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$$\hat{H}(\boldsymbol{X}(t))|\psi\rangle = E(\boldsymbol{X}(t))\,|\psi\rangle$$

Let's call the ground state $E_0(\boldsymbol{X}(t))$. Excited states E_1, E_2, ... Assume that the electrons are always in the ground state of the instantaneous Schrödinger equations.

Adiabatic theorem: Evolution of a quantum system under slowly varying $\hat{H}(t)$. If the system is in an instantaneous eigenstate initially, it will remain there if $\hat{H}(t)$ varies sufficiently slowly.

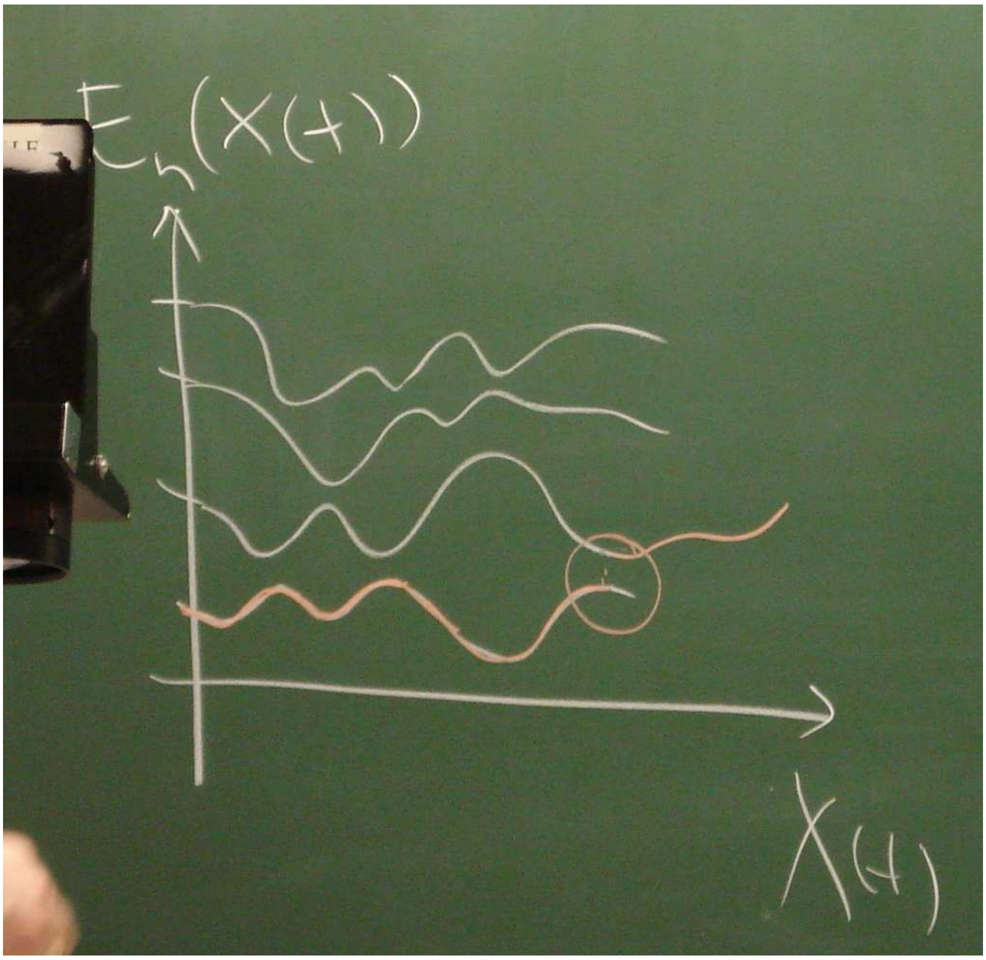

Figure 1. $E_n(\boldsymbol{X}(t))$ versus $\boldsymbol{X}(t)$. Typically they don't intersect. Landau, Zener calculated transition probabilities. Transitions happen for largish $\dot{\boldsymbol{X}}$.

