Adiabatic phase.

Consider the Hamiltonian:

$$H(\boldsymbol{k})|n,\boldsymbol{k}\rangle = E_n(\boldsymbol{k})|n,\boldsymbol{k}\rangle$$

The time evolution is given by:

$$H|n,t\rangle = i\hbar\frac{d}{dt}|n,t\rangle$$

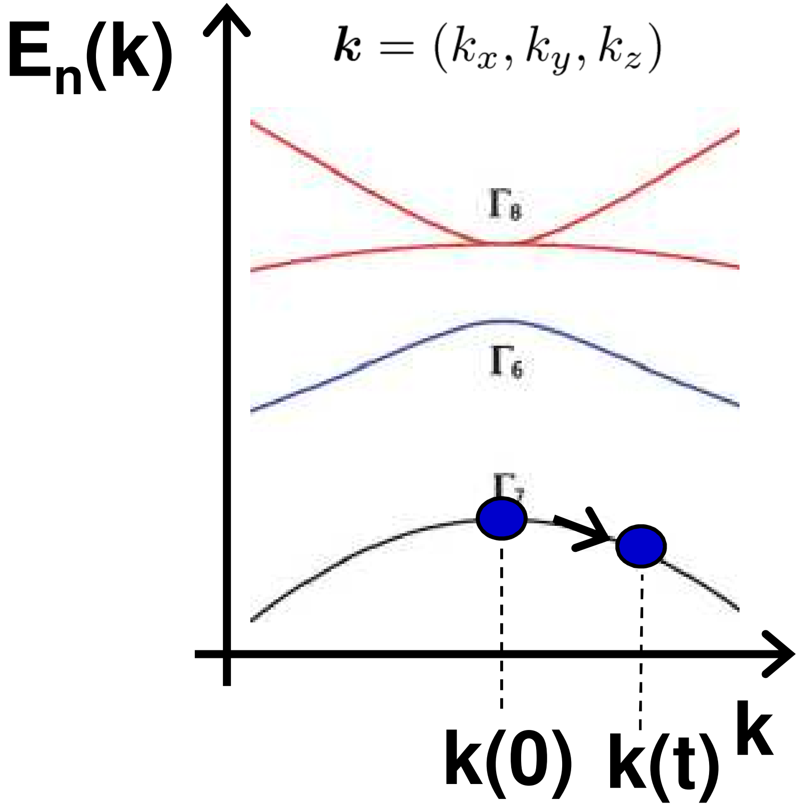
Now, suppose that k changes slowly with time :

$$|n,\boldsymbol{k}(0)\rangle \rightarrow |n,\boldsymbol{k}(t)\rangle$$

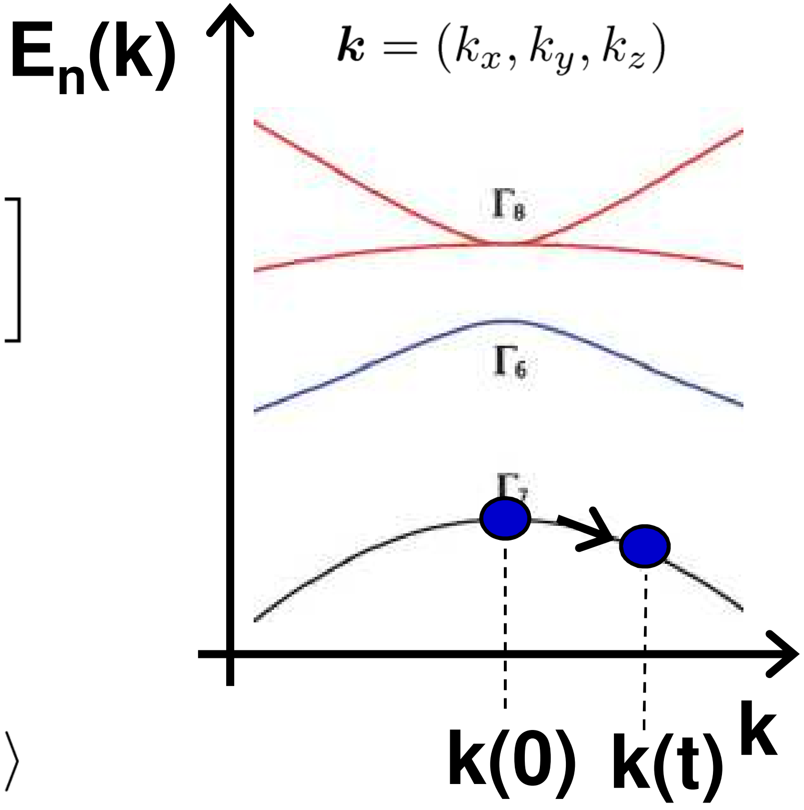
Notice that $|n,t\rangle$ IS NOT EQUAL to $|n,\boldsymbol{k}(t)\rangle$!

