Adiabatic methods in Quantum Control Theory

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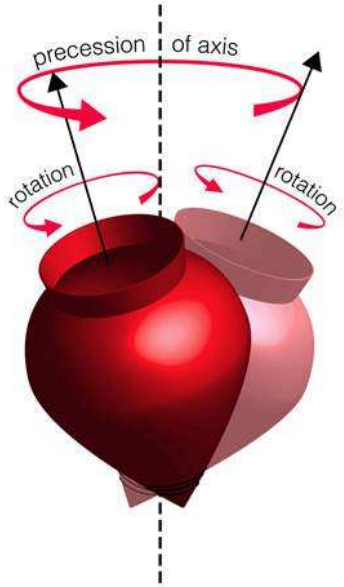
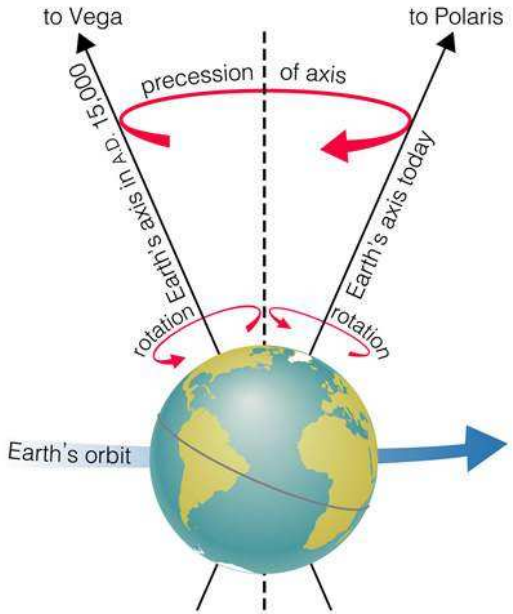
Separation of **time-scales**

$$\boxed{\text{slow degrees of freedom}} \leftrightarrow \boxed{\text{fast degrees of freedom}}$$

Fast degrees of freedom readjust ε-**istantaneuosly** to the evolution of the slow ones, where ε is the ratio between the two time scales.





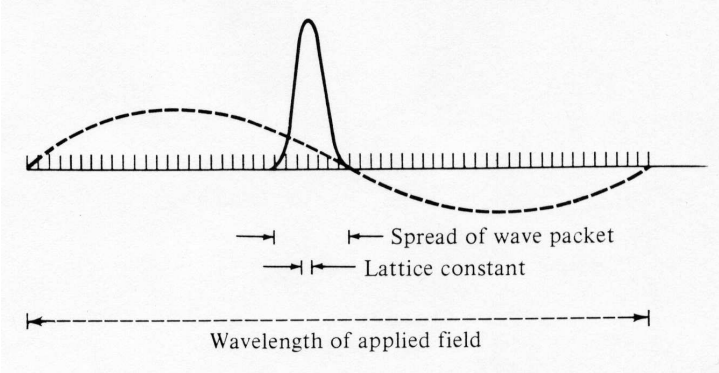
Examples from the **microphysical** world:

(i) molecular physics (**Born-Oppenheimer approx**)

$$\boxed{\text{nuclei}} \leftrightarrow \boxed{\text{electrons}}$$

(ii) **Bloch electron:** an electron in a crystal with a **slowly** varying external electromagnetic potential

$$\boxed{\begin{array}{c}\text{macroscale}\\ \text{dynamics}\end{array}} \leftrightarrow \boxed{\begin{array}{c}\text{lattice scale}\\ \text{dynamics}\end{array}}$$



Adiabatic methods in Quantum Control Theory ?

Part I

Adiabatic decoupling in a prototypical example: Born-Oppenheimer approximation in molecular physics

The framework

K nuclei:	coordinates	$x = (x_1, \ldots, x_K) \in \mathbb{R}^{3K} =: X$	$\mathcal{H}_{\mathrm{n}} = L^2(X, dx)$
N electrons:	coordinates	$y = (y_1, \ldots, y_N) \in \mathbb{R}^{3N} =: Y$	$\mathcal{H}_{\mathrm{el}} = \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3, dy_i)$

Hilbert space : $\mathcal{H} := L^2(X) \otimes \mathcal{H}_{\mathrm{el}} \cong L^2(X, \mathcal{H}_{\mathrm{el}})$

