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 :

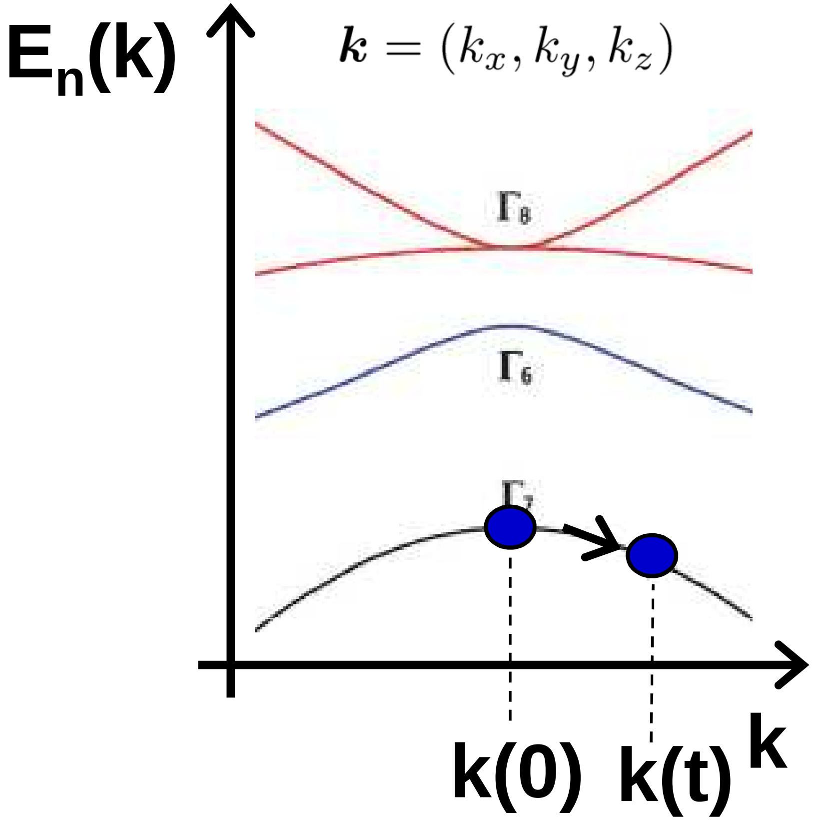
$$|n,\boldsymbol{k}(0)\rangle \rightarrow |n,\boldsymbol{k}(t)\rangle$$

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

In fact, they are related by a PHASE FACTOR:

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

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

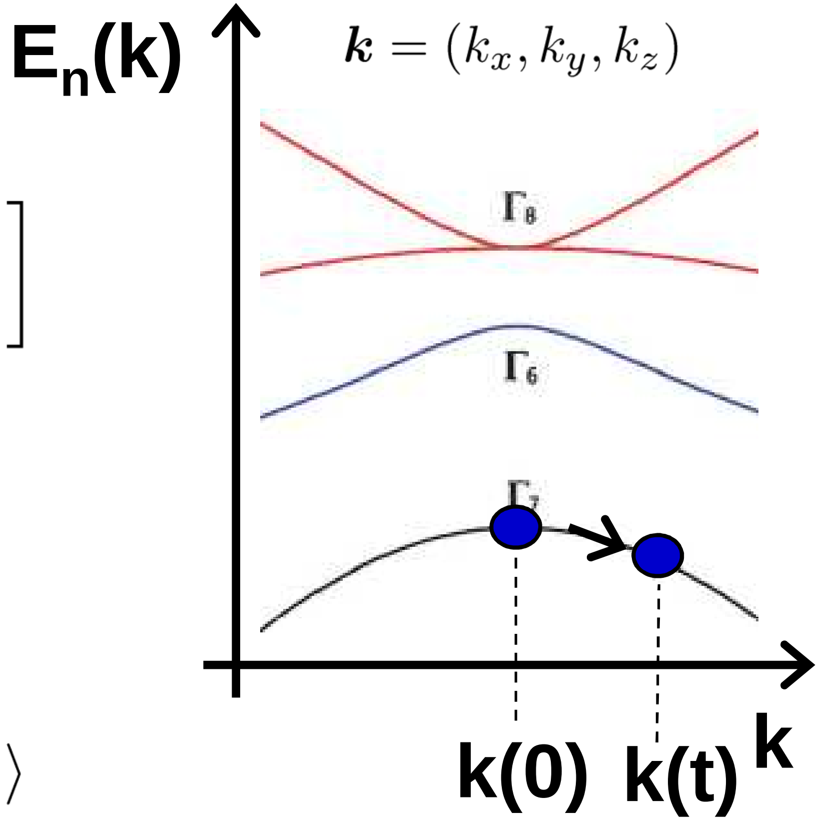


Adiabatic phase.