In fact, they are related by a PHASE FACTOR:

$$\boxed{|n,\boldsymbol{k}(t)\rangle = e^{+i\theta(t)}|n,t\rangle} \qquad \left(|n,t\rangle = e^{-i\theta(t)}|n,\boldsymbol{k}(t)\rangle\right)$$



Adiabatic phase.



We have:

1) $$i\hbar\frac{d|n,t\rangle}{dt} = i\hbar e^{-i\theta(t)}\left[\frac{d|n,\boldsymbol{k}(t)\rangle}{dt} - i\frac{d\theta(t)}{dt}|n,\boldsymbol{k}(t)\rangle\right]$$

2) $$\frac{d}{dt}|n,\boldsymbol{k}(t)\rangle = \frac{d\boldsymbol{k}(t)}{dt}\cdot\nabla_{\boldsymbol{k}}|n,\boldsymbol{k}(t)\rangle$$

Using the time-dependent Schrodinger's equation:

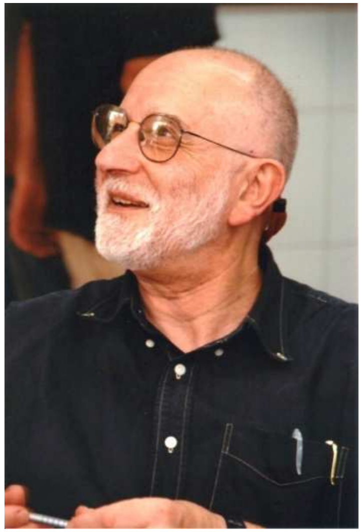
$$\hbar\frac{d\theta(t)}{dt} = E_n(\boldsymbol{k}(t)) - i\hbar\frac{d\boldsymbol{k}(t)}{dt}\cdot\langle n,\boldsymbol{k}(t)|\nabla_{\boldsymbol{k}}|n,\boldsymbol{k}(t)\rangle$$

Finally:

$$\boxed{|n,t\rangle = \exp\left(\frac{i}{\hbar}\int_0^t L_n[\boldsymbol{k}(t')]dt'\right)|n,\boldsymbol{k}(t)\rangle}$$

$$L_n[\boldsymbol{k}(t)] = i\hbar\frac{d\boldsymbol{k}(t)}{dt}\cdot\langle n,\boldsymbol{k}(t)|\nabla_{\boldsymbol{k}}|n,\boldsymbol{k}(t)\rangle - E_n[\boldsymbol{k}(t)]$$

Berry phase.



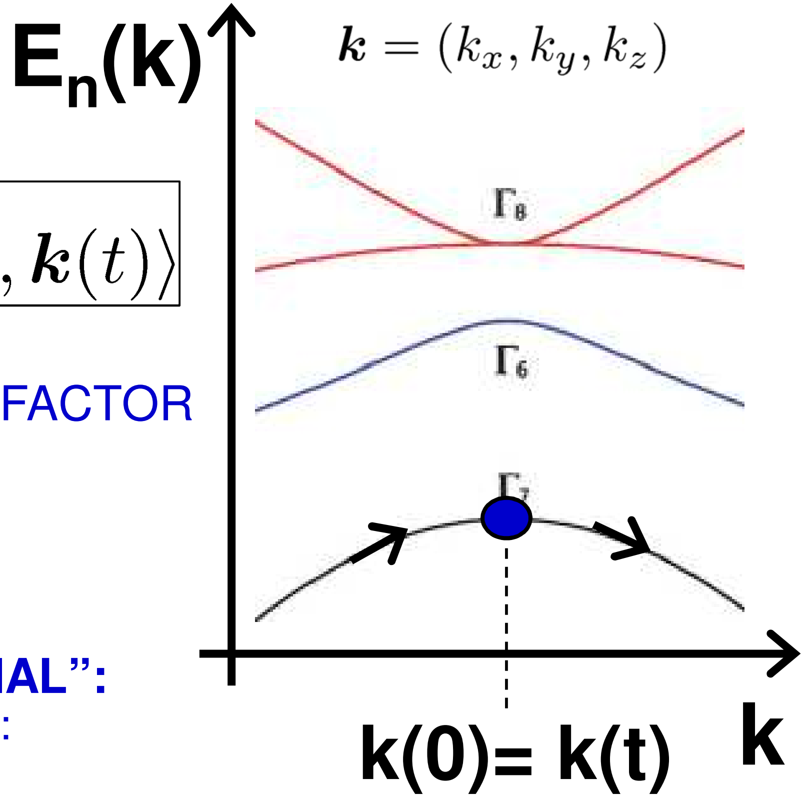
Sir Michael Berry

We can write as

$$|n,t\rangle = e^{i\gamma_n} e^{\frac{-i}{\hbar}\int_0^t E_n[\boldsymbol{k}(t')]dt'} |n, \boldsymbol{k}(t)\rangle$$