Molecular dynamics is described by the **Schrödinger equation**

$$i\frac{\partial}{\partial s}\Psi_s = H_{\mathrm{mol}}\Psi_s, \qquad s\text{: microscopic time}$$

with Hamiltonian

$$H_{\mathrm{mol}} = -\sum_{k=1}^{K} \frac{\hbar^2}{2M_k}\Delta_{x_k} - \sum_{i=1}^{N} \frac{\hbar^2}{2m_e}\Delta_{y_i} + V_{\mathrm{e}}(y) + V_{\mathrm{n}}(x) + V_{\mathrm{en}}(x, y)$$

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Hilbert space : $\mathcal{H} := L^2(X) \otimes \mathcal{H}_{\mathrm{el}} \cong L^2(X, \mathcal{H}_{\mathrm{el}})$

The Hamiltonian operator contains the following terms

$$V_{\mathrm{n}}(x) = \sum_{k=1}^{K} \sum_{l \neq k}^{K} \frac{e^2 Z_k Z_l}{|x_k - x_l|} \qquad V_{\mathrm{e}}(y) = \sum_{i=1}^{N} \sum_{j \neq i}^{N} \frac{e^2}{|y_i - y_j|}$$

$$V_{\mathrm{e,n}}(x, y) = \sum_{k=1}^{K} \sum_{i=1}^{N} -\frac{e^2 Z_k}{|x_k - y_i|}$$

where eZ_k, for $Z_k \in \mathbb{Z}$, is the **electric charge** of the k-th nucleus. A cut-off on the coulomb singularity is sometimes assumed to get rigorous results.

The framework

The large number of degrees of freedom makes convenient to elaborate an **approximation scheme**, exploiting the smallness of the parameter

$$\varepsilon = \sqrt{\frac{\mathbf{m_e}}{\mathbf{M}}} \simeq \mathbf{10^{-2}}$$

By introducing atomic units ($\hbar = 1, m_e = 1$) and the **adiabatic parameter** ε the Hamiltonian H_{mol} reads (up to a change of energy scale)

$$H_\varepsilon = -\sum_{k=1}^{K} \frac{\varepsilon^2}{2}\Delta_{x_k} + \underbrace{V_{\text{n}}(x) + \sum_{i=1}^{N} -\frac{1}{2}\Delta_{y_i} + V_{\text{e}}(y) + V_{\text{en}}(x,y)}_{H_{\text{el}}(x)}$$

For each fixed nuclei configuration $x = (x_1, \dots, x_K) \in X$ the operator $H_{\text{el}}(x)$ is an operator acting on the space $\mathcal{H}_{\text{el}}$.

The framework

If the kinetic energies of the nuclei and the electrons are comparable, then the velocities scale as

$$|v_n| \approx \sqrt{\frac{m_e}{M}}|v_e| = \varepsilon|v_e|.$$

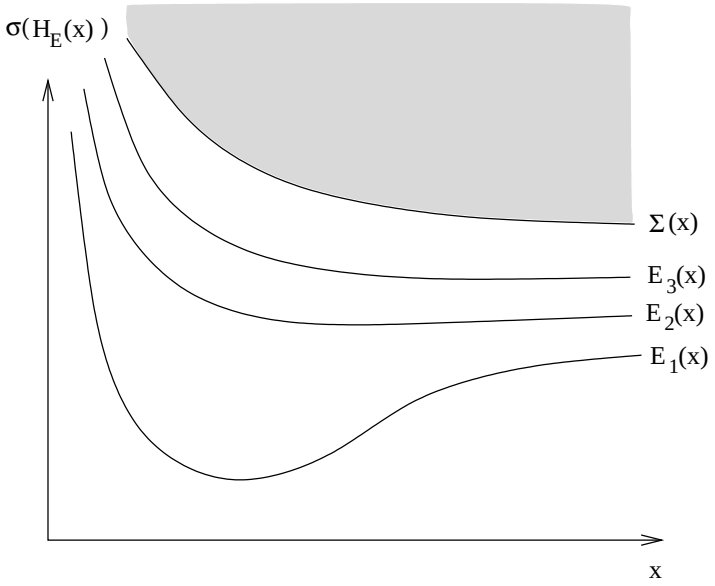
We have to wait a **microscopically long time**, namely $\mathcal{O}(\varepsilon^{-1})$, in order to see a non-trivial dynamics for the nuclei. This scaling fixes the **macroscopic time scale** $t = \varepsilon s$.

