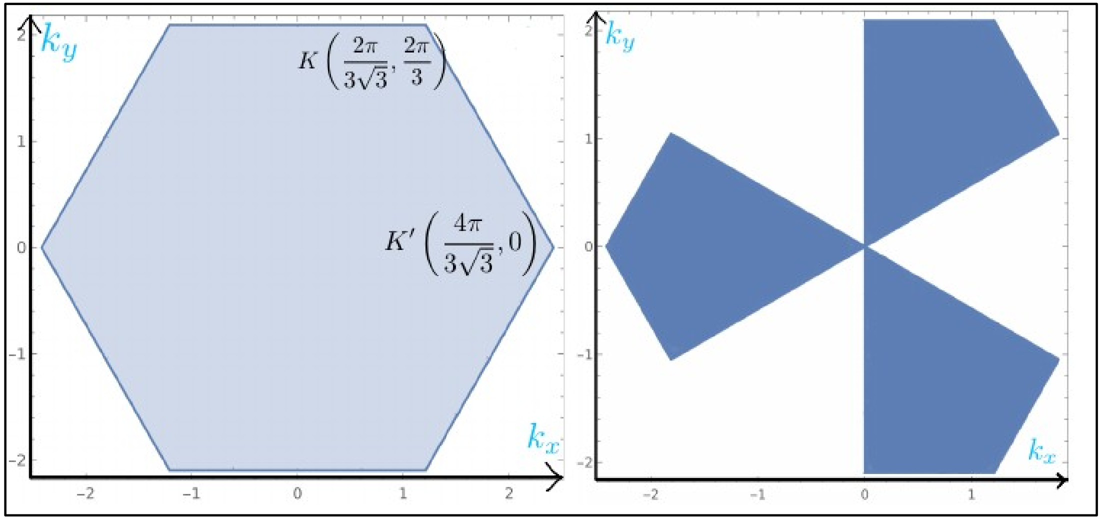
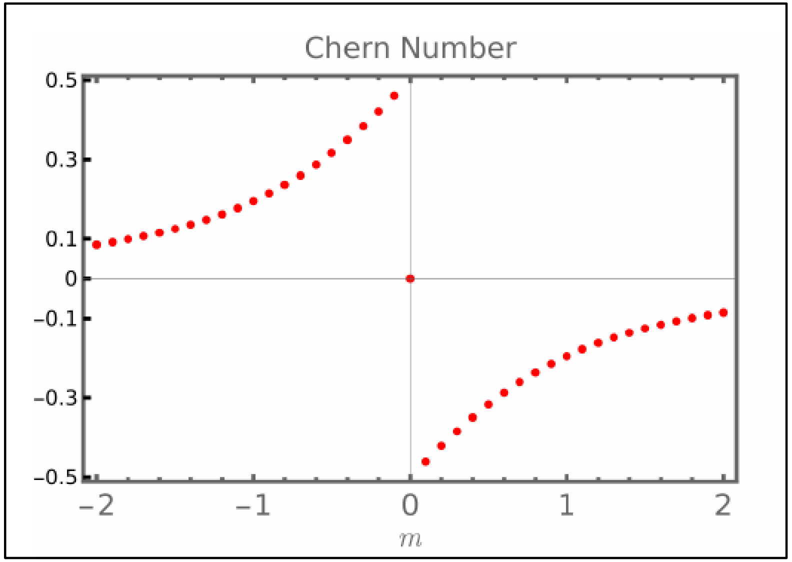