The first term is a GEOMETRICAL PHASE FACTOR

$$\gamma_n \equiv i \int_{\mathcal{C}} \langle n, \boldsymbol{k} | \nabla_{\boldsymbol{k}} | n, \boldsymbol{k}\rangle \cdot d\boldsymbol{k}$$



We define the "BERRY VECTOR POTENTIAL":
or "Berry connection":

$$\boldsymbol{A}_n(\boldsymbol{k}) \equiv i \langle n, \boldsymbol{k} | \nabla_{\boldsymbol{k}} | n, \boldsymbol{k}\rangle$$

Such that, if k(t)=k(0) (closed path): $\gamma_n = \oint_{\mathcal{C}} \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$ **BERRY PHASE**

"BERRY CURVATURE": $\boldsymbol{\Omega}_n(\boldsymbol{k}) \equiv \nabla_{\boldsymbol{k}} \times \boldsymbol{A}_n(\boldsymbol{k}) \Rightarrow \gamma_n = \iint_{\mathcal{S}} \boldsymbol{\Omega}_n(\boldsymbol{k}) \cdot d\boldsymbol{S}$

How to calculate Ω in a gauge-invariant way?

1) Vector identity (m =n):

$$\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\nabla_{\boldsymbol{k}} \times \langle n, \boldsymbol{k}|\nabla_{\boldsymbol{k}}|n, \boldsymbol{k}\rangle = i\left(\nabla_{\boldsymbol{k}}\langle n, \boldsymbol{k}|\right) \times \left(\nabla_{\boldsymbol{k}}|n, \boldsymbol{k}\rangle\right)$$

2) Identity (m ≠n):

$$\langle m, \boldsymbol{k}|\left[\nabla_{\boldsymbol{k}}|n, \boldsymbol{k}\rangle\right] = \left[\nabla_{\boldsymbol{k}}\langle n, \boldsymbol{k}|\right]|m, \boldsymbol{k}\rangle = \frac{\langle m, \boldsymbol{k}|\left(\nabla_{\boldsymbol{k}}H\right)|n, \boldsymbol{k}\rangle}{E_n - E_m}$$

$$\boxed{\boldsymbol{\Omega}_n(\boldsymbol{k}) = i\sum_{m\neq n}\frac{\langle n, \boldsymbol{k}|\left(\nabla_{\boldsymbol{k}}H\right)|m, \boldsymbol{k}\rangle \times \langle m, \boldsymbol{k}|\left(\nabla_{\boldsymbol{k}}H\right)|n, \boldsymbol{k}\rangle}{(E_n - E_m)^2}}$$

It is much easier to apply the $\nabla_{\mathbf{k}}$ operator in ***H*** rather than in the state!

Example: two-band system (Dirac-Weyl).

Consider the Hamiltonian of the form:

$$H(\mathbf{k}) = \mathbf{k} \cdot \boldsymbol{\sigma} \qquad H(k_x, k_y, k_z) = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix}$$

Eigenvalues **(Tarefa 19)**: $E_\pm(\mathbf{k}) = \pm|\mathbf{k}|$

$$k_z = |\mathbf{k}| \cos\theta$$

$$k_x + ik_y = |\mathbf{k}| \sin\theta e^{+i\phi}$$

Eigenvectors (up to a phase) **(Tarefa 19)**:

$$|+\rangle = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ \sin\left(\frac{\theta}{2}\right) e^{+i\phi/2} \end{pmatrix} \qquad |-\rangle = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ -\cos\left(\frac{\theta}{2}\right) e^{+i\phi/2} \end{pmatrix}$$

Example: two-band system (Dirac-Weyl).