In the macroscopic time scale, the Schrödinger equation reads

$$i\varepsilon\frac{\partial}{\partial t}\Psi_t = \left(-\frac{\varepsilon^2}{2}\Delta_x + H_{\mathrm{el}}(x)\right)\Psi_t, \qquad \Psi_{t=0} = \Psi_0$$

We are interested in the behavior of the solutions as $\varepsilon \downarrow 0$.

The band structure

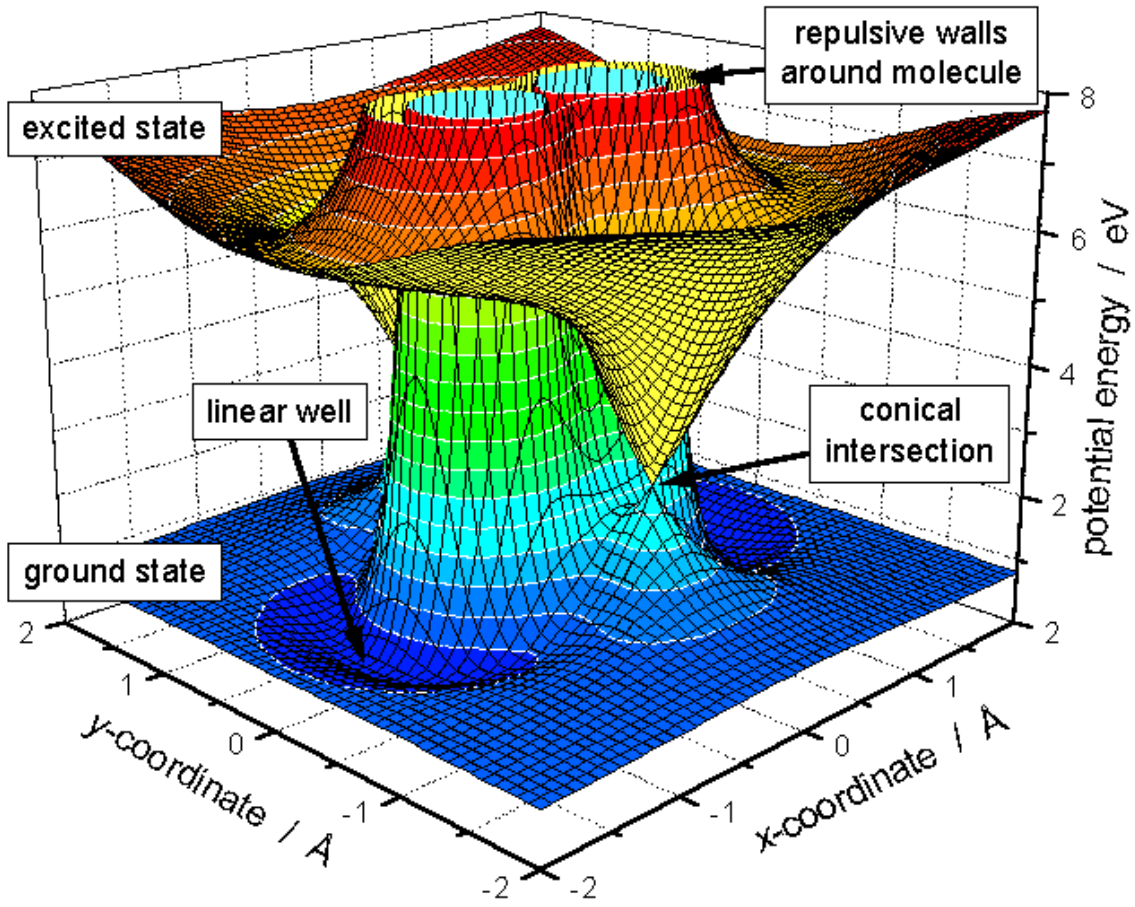


Solution of the **electronic structure** problem:

$$H_{\mathrm{el}}(x)\chi_n(x,y) = E_n(x)\chi_n(x,y)$$

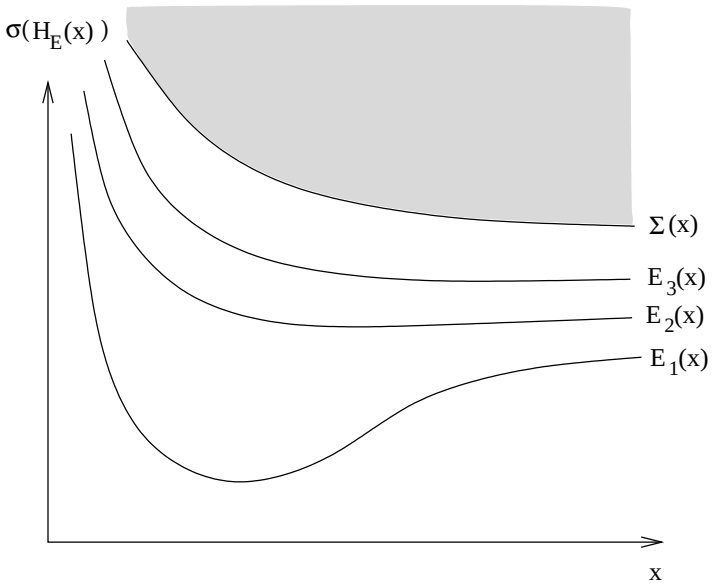
Eigenvalue:	$E_n(x)$
Eigenfunction:	$\chi_n(x,\cdot) \in \mathcal{H}_{\mathrm{el}}$
Eigenprojector:	$P_n(x) = \lvert\chi_n(x)\rangle\langle\chi_n(x)\rvert$
Total projector:	$P_n = \{P_n(x)\}_{x\in X}$

A real-life example: the hydrogen quasi-molecule



Credits: Eckart Wrede, University of Durham (UK)

The band structure



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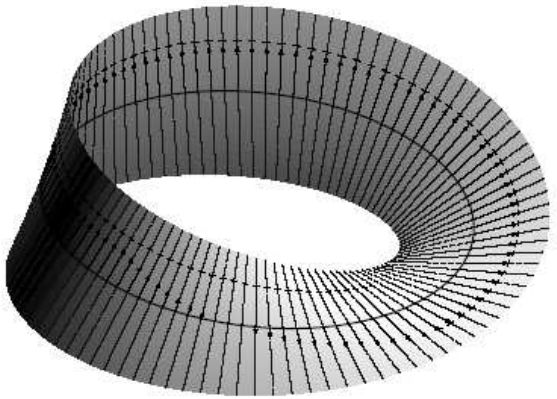
The family $\{\mathrm{Ran}\, P_n(x)\}_{x\in X}$, defines a complex **vector bundle** over $X \setminus C$, where C is the crossing manifold.



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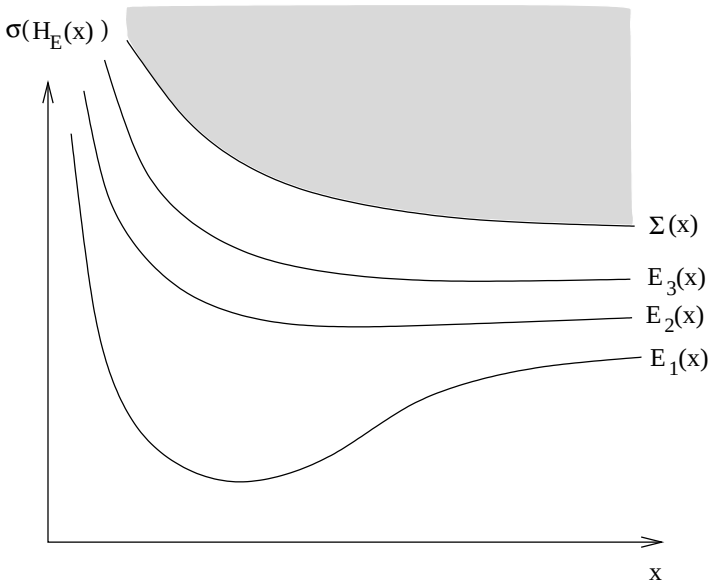

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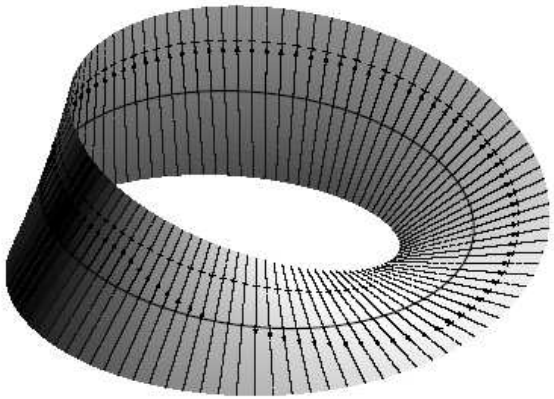
Geometric information is encoded in the **Berry connection**,

$$\mathcal{A}_n(x) := i\,\langle\chi_n(x), \nabla_x\chi_n(x)\rangle_{\mathcal{H}_{\mathrm{el}}}\,.$$

defined over $X \setminus C$.