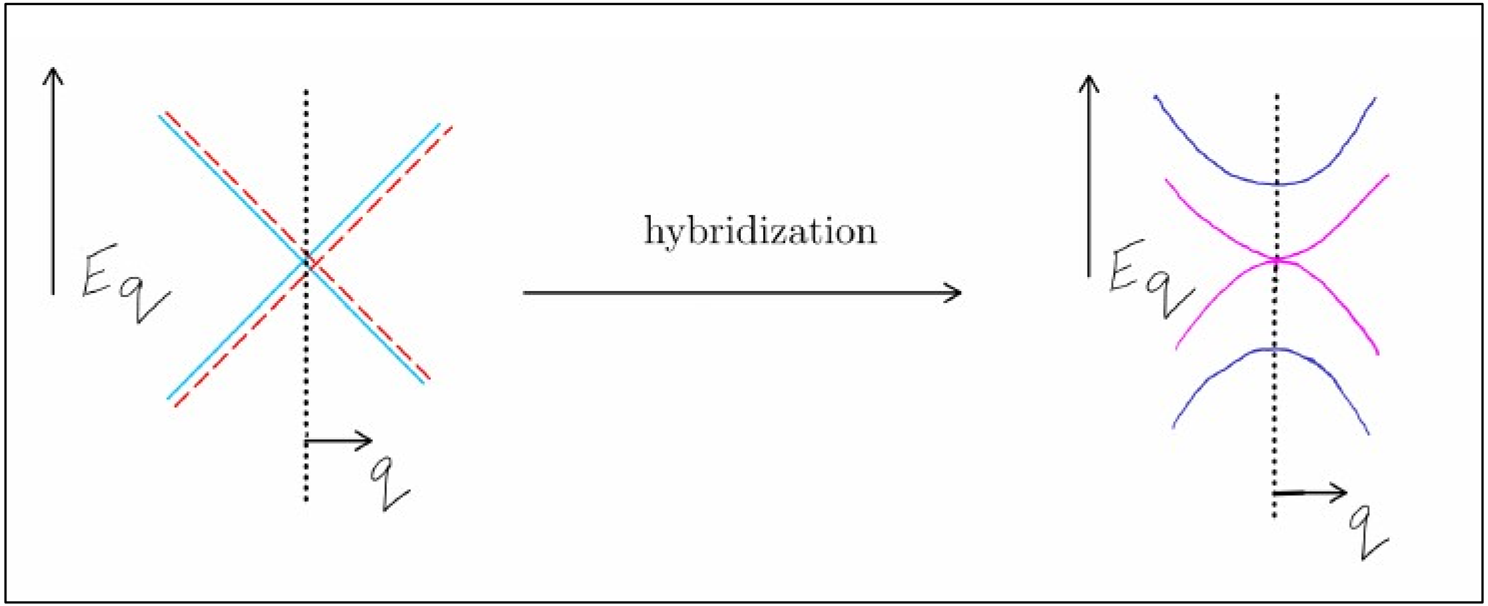