Gradient of the Hamiltonian: $H(\mathbf{k}) = \mathbf{k}\cdot\boldsymbol{\sigma} \Rightarrow \nabla_{\mathbf{k}} H = \boldsymbol{\sigma}$

Berry curvatures:

$$\begin{cases} \boldsymbol{\Omega}_{+}(\mathbf{k}) = i\dfrac{\langle +|\boldsymbol{\sigma}|-\rangle \times \langle -|\boldsymbol{\sigma}|+\rangle}{(E_{+}-E_{-})^2} \\ \boldsymbol{\Omega}_{-}(\mathbf{k}) = i\dfrac{\langle -|\boldsymbol{\sigma}|+\rangle \times \langle +|\boldsymbol{\sigma}|-\rangle}{(E_{-}-E_{+})^2} \end{cases}$$

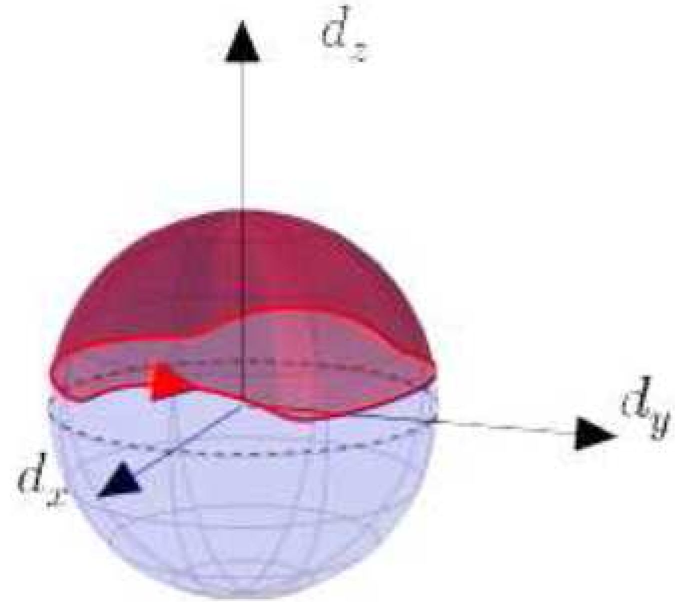
After a looong calculation (Lista 5): $\boxed{\boldsymbol{\Omega}_{\pm}(\mathbf{k}) = \mp\dfrac{\hat{\mathbf{k}}}{2|\mathbf{k}|^2}}$ (NOT gauge-dependent!) (Lista 5)

A "Berry curvature monopole" irradianting at the origin (k=0):

Chern number: $n_c = \dfrac{1}{2\pi}\oiint_{\mathcal{S}} \boldsymbol{\Omega}_{\pm}(\boldsymbol{k})\cdot d\boldsymbol{S} \Rightarrow \boxed{n_c = \pm 1}$

Example: two-band system (Dirac-Weyl).

Berry phase: $$\gamma_n = \oint_{\mathcal{C}} \boldsymbol{A}_n(\boldsymbol{k}) \cdot d\boldsymbol{k}$$



For a **closed path *C***, the Berry phase is the Berry connection flux through the **open surface *S*** :

$$\gamma_n = \iint_{\mathcal{S}} \boldsymbol{\Omega}_n(\boldsymbol{k}) \cdot d\boldsymbol{S}$$

Using :

$$\boldsymbol{\Omega}_{\pm}(\mathbf{k}) = \mp \frac{\hat{\mathbf{k}}}{2|\mathbf{k}|^2}$$

$$\gamma_{\pm} = \mp \frac{1}{2} \iint_{\mathcal{S}} \frac{\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{n}}}{|\boldsymbol{k}|^2} dS = \mp \frac{1}{2} \iint_{\mathcal{S}} \sin\theta d\theta d\phi$$

We find that the Berry phase is half of the solid angle enclosed by *C*:

$$\gamma_{\pm} = \mp \frac{1}{2} \Omega_C \qquad 0 \leq \Omega_C \leq 4\pi$$

Tarefa 19: two-band system (Dirac-Weyl).

Consider the Hamiltonian of the form:

$$H(\mathbf{k}) = \mathbf{k} \cdot \boldsymbol{\sigma} \qquad H(k_x, k_y, k_z) = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix}$$

1) Calculate the two eigenvalues of H(k)

2) Calculate the eigenvectors (up to a phase) in terms of the angles θ and ϕ:

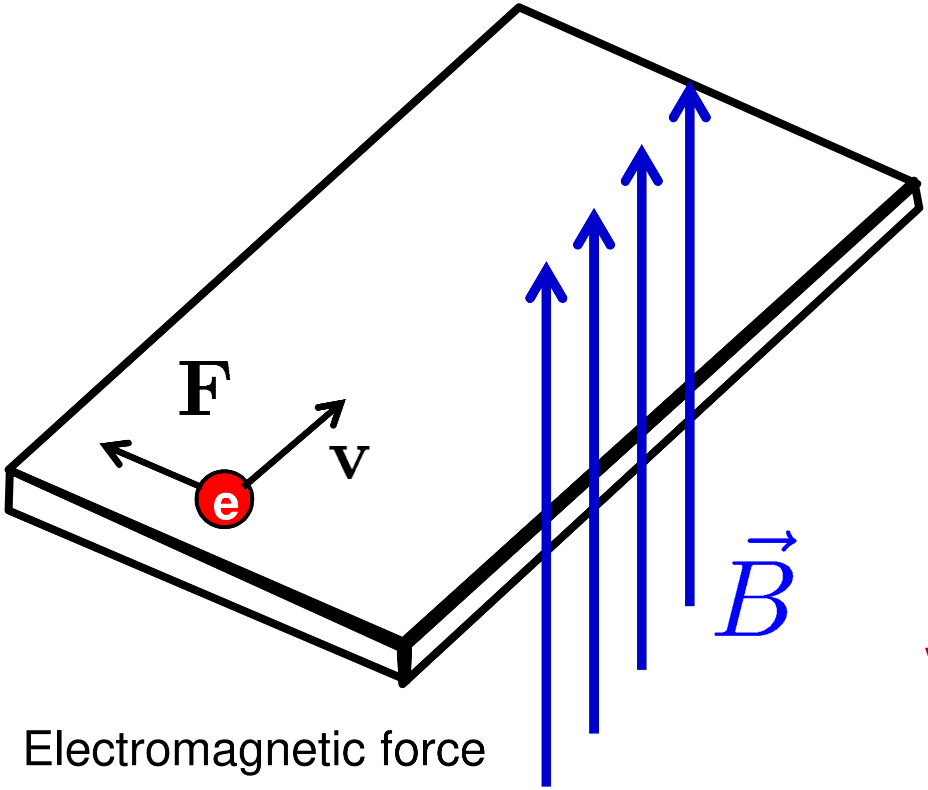
$$k_z = |\mathbf{k}| \cos\theta$$

$$k_x + ik_y = |\mathbf{k}| \sin\theta e^{+i\phi}$$

3) Calculate the Berry curvatures for each eigenstate:

$$\boldsymbol{\Omega}_+(\mathbf{k}) = i\frac{\langle +|\boldsymbol{\sigma}|-\rangle \times \langle -|\boldsymbol{\sigma}|+\rangle}{(E_+ - E_-)^2} \qquad \boldsymbol{\Omega}_-(\mathbf{k}) = i\frac{\langle -|\boldsymbol{\sigma}|+\rangle \times \langle +|\boldsymbol{\sigma}|-\rangle}{(E_- - E_+)^2}$$

Velocity and Berry curvature in the QHE



Electromagnetic force

$$\mathbf{F} = (-e)\mathbf{E} + (-e)\mathbf{v} \times \mathbf{B}$$

Electric potential and Vector potential.

$$\begin{cases} \mathbf{B} = \nabla_{\mathbf{r}} \times \mathbf{A}(\mathbf{r}) \\ \mathbf{E} = -\nabla_{\mathbf{r}} V(\mathbf{r}) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}, t) \end{cases}$$

In the absence of other charges:

$$V(\mathbf{r}) = 0 \Rightarrow \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}, t)$$

Hamiltonian:

$$H = \frac{(\mathbf{p} + e\mathbf{A}(t))^2}{2m^*} \equiv \frac{\hbar^2 (\mathbf{k}(t))^2}{2m^*}$$

Velocity: $m^*\mathbf{v}(t) = \mathbf{p} + e\mathbf{A}(t) = \hbar\mathbf{k}(t)$

Thus: $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} H(\mathbf{k})$

Tarefa 20: identity for the velocity

Using:

$$\begin{cases} \mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} H(\mathbf{k}) = \frac{1}{\hbar}\left(\frac{\partial H}{\partial k_x}\mathbf{i} + \frac{\partial H}{\partial k_y}\mathbf{j} + \frac{\partial H}{\partial k_z}\mathbf{k}\right) \\ H|n,\mathbf{k}(t)\rangle = E_n[\mathbf{k}(t)]|n,\mathbf{k}(t)\rangle \\ i\hbar\frac{d}{dt}|n,\mathbf{k}(t)\rangle = i\hbar\frac{d\mathbf{k}(t)}{dt}\cdot\nabla_{\mathbf{k}}|n,\mathbf{k}(t)\rangle \\ H|\Psi(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)\rangle \end{cases}$$

Show that:

1) $$\nabla_{\mathbf{k}}(H|n,\mathbf{k}\rangle) = (\nabla_{\mathbf{k}} H)|n\mathbf{k}(t)\rangle + H(\nabla_{\mathbf{k}}|n,\mathbf{k}\rangle)$$