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:

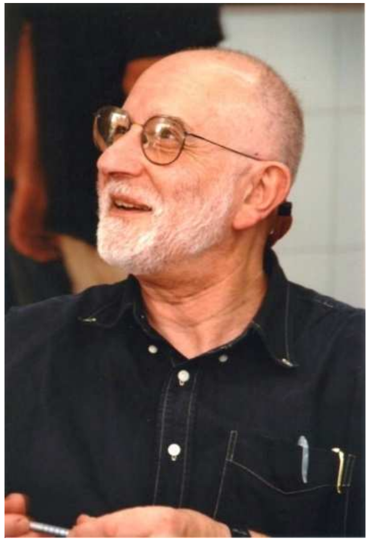
$$\hbar\frac{d\theta(t)}{dt} = E_n(\boldsymbol{k}(t)) - i\hbar\frac{d\boldsymbol{k}(t)}{dt}\cdot\langle n,\boldsymbol{k}(t)|\nabla_{\boldsymbol{k}}|n,\boldsymbol{k}(t)\rangle$$

Finally:

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

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

Berry phase.



Sir Michael Berry

We can write as

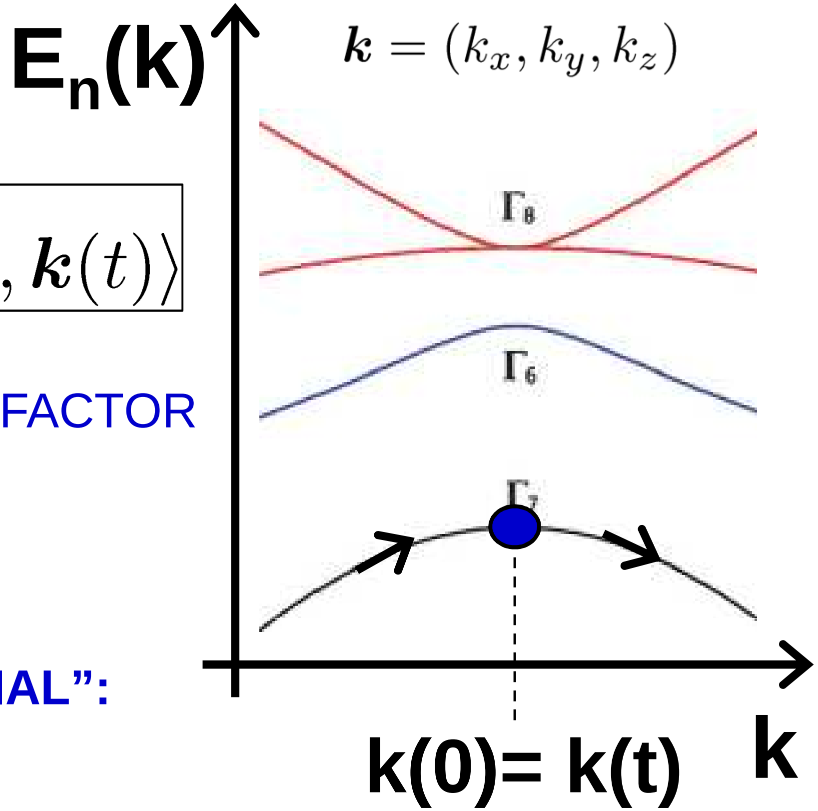
$$|n,t\rangle = e^{i\gamma_n} e^{\frac{-i}{\hbar}\int_0^t E_n[\boldsymbol{k}(t')]dt'} |n,\boldsymbol{k}(t)\rangle$$

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":

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



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):

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

2) Identity (m ≠n):

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

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

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 17)**: $E_\pm(\mathbf{k}) = \pm|\mathbf{k}|$

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

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

Eigenvectors (up to a phase) **(Tarefa 17)**:

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

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:

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

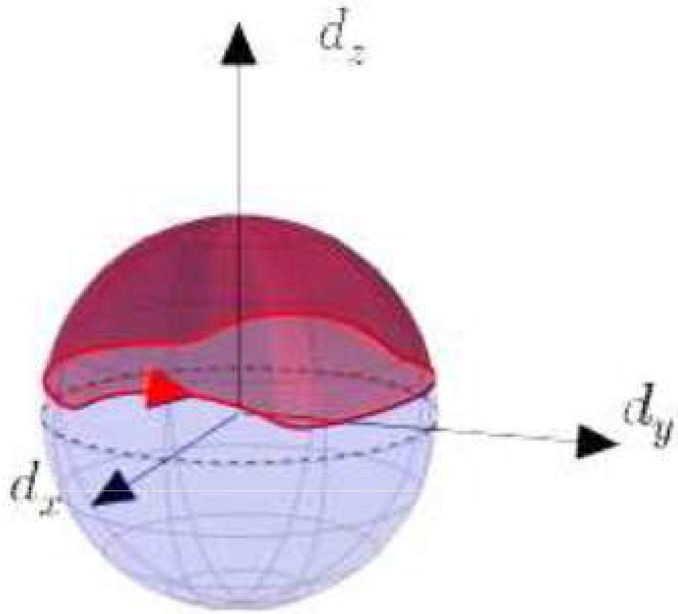
After a looong calculation (Lista 5): $\boxed{\boldsymbol{\Omega}_{\pm}(\mathbf{k}) = \pm \dfrac{\hat{\mathbf{k}}}{2|\mathbf{k}|^2}}$ (NOT gauge-dependent!) (Lista 5)

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

Chern number: $$\oiint_{\mathcal{S}} \boldsymbol{\Omega}_n(\boldsymbol{k}) \cdot d\boldsymbol{S} = 2\pi$$

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 :

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

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

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

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