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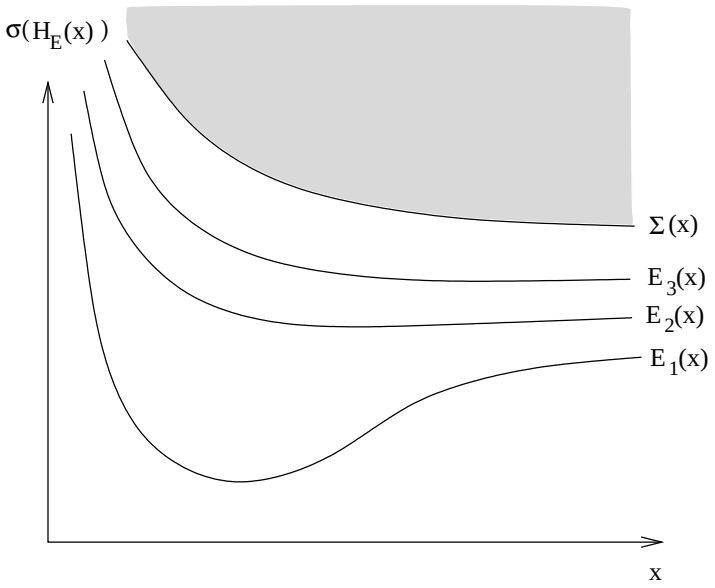

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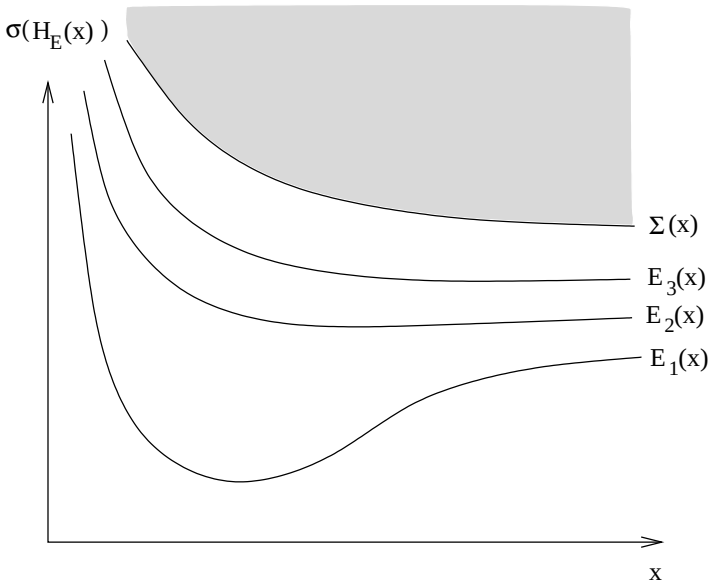
We focus on an **isolated** (non degenerate) energy band. We assume the initial state is **concentrated on the n-th band**, *i. e.* in the closed subspace

$$\mathrm{Ran}\, P_n = \{\Psi \in \mathcal{H} :\ \Psi(x,y) = \varphi(x)\ \chi_n(x,y) \text{ for } \varphi \in L^2(X)\}$$

The band structure



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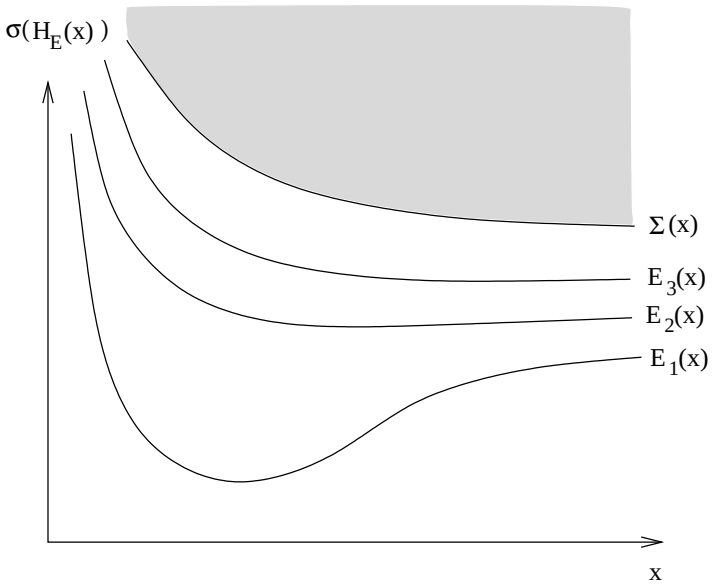
Transitions from an isolated band are $\mathcal{O}(\varepsilon)$:

$$\|(1-P_n)\, e^{-iH_\varepsilon t/\varepsilon}\, P_n\ \Psi_0\| = \mathcal{O}(\varepsilon)$$

