Effects of Berry Curvature on Thermoelectric Transport

Archisman Panigrahi

UG 4th Year

20th June 2021

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

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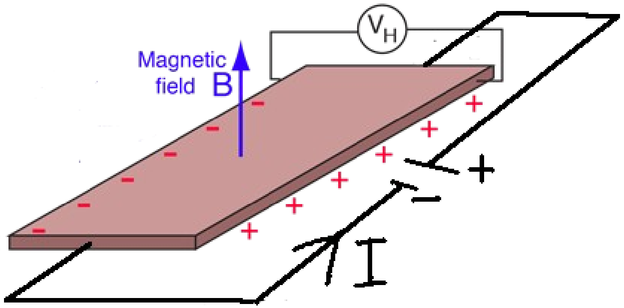

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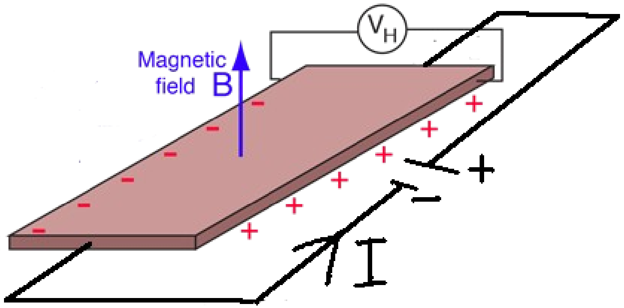

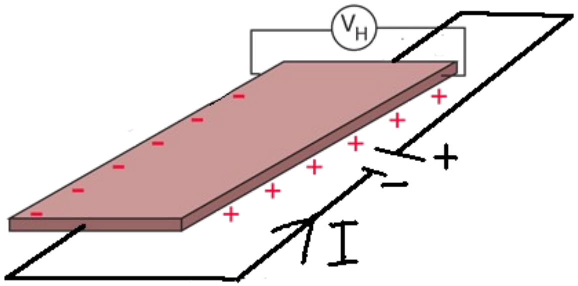

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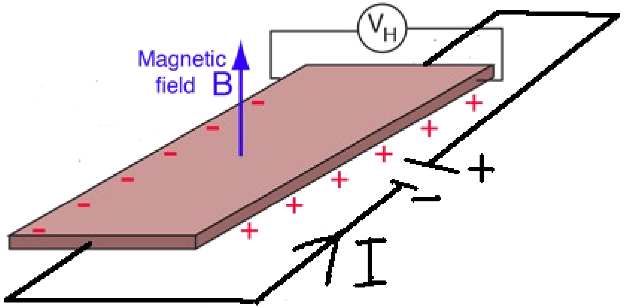

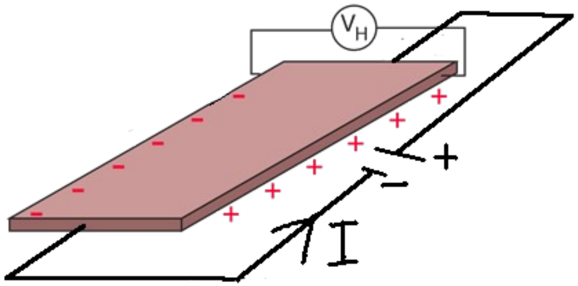

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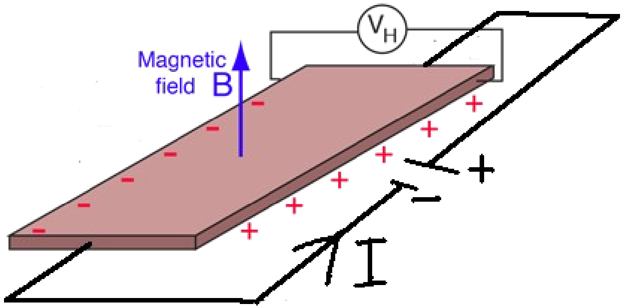

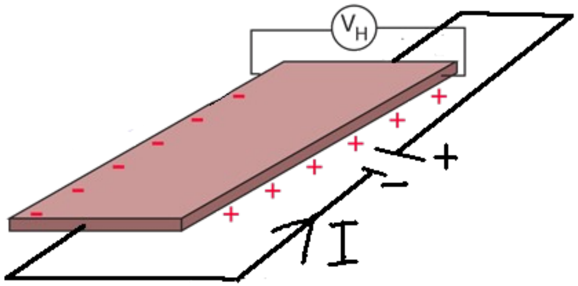

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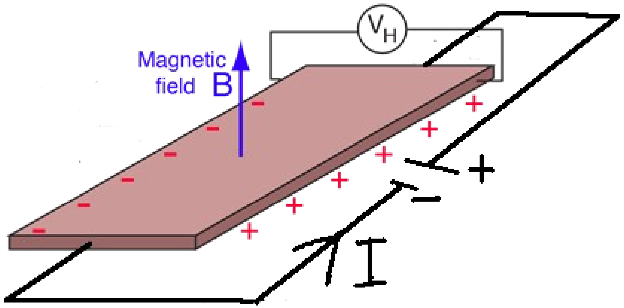

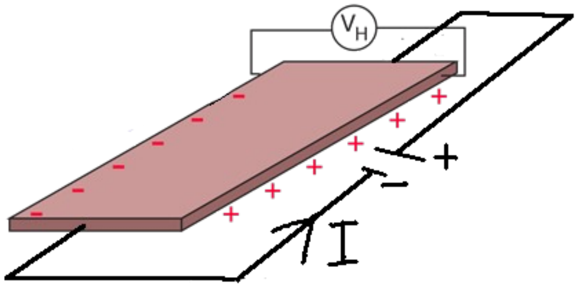

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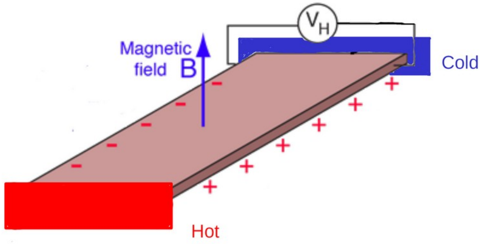

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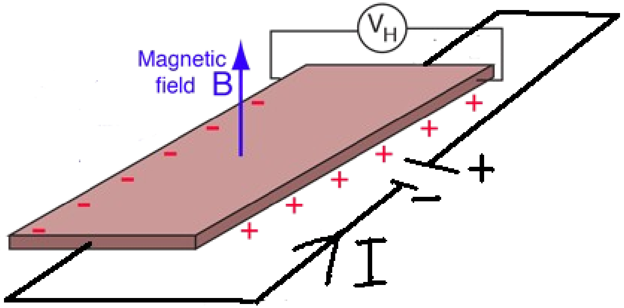

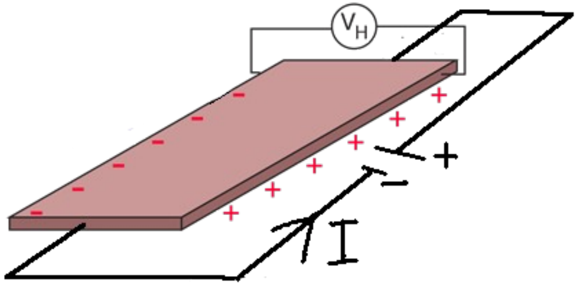

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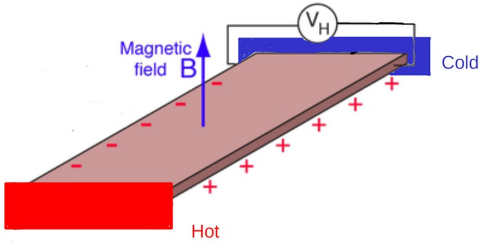

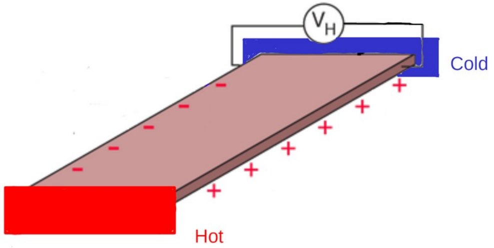

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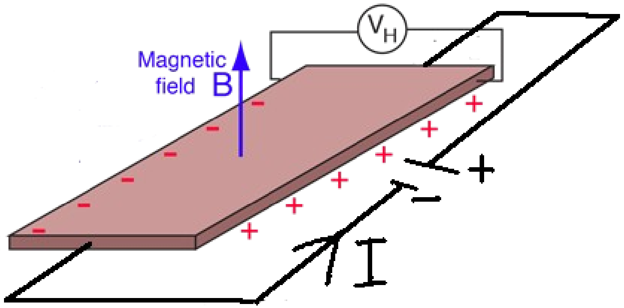