Adiabatic basis

$$\hat{H}(\boldsymbol{X}(t))\,|\phi_n(t)\rangle = E_n(t)\,|\phi_n(t)\rangle$$

$$|\psi\rangle = \sum_n a_n(t)\;\mathrm{e}^{-\mathrm{i}\theta_n(t)}|\phi_n(t)\rangle$$

where $|\psi\rangle$ is the solution of the time-dependent Schrödinger equation, and $\theta_n(t)$ is defined by

$$\theta_n(t) = \frac{1}{\hbar}\int_0^t \mathrm{d}t'\,E_n(t')$$

Initially $a_n(0) = \delta_{ni}$. The adiabatic theorem $\Rightarrow a_n(t) = \delta_{ni}$.

$$\mathrm{i}\,\hbar\,\partial_t|\psi\rangle = \sum_n \left[\mathrm{i}\hbar\,\dot{a}_n(t)|\phi_n\rangle + a_n\,E_n\,|\phi_n\rangle + \mathrm{i}\hbar\,a_n\dot{X}\,|\frac{\partial\phi_n}{\partial X}\rangle\right]\mathrm{e}^{-\mathrm{i}\theta_n(t)} = \sum_n E_n\,\mathrm{e}^{-\mathrm{i}\theta_n}\,|\phi_n\rangle$$

Multiply with $\langle\phi_n|$ from the left:

$$0 = \mathrm{i}\,\hbar\,\dot{a}_m\,\mathrm{e}^{-\mathrm{i}\theta_n} + \mathrm{i}\hbar\,\dot{X}\sum_n a_n\,\langle\phi_m|\frac{\partial\phi_n}{\partial X}\rangle\,\mathrm{e}^{-\mathrm{i}\theta_n}$$

$$\dot{a}_m = -\,\dot{X}\sum_n a_n\,\langle\phi_m|\frac{\partial\phi_n}{\partial X}\rangle\,\mathrm{e}^{-\mathrm{i}(\theta_n-\theta_m)}$$

This is called the adiabatic Schrödinger equation. $a_m(0) = \delta_{mi}$. Try to show that

$$\Delta a_m(t) = a_m(t) - a_m(0)$$

is exponentially small if $m \neq i$. By normalisation $|a_i(t)|^2 \approx 1$.

$$\Delta a_m = \int_0^t \mathrm{d}t'\,\dot{a}_m(t') = -\int_0^t \mathrm{d}t'\,\dot{X}\sum_n a_n\,\langle\phi_m|\frac{\partial\phi_n}{\partial X}\rangle\,\mathrm{e}^{-\mathrm{i}(\theta_n-\theta_m)}$$

$\mathrm{d}X' = \dot{X}\,\mathrm{d}t'$, $\dot{X} = \mathrm{const} \equiv \varepsilon$.

$$= -\sum_n \int^X \mathrm{d}X'\,a_n(X')\,\langle\phi_m|\frac{\partial\phi_n}{\partial X}\rangle \times \exp\left(-\frac{\mathrm{i}}{\varepsilon\hbar}\int^{X'}\mathrm{d}X''\,(E_n(X'') - E_m(X''))\right)$$

As $\varepsilon \to 0$ this is a rapidly oscillating function. Rapidly oscillating integrands ensures that $a_m(t)$ remains exponentially small (for $m \neq i$) provided $E_n(X) \neq E_m(X)$. A little more technical assumption: $\langle\phi_m|\frac{\partial\phi_n}{\partial X}\rangle$ analytic.

$a_m(0) = \delta_{mi} \rightarrow a_m(t) = 0$ if $m \neq i$, $|a_i(t)| = 1$.

The adiabatic basis is only defined up to a phase.

$$|\phi_n(X)\rangle \quad \rightarrow \quad |\phi_n'(X) = \mathrm{e}^{\mathrm{i}\chi_n(X)}|\phi_n(X)\rangle$$

Suggestion:

$$\langle\phi_n'(X)|\frac{\partial\phi'}{\partial X}\rangle = 0$$

$$a_m(t) = \begin{cases} 1 & \text{if } m = i \\ 0 & \text{if } m \neq i \end{cases}$$

Let us calculate $\langle\phi_n'(X)|\frac{\partial\phi'}{\partial X}\rangle$:

$$\langle\phi_n'(X)|\frac{\partial\phi'}{\partial X}\rangle = \langle\phi_n(X)|\frac{\partial\phi_n}{\partial X}\rangle + \mathrm{i}\,\frac{\partial\chi_n(X)}{\partial X} = 0$$

$$\chi_n(X) = \int^X \mathrm{d}X'\,\langle\phi_n|\frac{\partial\phi_n}{\partial X}\rangle$$

$$|\psi\rangle \approx \mathrm{e}^{-\mathrm{i}\theta_i}|\phi_i'\rangle = \mathrm{e}^{-\mathrm{i}\chi_i}\,\mathrm{e}^{-\mathrm{i}\theta_i}|\phi_i\rangle$$

$e^{-i\theta_i}$: the dynamical phase.

$e^{-i\chi_i}$: Berry's phase.