We say that an **isolated band is adiabatically protected against transitions.**

▷ Note: the upper bound holds for any Ψ_0 such that $\|-i\varepsilon\nabla_x\Psi_0\| = \mathcal{O}(1) \leq \mathcal{E}$, corresponding to the fact that the **kinetic energy of the nuclei** is supposed to be $\mathcal{O}(1)$, *i. e.* comparable with that of the electrons.

The band structure



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For a fixed band, the dynamics of the nuclei is governed by the Hamiltonian

$$P_n\, H_\varepsilon P_n = -\frac{\varepsilon^2}{2}\sum_{k=1}^{K}\Delta_{x_k} + E_n(x) + \mathcal{O}(\varepsilon)$$

in $\mathrm{Ran}\, P_n \cong \mathcal{H}_{\mathrm{n}} = L^2(X)$. Notice the impressive dimensional reduction!

This is the **time-dependent Born-Oppenheimer approximation**.

References

(i) Predecessors: time-adiabatic theorems

▷ [Kato, Nenciu, Avron, Seiler, Simon, Sjöstrand ... and many others]

(ii) Dynamical Born-Oppenheimer approximation

▷ Propagation of generalized Gaussian wavepackets [Hagedorn and Joye]

▷ Matrix valued pseudodifferential operators
[Brummelhaus, Nourrigat; Martinez, Nenciu, Sordoni; Panati, Spohn, Teufel]

▷ Scattering theory including resonances
[Martinez, Nakamura, Nenciu, Sordoni]

▷ Exponentially small transitions [Hagedorn and Joye]

▷ Optimal truncation [Betz and Teufel]

(iii) Stationary Born-Oppenheimer approximation

▷ [Combes, Duclos and Seiler; Klein, Martinez, Seiler, Wang]

(iv) Dynamics near conical eigenvalue intersections

▷ [P. Gerard, Fermannian, Lasser, Teufel, Colin de Verdiére]

To prove the claim, one has to bound the difference

$$\left(\mathrm{e}^{-\mathrm{i}\,H_\varepsilon\,t/\varepsilon} - \mathrm{e}^{-\mathrm{i}\,P_nH_\varepsilon P_n\,t/\varepsilon}\right)\,P_n.$$

The **Duhamel formula** yields

$$\begin{aligned}\left(\mathrm{e}^{-\mathrm{i}\,H_\varepsilon\,t/\varepsilon} - \mathrm{e}^{-\mathrm{i}\,P_nH_\varepsilon P_n\,t/\varepsilon}\right)\,P_n &= \mathrm{i}\mathrm{e}^{-\mathrm{i}H_\varepsilon t/\varepsilon}\int_0^{t/\varepsilon} ds\,\mathrm{e}^{\mathrm{i}H_\varepsilon s}\,(P_nH_\varepsilon P_n - H_\varepsilon)\,\mathrm{e}^{-\mathrm{i}P_nH_\varepsilon P_n s}\,P_n\\ &= \mathrm{i}\mathrm{e}^{-\mathrm{i}H_\varepsilon t/\varepsilon}\int_0^{t/\varepsilon} ds\,\mathrm{e}^{\mathrm{i}H_\varepsilon s}\,(P_nH_\varepsilon P_n - H_\varepsilon)\,P_n\,\mathrm{e}^{-\mathrm{i}P_nH_\varepsilon P_n s}\\ &= \mathrm{i}\mathrm{e}^{-\mathrm{i}H_\varepsilon t/\varepsilon}\int_0^{t/\varepsilon} ds\,\mathrm{e}^{\mathrm{i}H_\varepsilon s}\,\underbrace{[P_n, H_\varepsilon]\,P_n}_{\mathcal{O}(\varepsilon)}\,\mathrm{e}^{-\mathrm{i}P_nH_\varepsilon P_n s}\,.\end{aligned}$$

The commutator is

$$[P_n, H_\varepsilon]P_n = \left[|\chi_n(x)\rangle\langle\chi_n(x)|, -\frac{\varepsilon^2}{2}\Delta_x\right]P_n = \mathcal{O}(\varepsilon)$$

but the integration interval is $\mathcal{O}(\varepsilon^{-1})$. Thus the **naïf approach fails**.