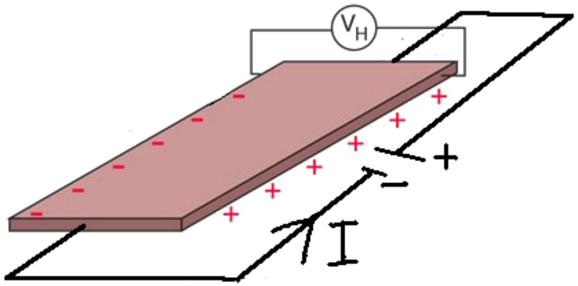

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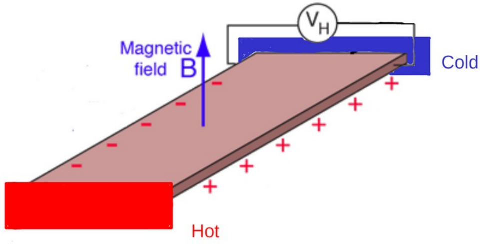
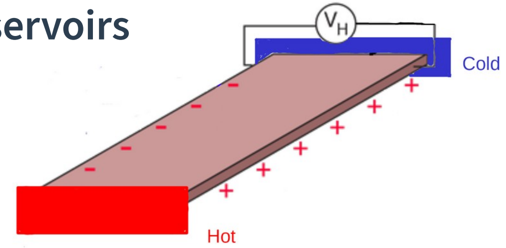


Electrically insulating temperature reservoirs



Thermoelectric transport: Einstein and Onsager relations

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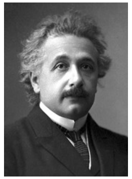

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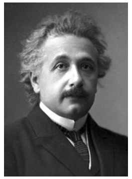

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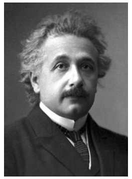

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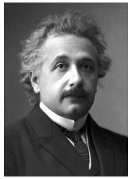

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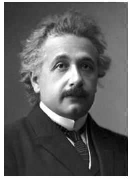

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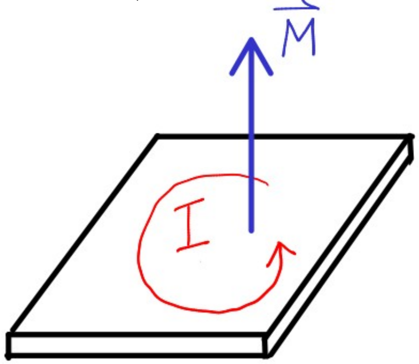

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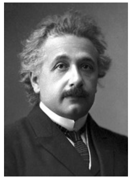

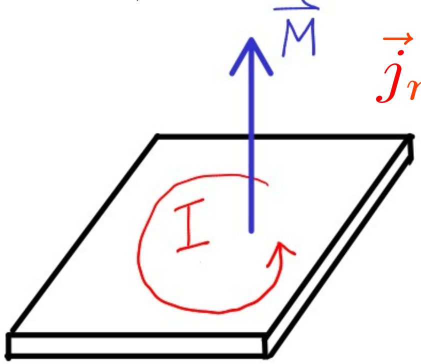

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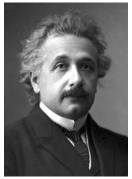

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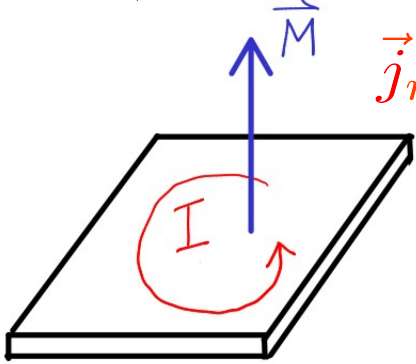

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N. R. Cooper, B. I. Halperin, and I. M. Ruzin. PRB **55** 2344 (1997)

Geometric phase and Berry Curvature

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

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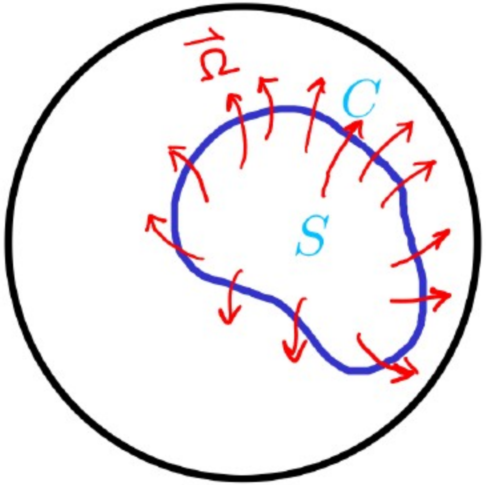

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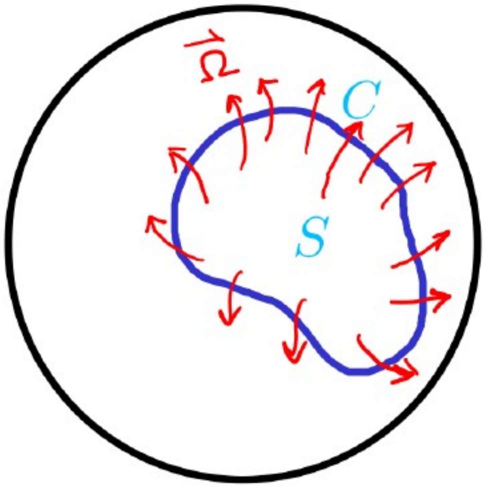

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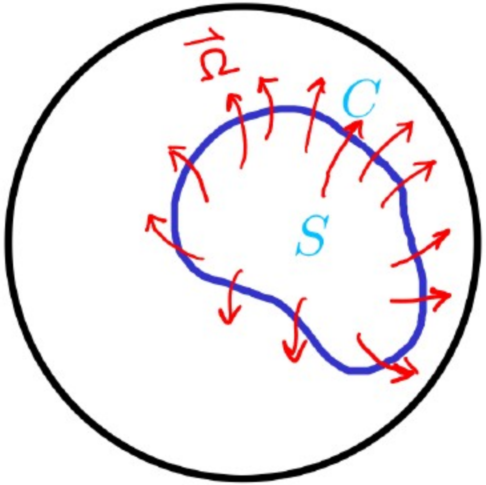

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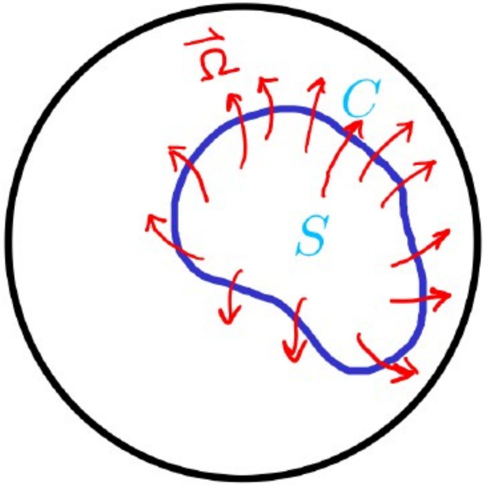

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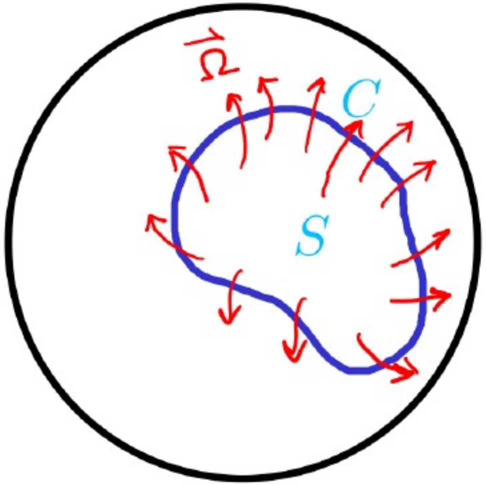

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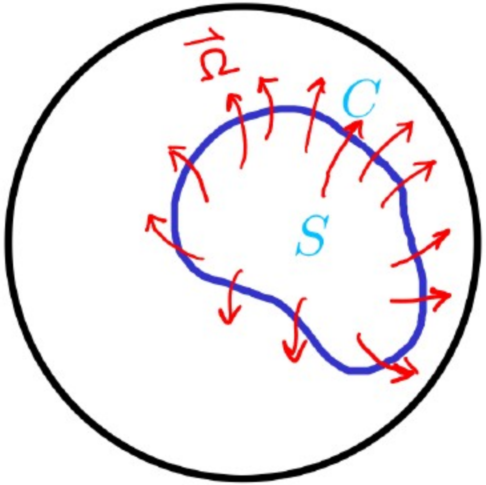