2) $$H(\nabla_{\mathbf{k}}|n,\mathbf{k}\rangle) = i\hbar\nabla_{\mathbf{k}}\left(\frac{d\mathbf{k}(t)}{dt}\cdot\nabla_{\mathbf{k}}|n,\mathbf{k}\rangle\right)$$

3) $$\hbar\mathbf{v}|n\mathbf{k}(t)\rangle = \nabla_{\mathbf{k}}(E_n[\mathbf{k}]|n,\mathbf{k}\rangle) - i\hbar\nabla_{\mathbf{k}}\left(\frac{d\mathbf{k}(t)}{dt}\cdot\nabla_{\mathbf{k}}|n,\mathbf{k}\rangle\right)$$

Tip: Do it by components so you don't get confused!!

Velocity and Berry curvature in the QHE

From the previous result, it follows(*):

$$\mathbf{v}_n(\mathbf{k}) = \langle n, \mathbf{k}(t)|\mathbf{v}|n, \mathbf{k}(t)\rangle = \frac{1}{\hbar}\nabla_{\mathbf{k}} E[\mathbf{k}] + \frac{d\mathbf{k}(t)}{dt} \times \nabla_{\mathbf{k}} \times \langle n, \mathbf{k}|i\nabla_{\mathbf{k}}|n, \mathbf{k}\rangle$$

Remember the definition of the Berry curvature:

$$\boldsymbol{\Omega}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \langle n\mathbf{k}|i\nabla_{\mathbf{k}}|n, \mathbf{k}\rangle$$

and using:

$$\frac{d\mathbf{k}(\mathbf{t})}{dt} = \frac{e}{\hbar}\frac{\partial \mathbf{A}}{\partial t} = -\frac{e}{\hbar}\mathbf{E}$$

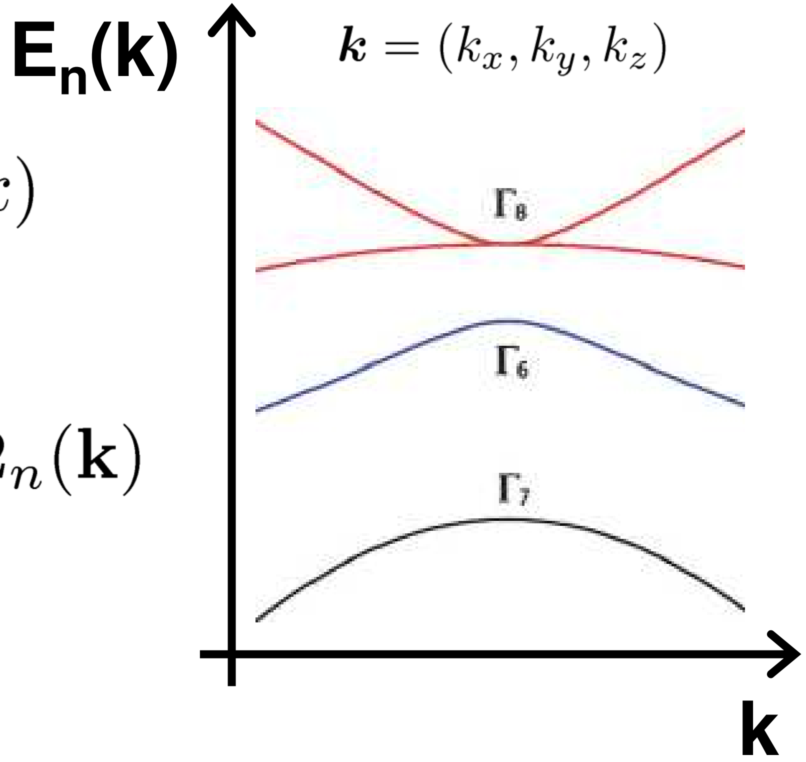
we get

$$\boxed{\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} E_n[\mathbf{k}] - \frac{e}{\hbar}\mathbf{E} \times \boldsymbol{\Omega}_n(\mathbf{k})}$$

(*) Should be on Lista 5!