A rigorous proof has been provided by [Spohn Teufel 2001], elaborating on [Kato 1950].

For a fixed band, the dynamics of the nuclei is governed by the Hamiltonian

$$P_n\, H_\varepsilon P_n = -\frac{\varepsilon^2}{2} \sum_{k=1}^{K} \Delta_{x_k} + E_n(x) + \mathcal{O}(\varepsilon)$$

acting in $\operatorname{Ran} P_n \cong \mathcal{H}_{\mathrm{n}} = L^2(X)$.

What about higher-order corrections?

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What about higher-order corrections?

The naïf expansion has no physical meaning since

$$\|(1 - P_n)\, e^{-iH_\varepsilon t/\varepsilon}\, P_n\, \Psi_0\| = \mathcal{O}(\varepsilon) \geq C\varepsilon$$

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Questions:

(i) **almost-invariant subspace:** is there a subspace of $\mathcal{H} = \mathcal{H}_{\mathrm{n}} \otimes \mathcal{H}_{\mathrm{el}}$ which is almost-invariant under the dynamics, up to errors ε^N ?

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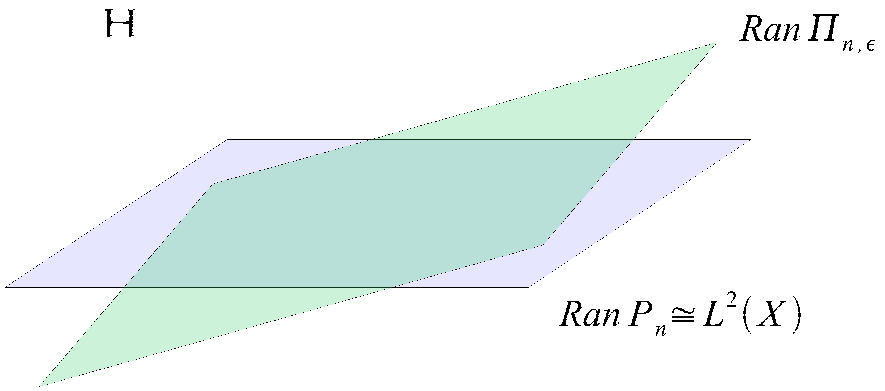
(ii) **intra-band dynamics:** is there any simple way to describe the dynamics inside this subspace?

Almost-invariant subspace

Answer 1: to any globally **isolated** energy band $E_n(\cdot)$ corresponds a subspace of the Hilbert space which is **almost-invariant under the dynamics** as $\varepsilon \downarrow 0$.

More precisely, one constructs an orthogonal projector $\Pi_{n,\varepsilon} \in \mathcal{B}(\mathcal{H})$ with $\Pi_{n,\varepsilon} = P_n + \mathcal{O}(\varepsilon)$, such that $\mathrm{Ran}\,\Pi_{n,\varepsilon}$ is almost invariant under the dynamics, *i. e.* for any $N \in \mathbb{N}$ there exists C_N such that

$$\|(1 - \Pi_{n,\varepsilon})\; e^{-iH_\varepsilon t/\varepsilon}\; \Pi_{n,\varepsilon}\Psi_0\| \leq C_N\, \varepsilon^N (1 + |t|)(1 + \mathcal{E})\|\Psi_0\|.$$



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Credits: [Sjöstrand], [Emmerich Weinstein], [Nenciu Sordoni] and [Martinez Sordoni], [Panati Spohn Teufel]

The intra-band dynamics

Problem: no natural identification between $\mathrm{Ran}\,\Pi_{n,\varepsilon}$ and $\mathcal{H}_{\mathrm{n}} \cong L^2(X)$, then no evident **reduction** in the number of degrees of freedom.

Solution: to construct a **intertwining unitary operator**

$$U_{n,\varepsilon} : \mathrm{Ran}\,\Pi_{n,\varepsilon} \longrightarrow \mathcal{H}_{\mathrm{n}} \cong L^2(X)$$

in order to map the intraband dynamics to the nuclei Hilbert space.