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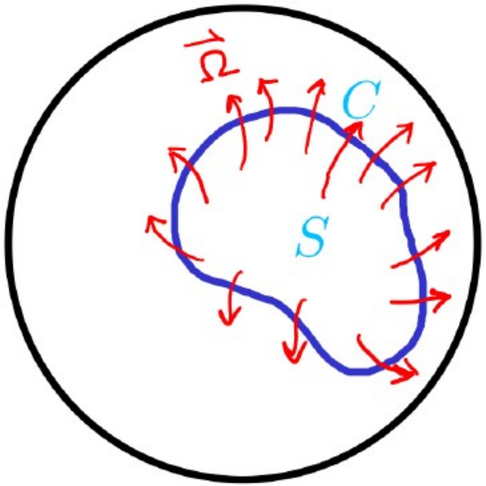

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Stokes' theorem:

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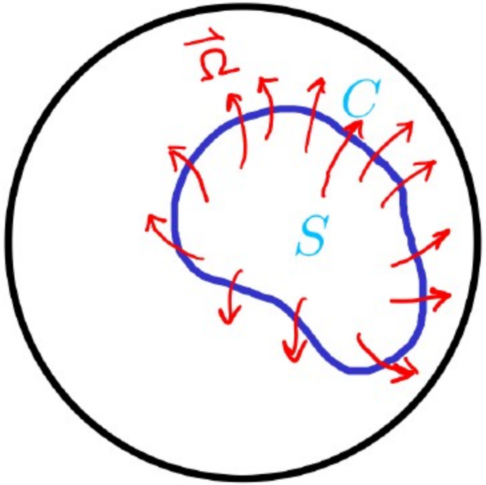

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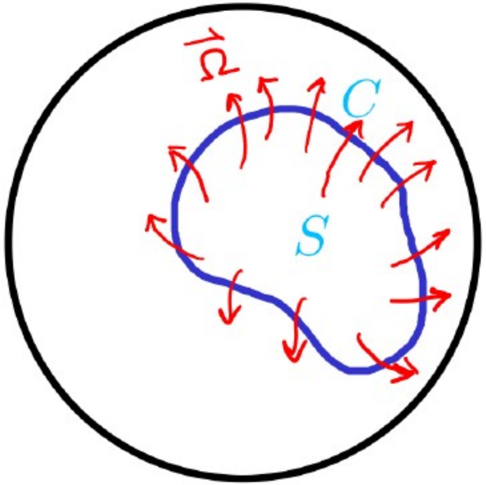

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Like magnetic field, but in parameter space

Berry Curvature in reciprocal space

- Block wavefunctions in periodic potential

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

Berry Curvature in reciprocal space

- **Block wavefunctions in periodic potential**

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

Effective Schrodinger equation

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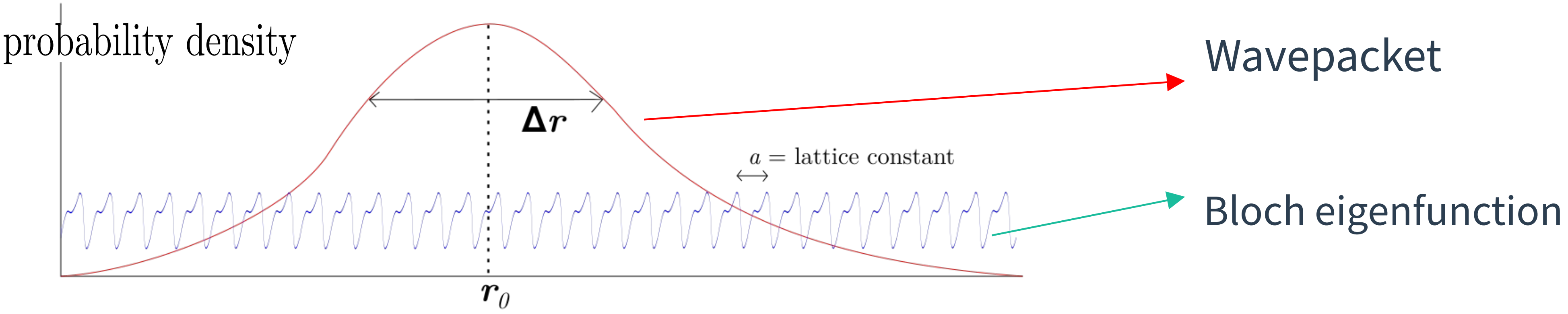
Construction of Bloch wavepacket, and its evolution



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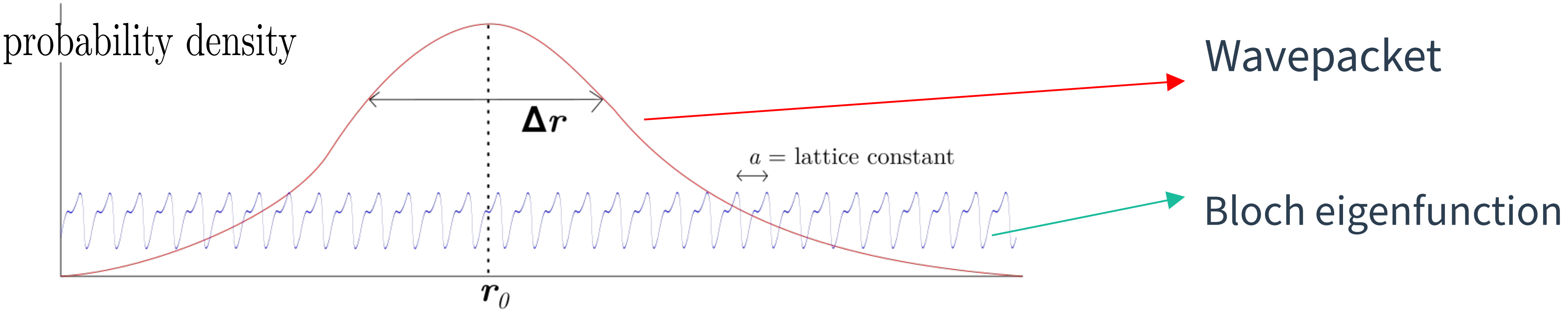

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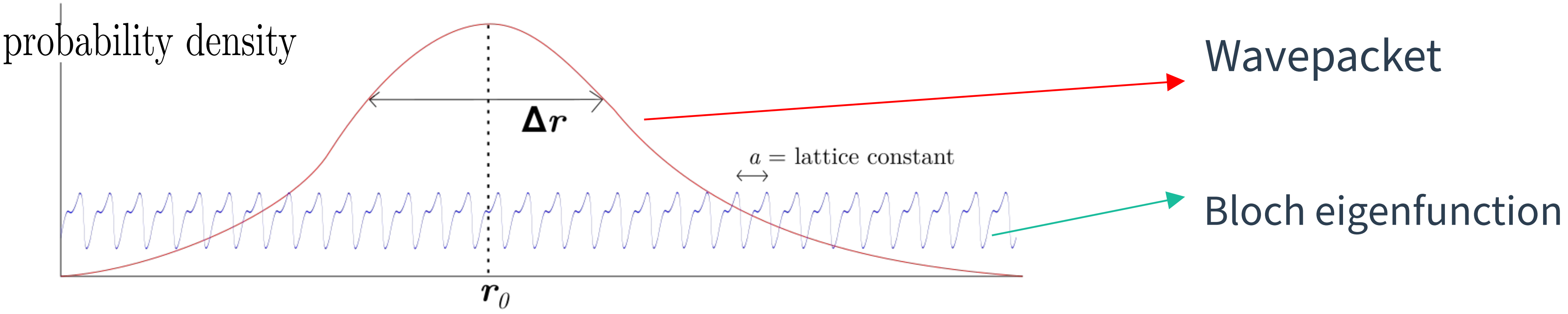

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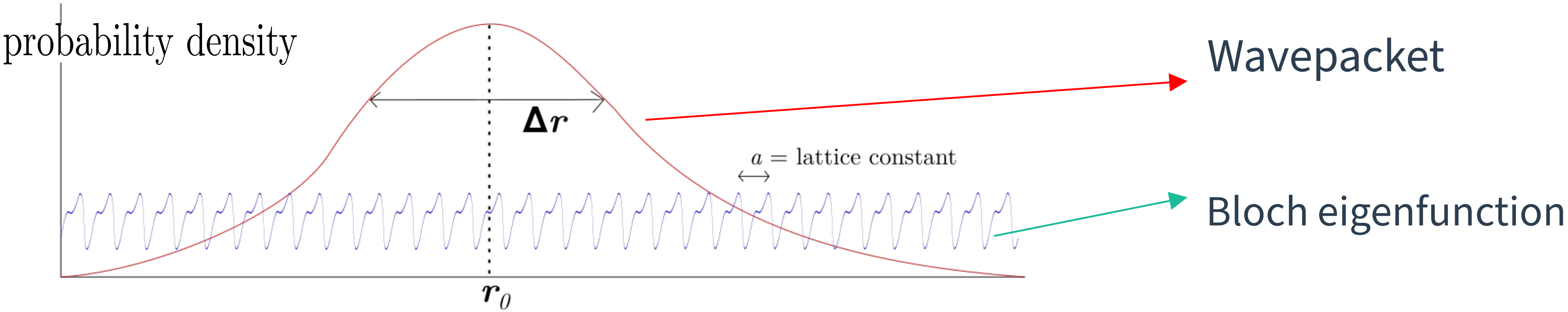