Hall Conductance and Chern number

Current density(*): $$\mathbf{J} = -e \sum_n \int \frac{d\mathbf{k}}{(2\pi)^2} \mathbf{v}_n(\mathbf{k}) f(k)$$



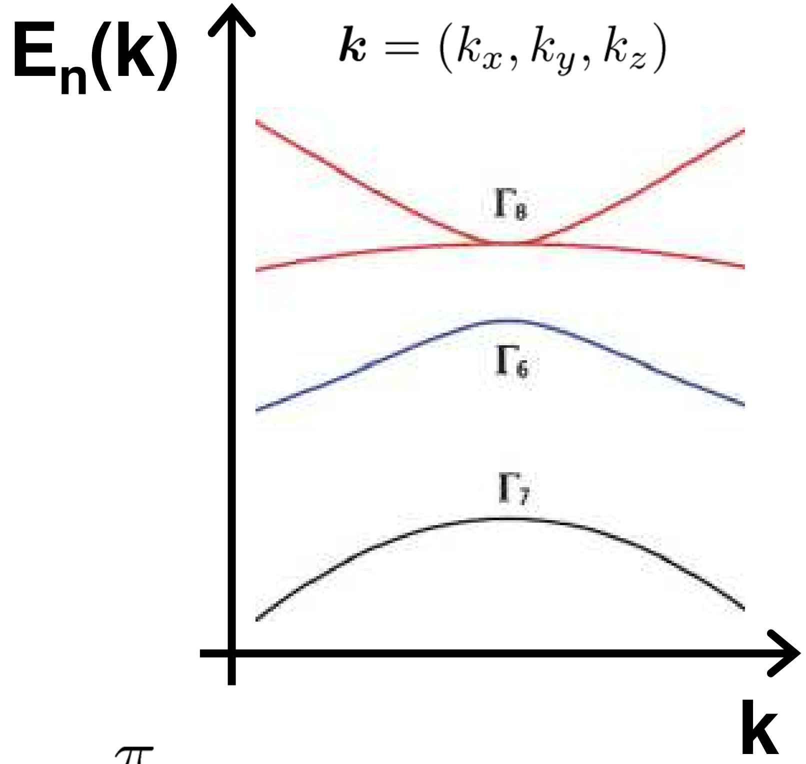
Using: $$\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} E_n[\mathbf{k}] - \frac{e}{\hbar} \mathbf{E} \times \mathbf{\Omega}_n(\mathbf{k})$$

we might calculate the conductance: $$\mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E}$$

If we have a gap and N filled levels $$\sum_{n \in \text{filled}} \int \frac{d\mathbf{k}}{(2\pi)^2} \nabla_{\mathbf{k}} E_n[\mathbf{k}] f(k) = 0$$

(*) Quantum version of the usual: $$\mathbf{J} = (-e) n \langle \mathbf{v} \rangle$$

Hall Conductance and Chern number



The conductance can then be calculated: $\mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E}$

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}\sum_{n\in\text{filled}}\int_{\text{BZ}} \mathbf{\Omega}_n(\mathbf{k})\cdot d\mathbf{k}$$

The integral will be carried out in the 1st BZ, which is a torus for the Berry curvature:

$$\mathbf{\Omega}_n(k_x,k_y) = \mathbf{\Omega}_n(k_x+\frac{\pi}{a},k_y) = \mathbf{\Omega}_n(k_x,k_y+\frac{\pi}{a})$$

Thus the integral will be 2π (Chern number) and the sum will give the number of filled bands ν :

$$\boxed{\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi}2\pi\nu = \frac{e^2}{h}\nu}$$

TKNN invariant: 1982

The Hall conductivity is proportional to a Chern number (Berry-phase-like)

$$\sigma_{xy} = \frac{e^2}{h} \sum_{n<N_F} \frac{1}{2\pi} \iint_{\text{BZ}} \boldsymbol{\Omega}_n(\boldsymbol{k}) \cdot d\boldsymbol{k} \equiv \nu \frac{e^2}{h}$$

Thouless, Kohmoto, Nightingale, den Nijs, *Phys. Rev. Lett*. 49, 405 (1982)

- System is periodic (BZ is a torus in k-space)
- There is an uniform magnetic field in the system.
- Fermi energy lies in a gap with N_F filled bands.