Bilayer Graphene



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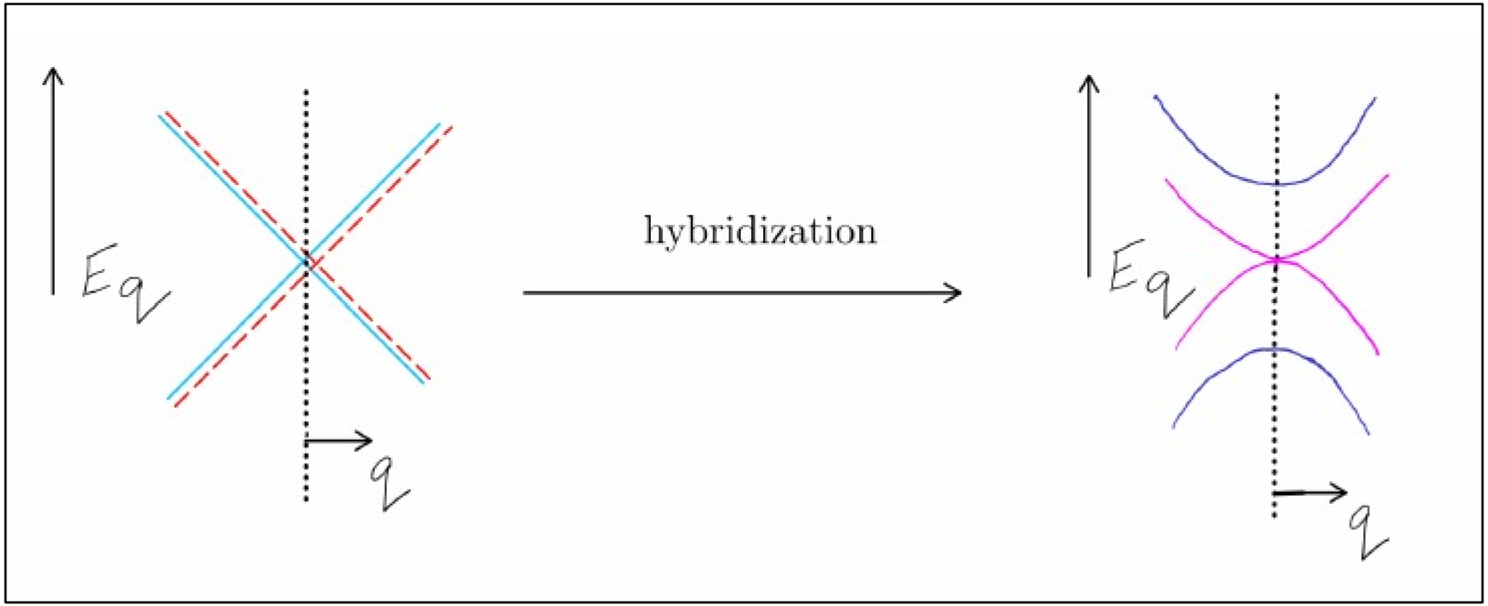
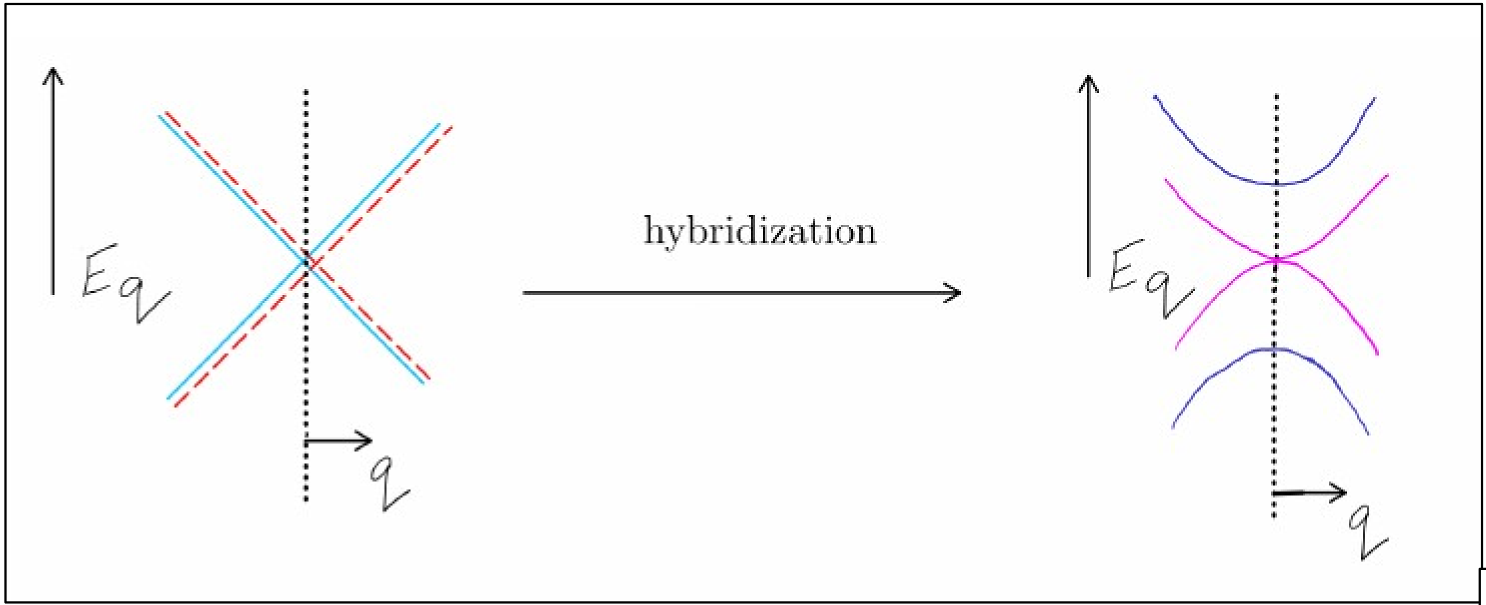
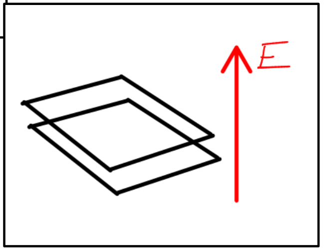


- We can generate a band gap by applying an electric field

Bilayer Graphene





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Results for valley Chern number

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

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

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