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Anomalous velocity

(2D)

0

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(2D)

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(2D)

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(2D)

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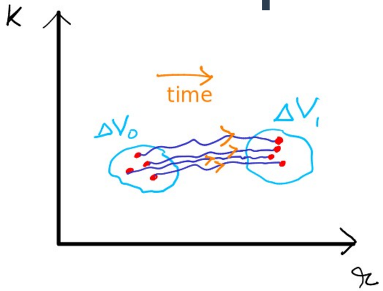

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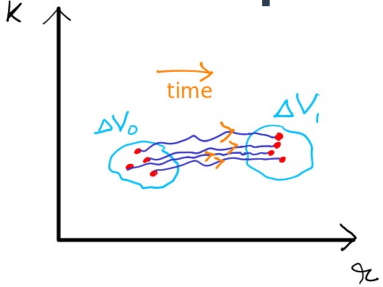

$$\Delta V \left(1 + \frac{e}{\hbar}\vec{B} \cdot \vec{\Omega}\right)$$

(2D)

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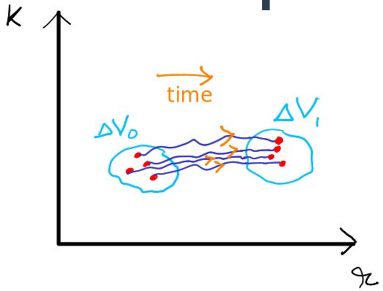

$$\Delta V \left(1 + \frac{e}{\hbar}\vec{B}\cdot\vec{\Omega}\right)$$

is a constant of motion

(2D)

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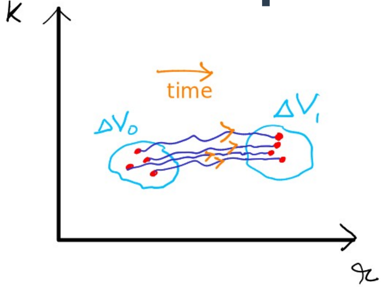
$$\dot{k} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial k}\times\boldsymbol{B} + \frac{e^2}{\hbar^2}(\boldsymbol{E}\cdot\boldsymbol{B})\boldsymbol{\Omega}}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}$$

- **Phase space density is modified**



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

is a constant of motion

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

(2D)

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

Effects of Berry curvature

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

- The semiclassical equation of velocity is modified

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

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

Anomalous velocity

(2D)

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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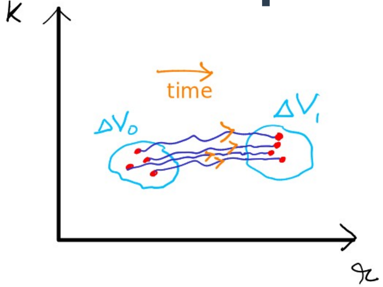

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(2D)

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

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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Semiclassical framework

Boltzmann Transport framework

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

Boltzmann Transport framework

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Semiclassical framework

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

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

Boltzmann Transport framework

Classical charge and energy currents

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

Semiclassical framework

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

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Heat current: From 1st law of thermodynamics,

Boltzmann Transport framework

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Boltzmann Transport framework

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Boltzmann Transport framework

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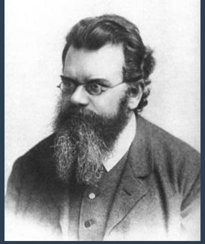
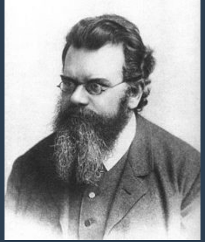
Boltzmann Transport Equation



- In equilibrium, $\tilde{g}_k$ is the Fermi distribution.
- The external fields are small, and it deviates slightly from the Fermi distribution

Boltzmann Transport Equation



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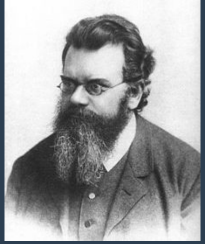

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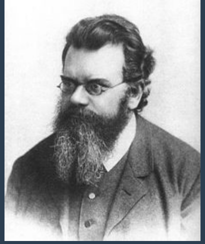

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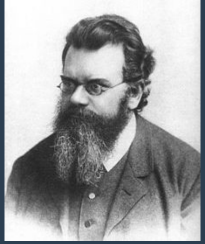

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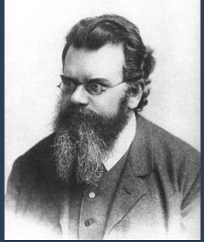

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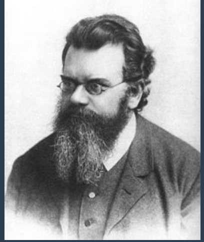

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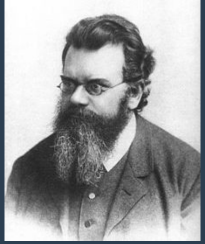

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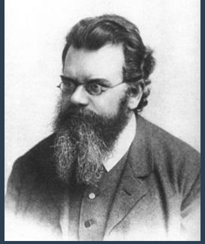
Boltzmann Transport Equation



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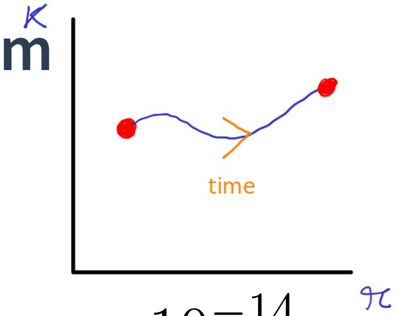

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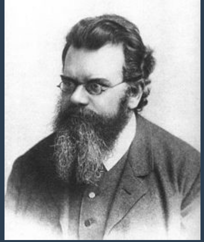

- In steady-state, and homogeneous fields, the equation in becomes,

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

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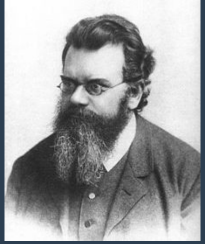

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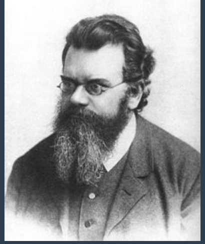
- Why is the perturbation theory valid?

Boltzmann Transport Equation



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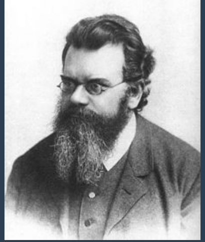
Boltzmann Transport Equation



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$\omega_c \tau \times$

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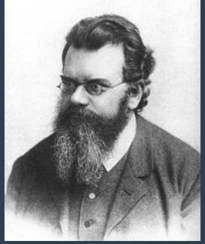

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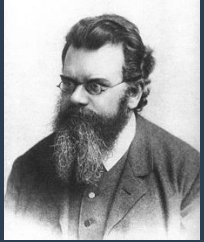

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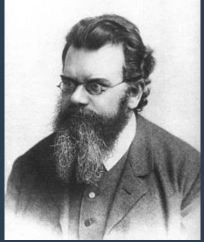
Boltzmann Transport Equation



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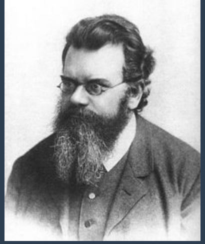

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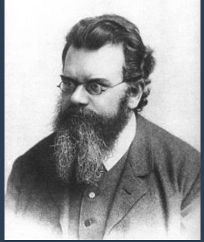
Boltzmann Transport Equation



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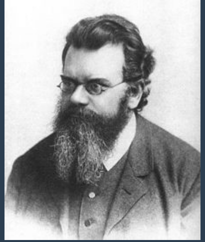
$$B < B_{critical} = \frac{m^*}{e\tau}$$

Boltzmann Transport Equation



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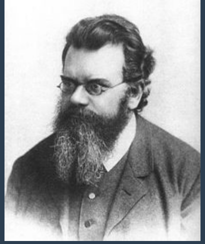
- Why is the perturbation theory valid?