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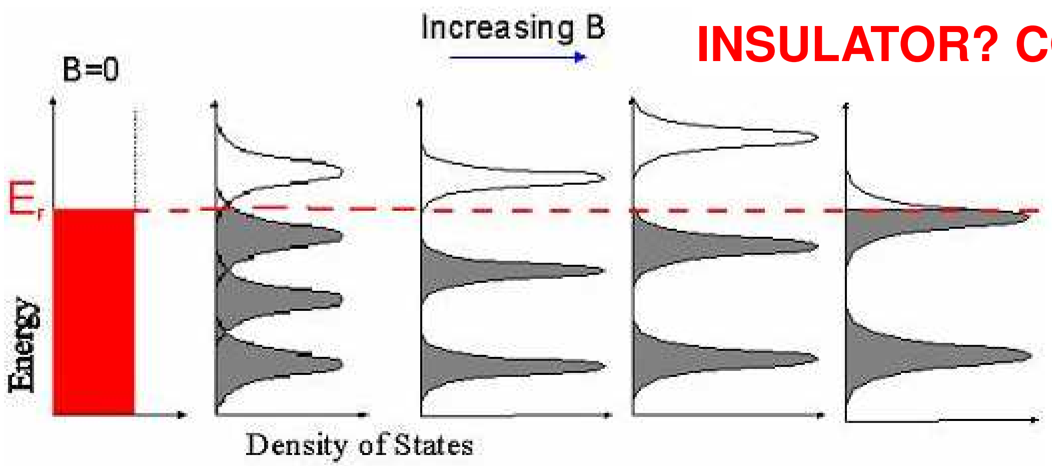

INSULATOR? CONDUCTOR? Neither?

ν = 0,1,2,... : filling factor. Depends only on the topology of the BZ states.

TKNN invariant: 1982

The Hall conductivity is proportional to a Chern number (Berry-phase-like)

$$\sigma_{xy} = \frac{e^2}{h} \sum_{n<N_F} \frac{1}{2\pi} \iint_{\mathrm{BZ}} \boldsymbol{\Omega}_n(\boldsymbol{k}) \cdot d\boldsymbol{k} \equiv \nu \frac{e^2}{h}$$

Thouless, Kohmoto, Nightingale, den Nijs, *Phys. Rev. Lett.* 49, 405 (1982)

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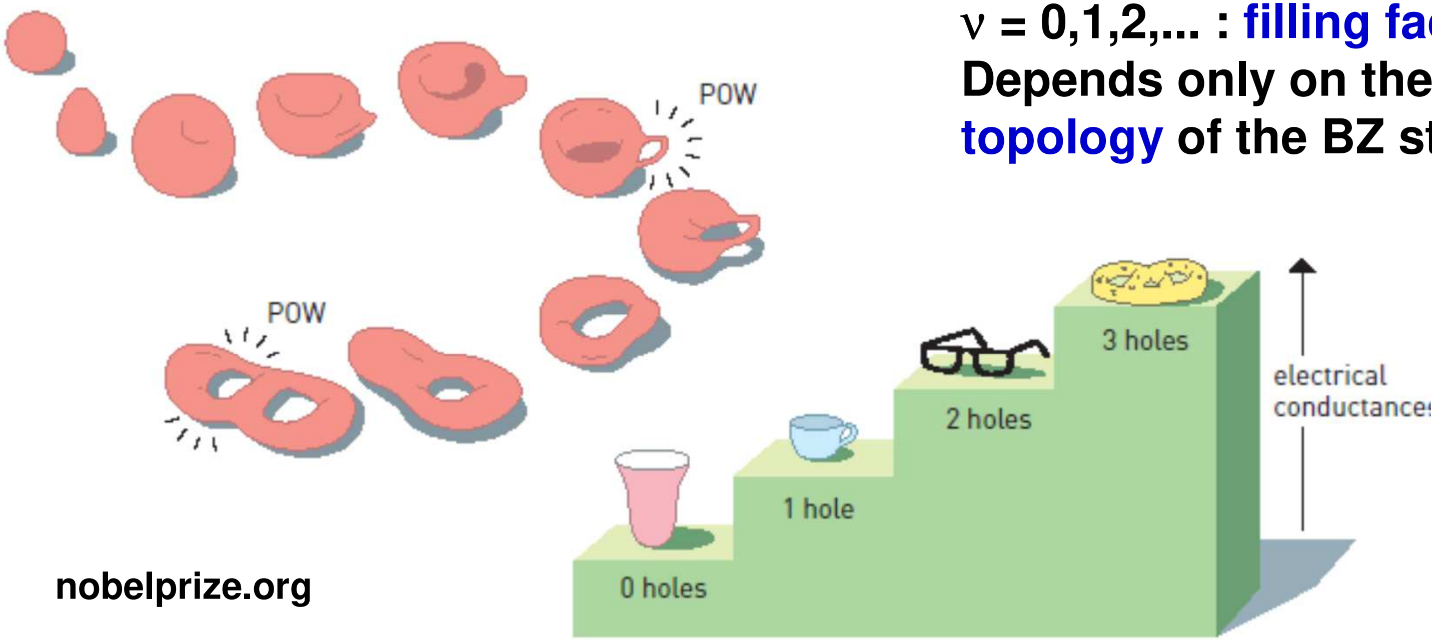

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