The phase χ cannot be eliminated when time evolution brings $\boldsymbol{X}(t)$ back to its starting point.

$$\chi_c = i \oint d\boldsymbol{X} \, \langle \phi_n | \frac{\partial \phi_n}{\partial X} \rangle$$

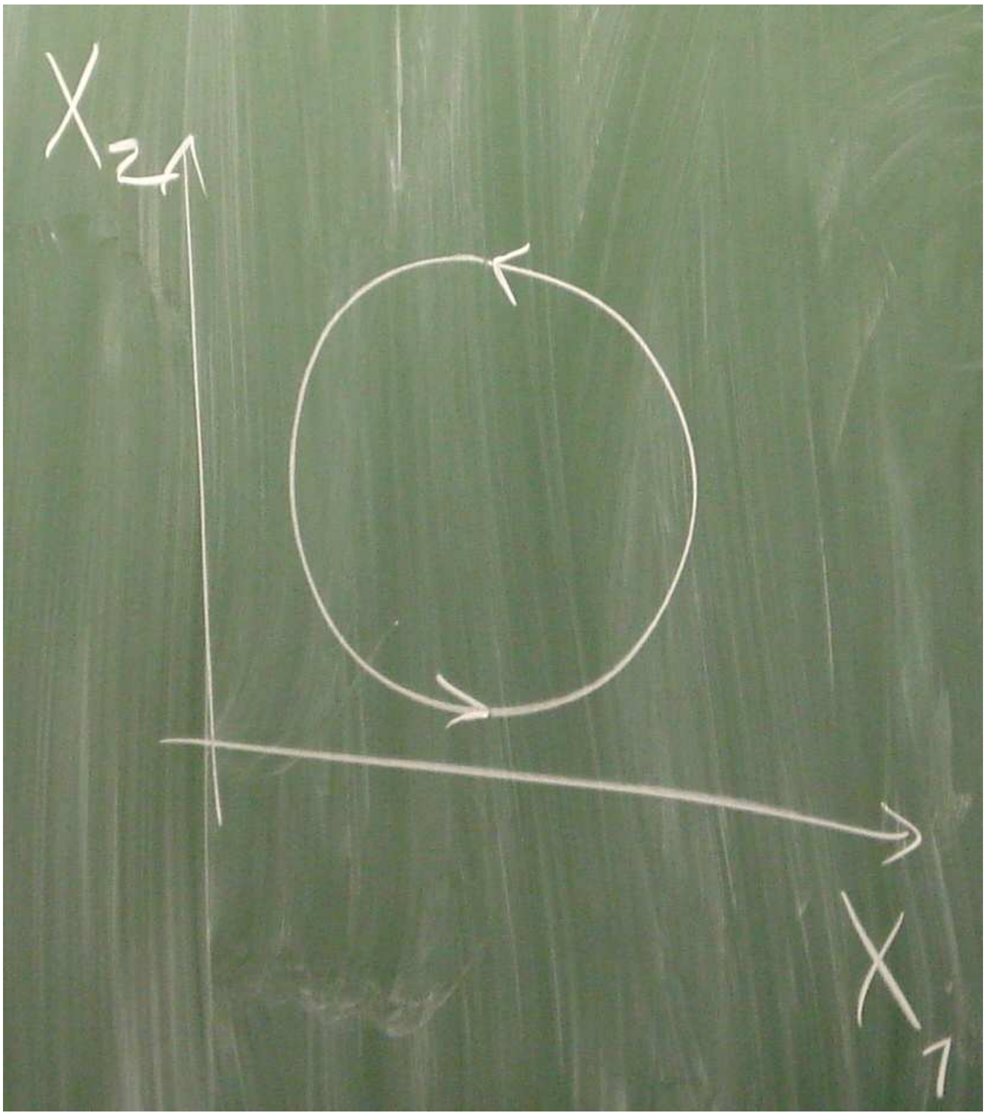

Figure 2. X_2, X_1

Interpret $i\langle \phi_n | \frac{\partial \phi_n}{\partial X} \rangle$ as a vector potential $\boldsymbol{A}_n(\boldsymbol{X})$. Stokes theorem:

$$\chi_c = i \int dX_1 \, dX_2 \left(\nabla \times \langle \phi_n | \frac{\partial \phi_n}{\partial X} \rangle \right) \hat{\boldsymbol{n}}_z = \int dX_1 \, dX_2 \, \beta_{12}^{(n)}(X_1, X_2)$$

where

$$\beta_{12}^{(n)}(X_1, X_2) = i \left[\langle \frac{\partial \phi_n}{\partial X_1} | \frac{\partial \phi_n}{\partial X_2} \rangle - \langle \frac{\partial \phi_n}{\partial X_2} | \frac{\partial \phi_n}{\partial X_1} \rangle \right]$$

This is Berry's two-form.