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

- This is less than the first term when $B < B_{critical} = \dfrac{m^*}{e\tau}$
- If then the critical field is ~ 570 T

Boltzmann Transport Equation



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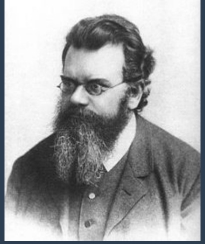

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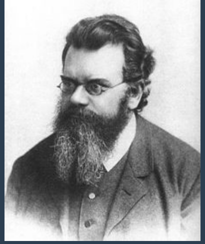

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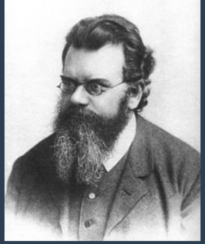
Why even consider this term, then??

Boltzmann Transport Equation



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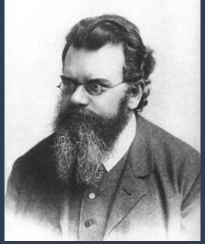

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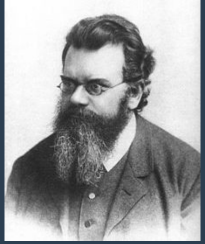
- The solution, with

Boltzmann Transport Equation



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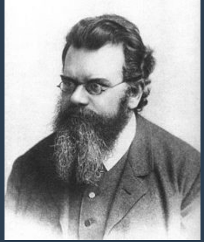
Boltzmann Transport Equation



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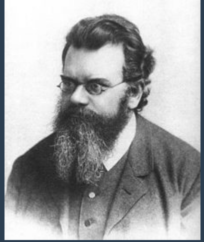

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Einstein and Onsager

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

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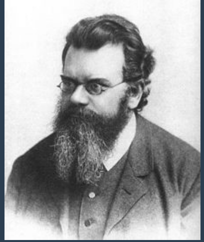

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Einstein and Onsager Relations are satisfied

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

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

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2[nd] order

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Which all terms contribute

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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,

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Independent of scattering!!

Which all terms contribute

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

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Independent of scattering!!

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- For a filled band, $\sigma_{xy} = -\sigma_{yx} = \frac{2e^2}{h}\mathcal{C}$
- This is not the (usual) quantum Hall effect

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Independent of scattering!!

Issue

- Apparently, a temp gradient or
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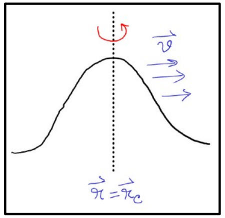
- No term like $\nabla\mu \times \vec{\Omega}$ and $\nabla T \times \vec{\Omega}$



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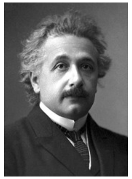

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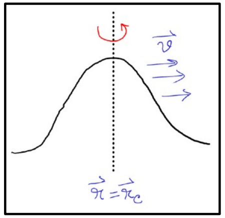

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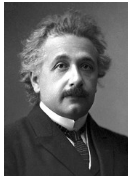

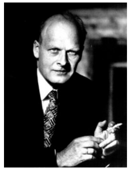

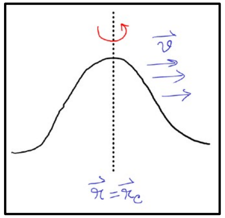

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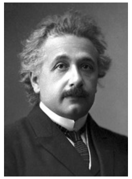
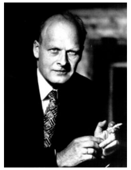


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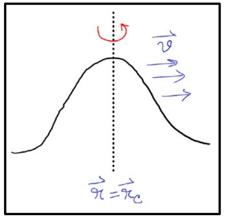

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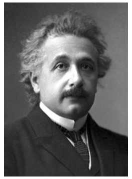
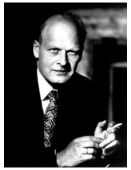
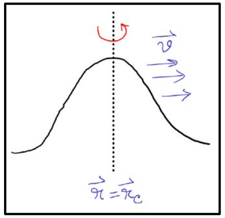




(Nernst)



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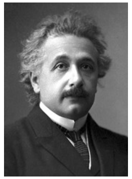

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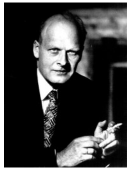

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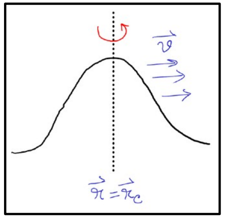

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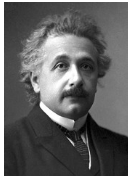 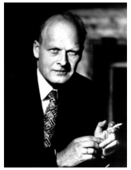 

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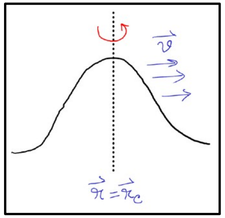

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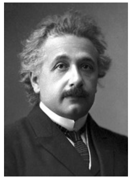
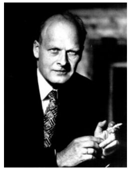


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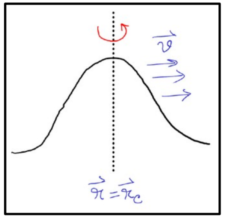

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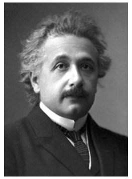
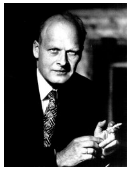


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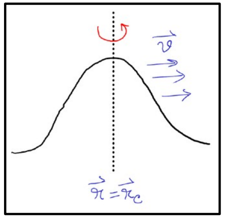

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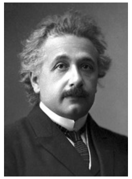
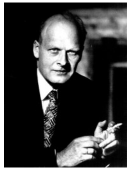


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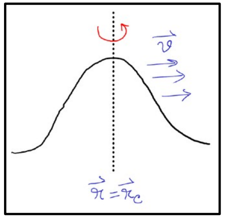

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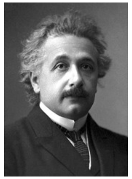
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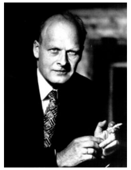
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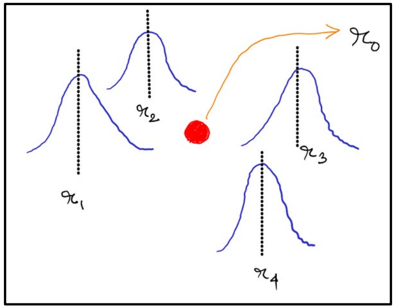

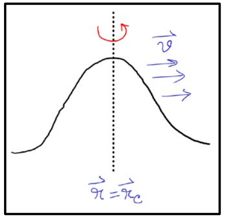

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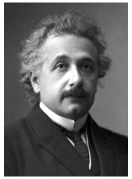
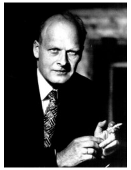


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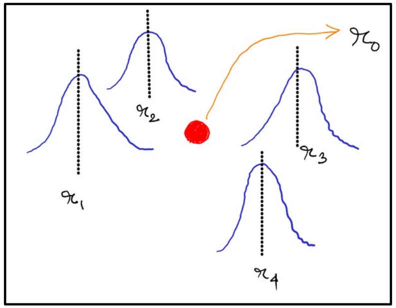

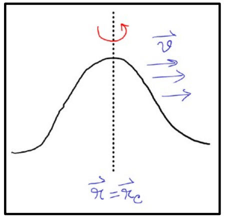

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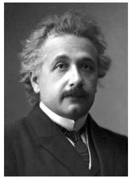
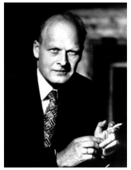


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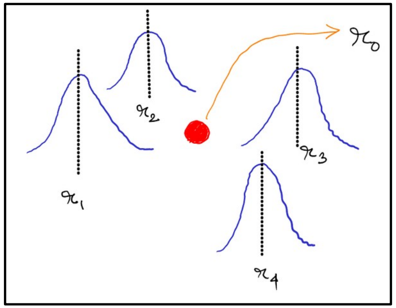

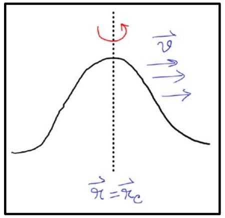

Orbital magnetic moment

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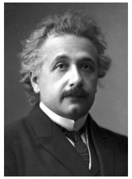
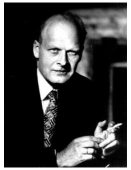


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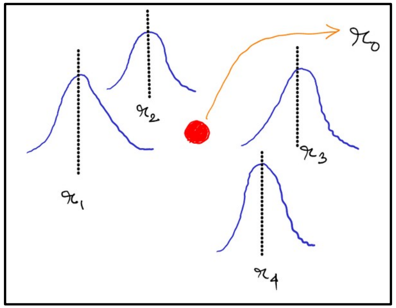

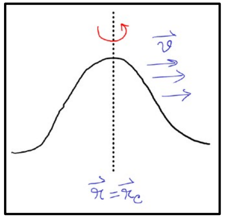

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$$\vec{m}_k = -\frac{e}{2m}\langle\psi_{k,r_0}|\,(\hat{\vec{r}} - \vec{r}_0) \times \hat{\vec{p}}\,|\psi_{k,r_0}\rangle$$

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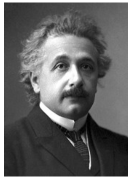 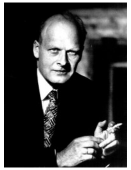 

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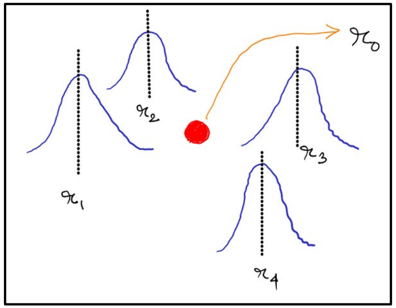

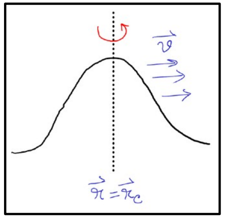

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Di Xiao, Yugui Yao, Zhong Fang, and Qian Niu. PRL **97**, 026603 (2006)

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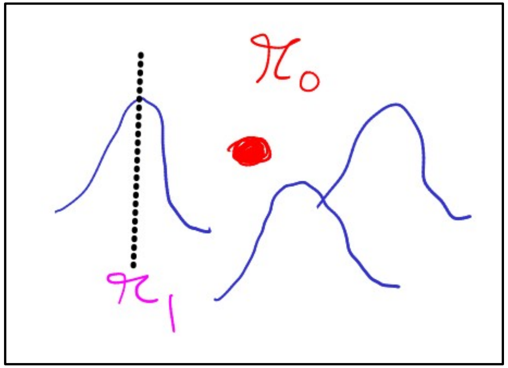

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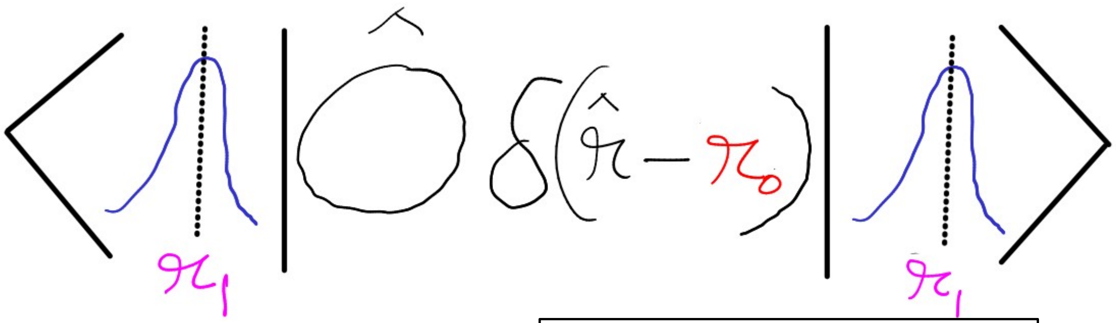

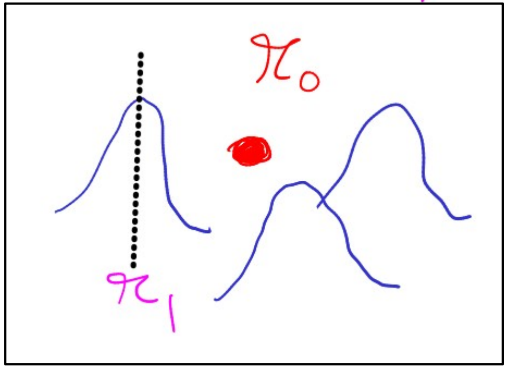

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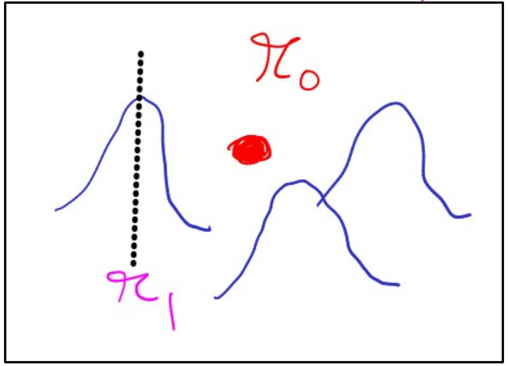

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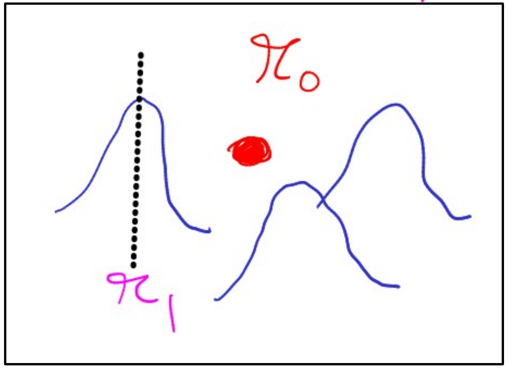

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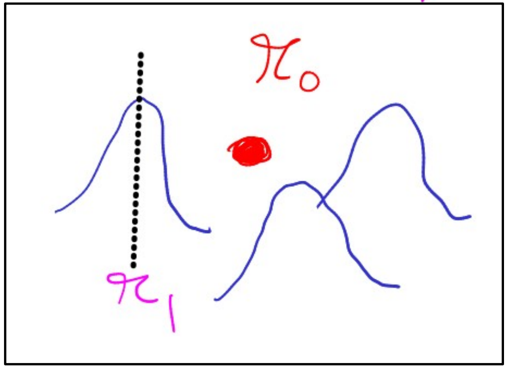

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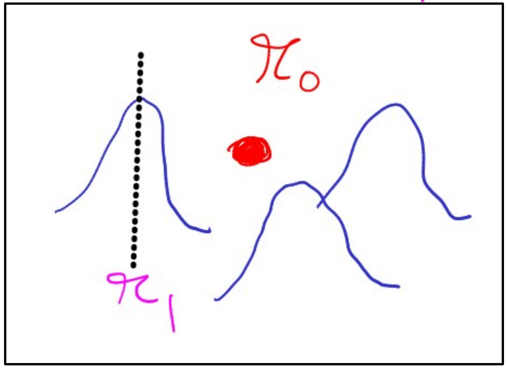
- To be technically correct, we should use the operator $\frac{\hat{O}\delta(\hat{r}-\vec{r}_0)+\delta(\hat{r}-\vec{r}_0)\hat{O}}{2}$ in case $\hat{O}$ does not commute with $\hat{r}$



- 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

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

Effects of orbital magnetization

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

Transport current

Now we are ready to calculate the transport current

$$
\begin{aligned}
\vec{j}^{\,e}_{\text{transport}} &= \left\langle \hat{\vec{j}}_e \right\rangle - \vec{j}^{\,e}_M \\
&= \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_BT\log\left(1+e^{-\beta(\varepsilon_0(\vec{k})-\mu)}\right)\right]
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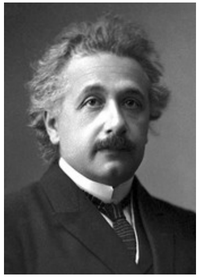

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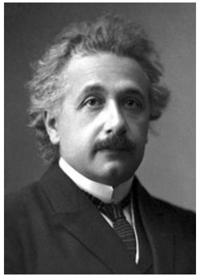

How about Onsager relation?

- 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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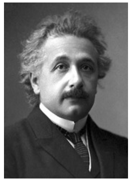

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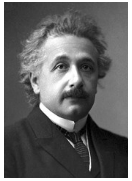


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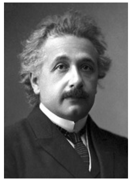


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Possible resolution

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Berry curvature and Chern numbers of some microscopic models

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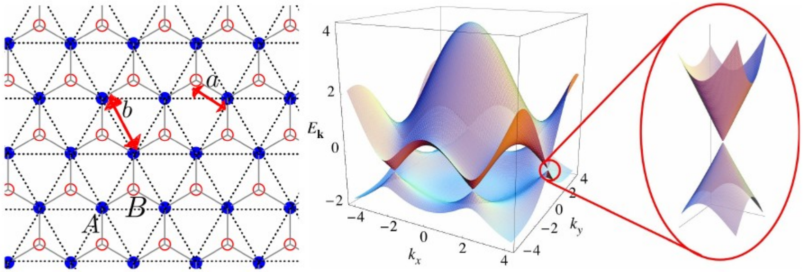

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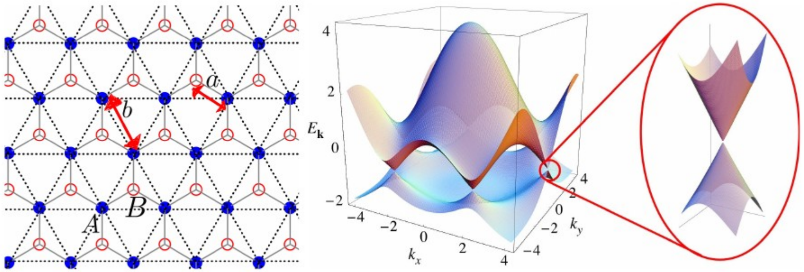

Non-zero Berry curvature when there is a finite band gap : Spin-Orbit Coupling

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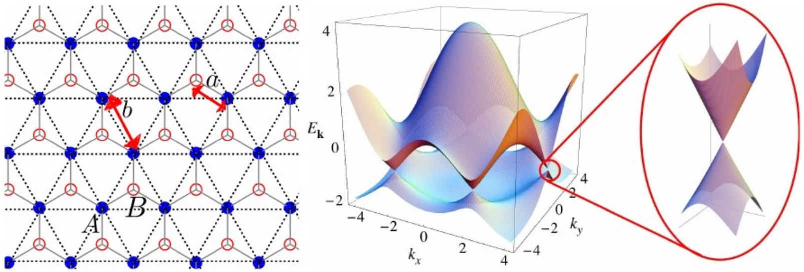

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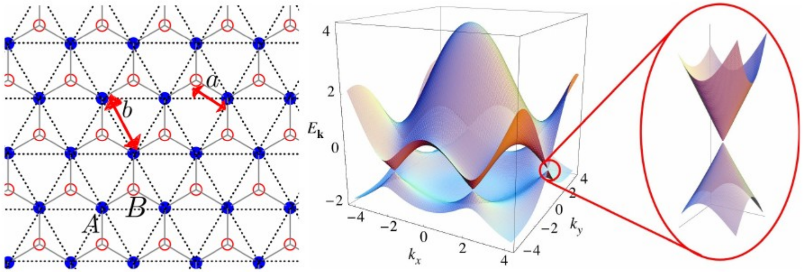

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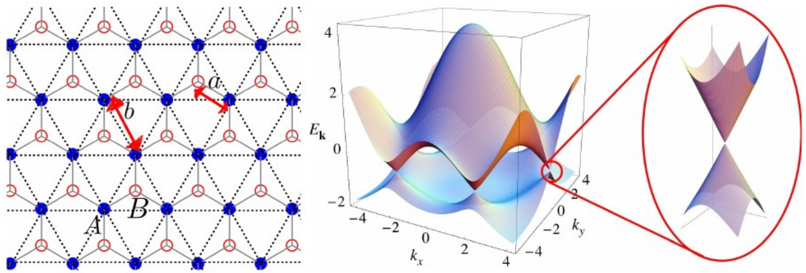

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Valley Polarization

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

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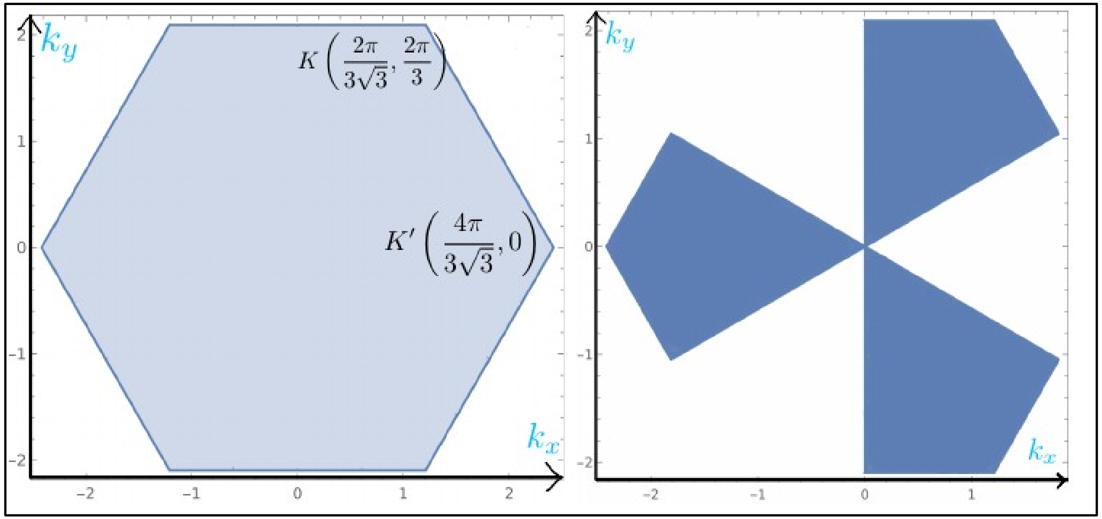

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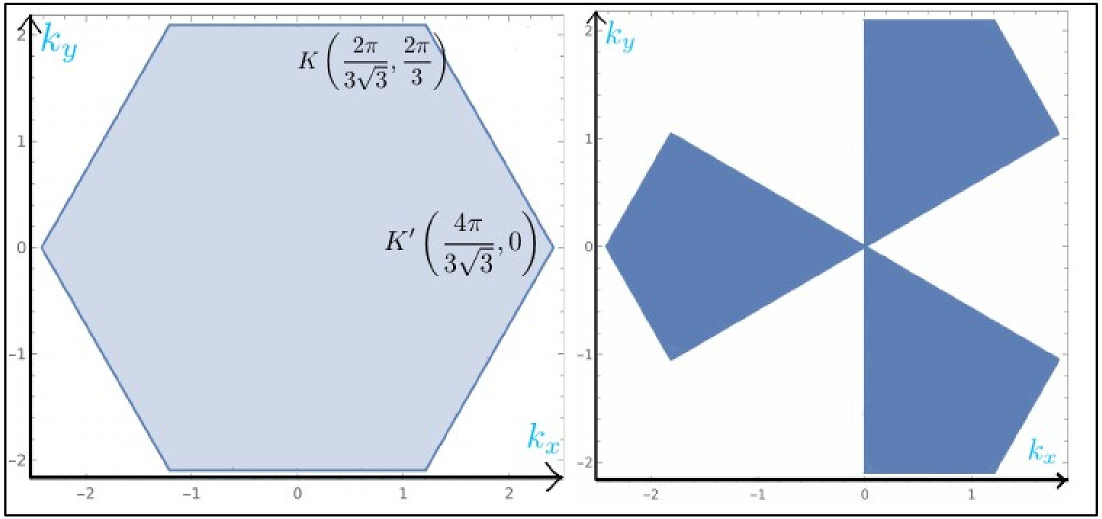

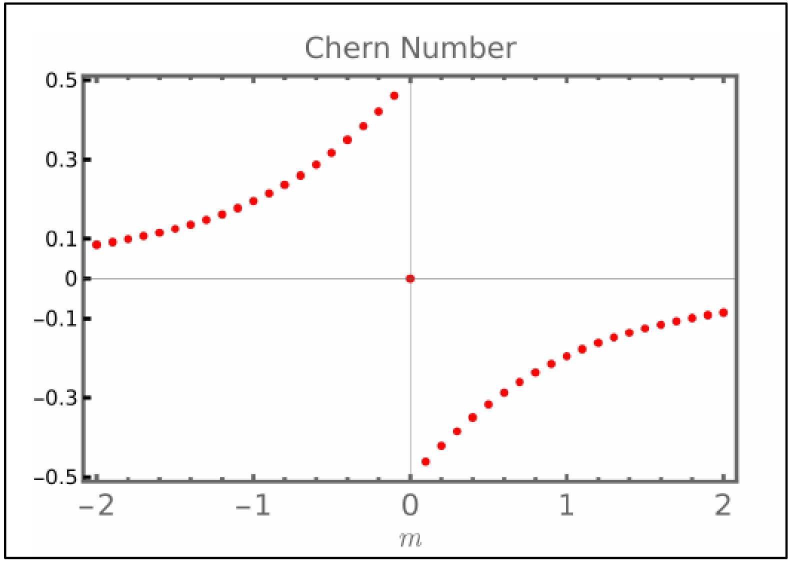

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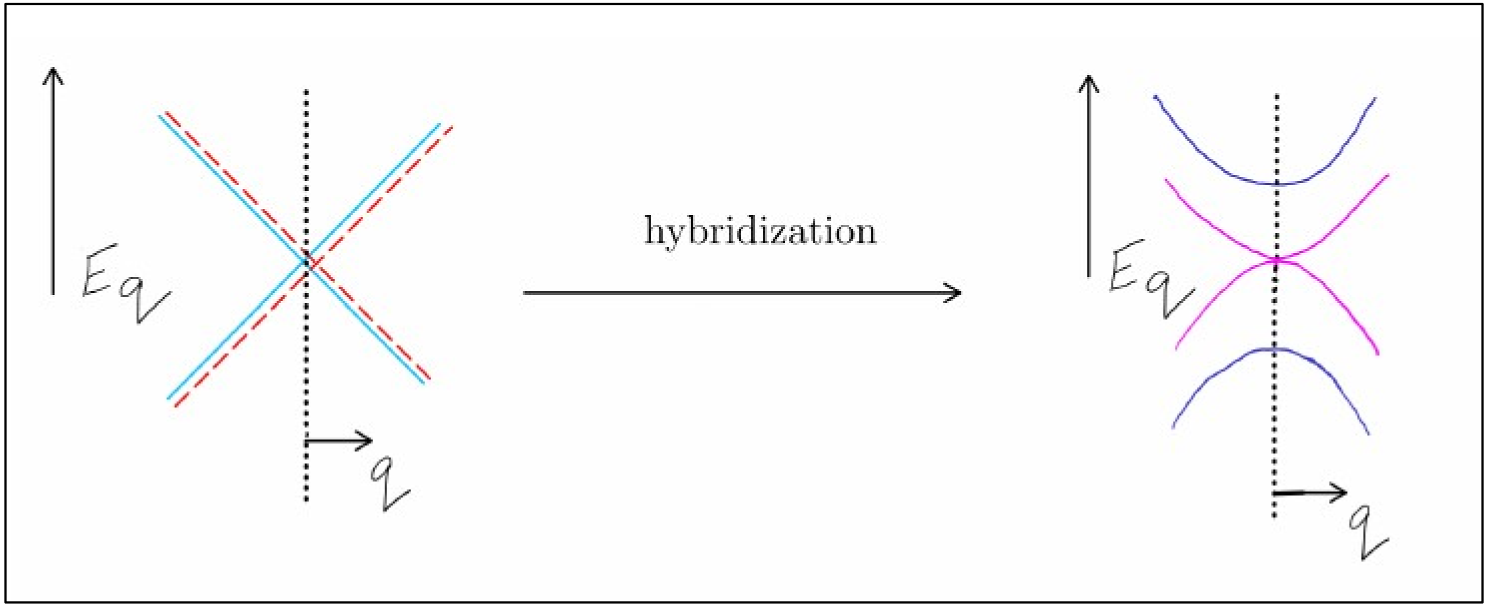

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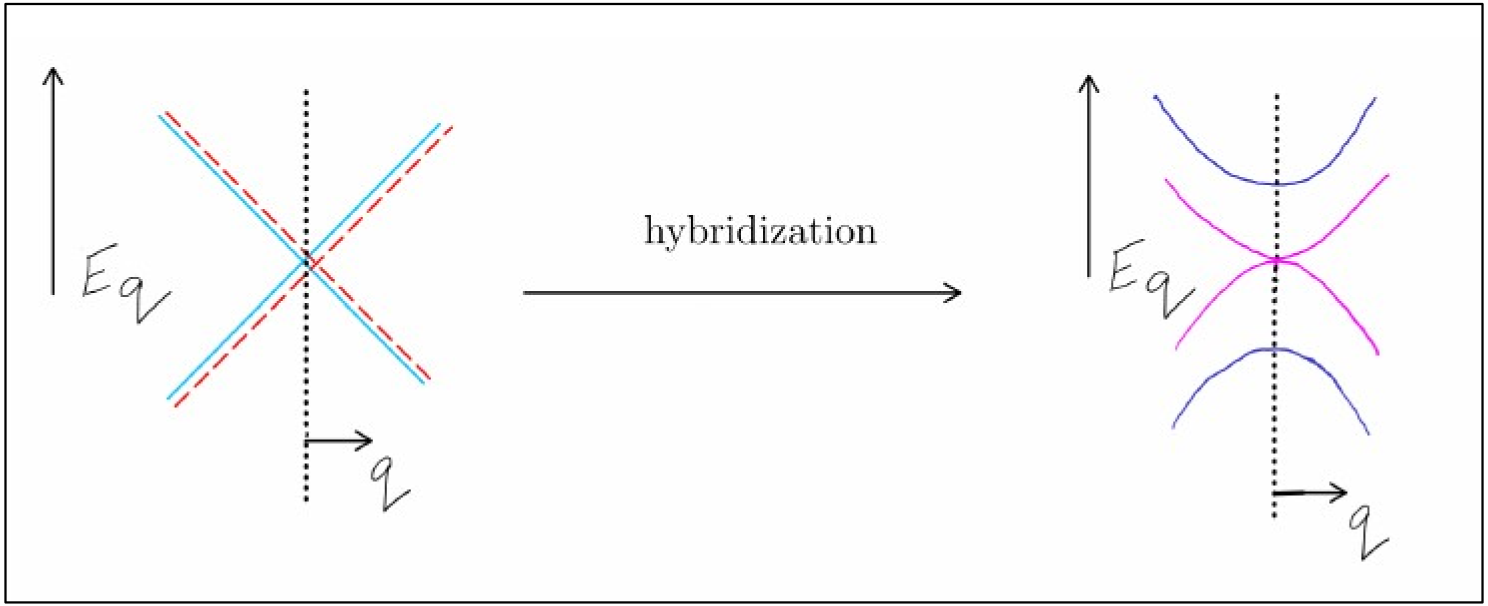

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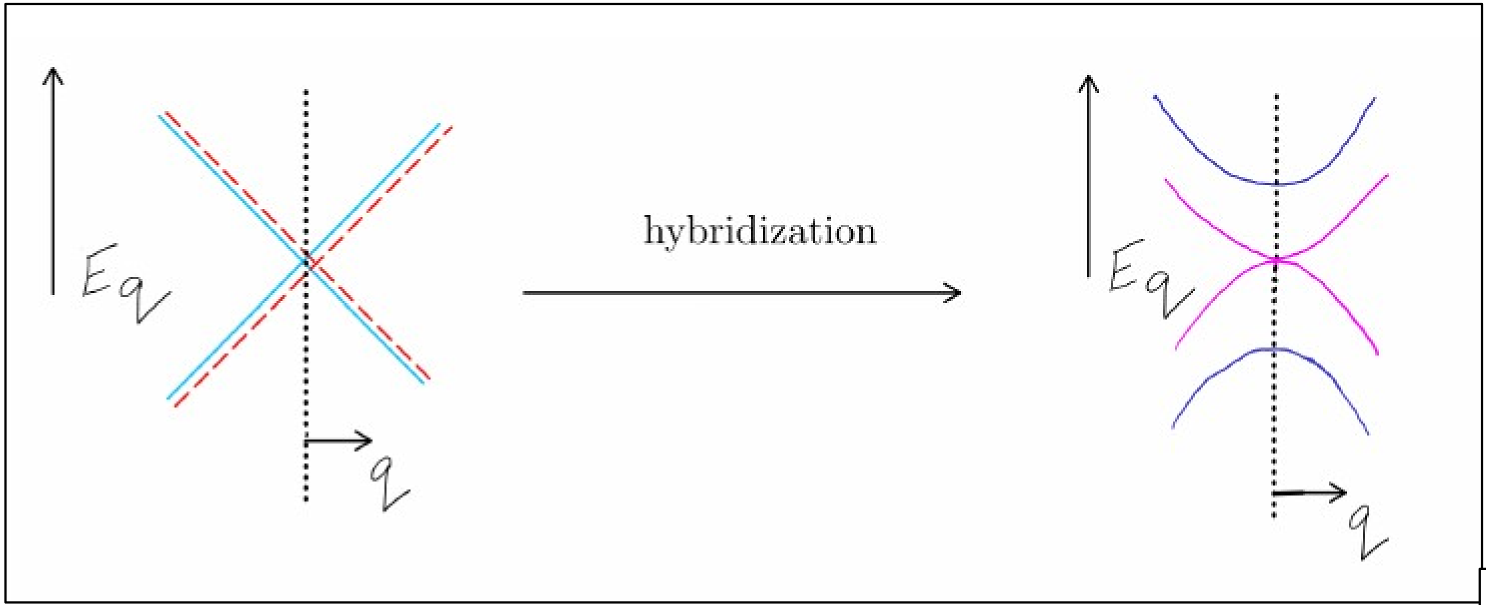

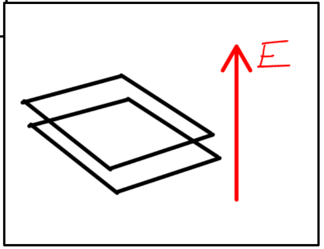

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Results for valley Chern number

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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