The intra-band dynamics

We construct a **intertwining unitary operator**

$$\begin{array}{ccc} \operatorname{Ran}\Pi_{n,\varepsilon} & \xrightarrow{U_{n,\varepsilon}} & \mathcal{H}_{\mathrm{n}} \cong L^2(X) \\ \Big\downarrow{\scriptstyle \Pi_{n,\varepsilon} H_\varepsilon \Pi_{n,\varepsilon}} & & \Big\downarrow{\scriptstyle \hat{H}_{\mathrm{eff},\varepsilon}} \\ \operatorname{Ran}\Pi_{n,\varepsilon} & \xrightarrow{U_{n,\varepsilon}} & \mathcal{H}_{\mathrm{n}} \cong L^2(X) \end{array}$$

Answer 2: the effective Hamiltonian $\hat{H}_{\mathrm{eff},\varepsilon} := U_{n,\varepsilon}\,\Pi_{n,\varepsilon}\,H_\varepsilon\,\Pi_{n,\varepsilon}\,U_{n,\varepsilon}^{-1}$ acting in $L^2(X)$ satisfies: for every $N \in \mathbb{N}$ there exist C_N such that

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H_\varepsilon t/\varepsilon} - U_{n,\varepsilon}^{-1}\, \mathrm{e}^{-\mathrm{i}\,\hat{H}_{\mathrm{eff},\varepsilon}\,t/\varepsilon}\, U_{n,\varepsilon} \right) \Pi_{n,\varepsilon}\Psi_0 \right\|_{\mathcal{H}} \leq C_N\,\varepsilon^N\,(1+|t|)\|\Psi_0\|,$$

and, more important, ...

The intra-band dynamics

... the operator $\hat{H}_{\text{eff},\varepsilon}$ is an ε-pseudodifferential operator*: it is the **ε-Weyl quantization** of a function

$$H_{\text{eff},\varepsilon} : X \times X^* \to \mathbb{R}, \qquad (q,p) \mapsto H_{\text{eff},\varepsilon}(q,p)$$

with expansion

$$H_{\text{eff},\varepsilon}(q,p) = h_0(q,p) + \varepsilon h_1(q,p) + \varepsilon^2 h_2(q,p) + \mathcal{O}(\varepsilon^3)$$

$$h_0(q,p) = \tfrac{1}{2}p^2 + E_n(q) \qquad \textbf{Born-Oppenheimer}$$

$$h_1(q,p) = \dots$$

▷ **Remark:** the effective Hamiltonian operator $\hat{H}_{\text{eff},\varepsilon}$ is obtained by using **ε-Weyl quantization**

$$(q,p) \mapsto (x, i\varepsilon\nabla_x), \qquad e^{i\alpha\cdot q}e^{i\beta\cdot p} \mapsto e^{i(\alpha\cdot x + \beta\cdot(i\varepsilon\nabla_x))}.$$

The intra-band dynamics

The dynamics corresponding to the n-th energy band is described by the effective Hamiltonian

$$H_{\mathrm{eff},\varepsilon}(q,p) = h_0(q,p) + \varepsilon h_1(q,p) + \varepsilon^2 h_2(q,p) + \mathcal{O}(\varepsilon^3)$$

where

$$h_0(q,p) = \tfrac{1}{2}p^2 + E_n(q) \qquad \textbf{Born-Oppenheimer}$$

$$h_1(q,p) = -ip \cdot \langle \chi_n(q), \nabla_q \chi_n(q) \rangle =: -p \cdot \mathcal{A}_n(q) \qquad \textbf{Berry connection}$$

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where

$$\begin{aligned}
h_0(q,p) &= \tfrac{1}{2}p^2 + E_n(q) \\
h_1(q,p) &= -ip \cdot \langle \chi_n(q), \nabla_q \chi_n(q) \rangle_{\mathcal{H}_{\mathrm{el}}} =: -p \cdot \mathcal{A}_n(q) \\
h_2(q,p) &= \tfrac{1}{2}\mathcal{A}^2(q) + \tfrac{1}{2}\left\langle \nabla_q \chi_n(q), (1 - P_n(q)) \cdot \nabla_q \chi_n(q) \right\rangle_{\mathcal{H}_{\mathrm{el}}} \\
&\quad - \Big\langle p \cdot \nabla_q \chi_n(q);\ (H_{\mathrm{el}}(q) - E_n(q))^{-1} (1 - P_n(q))\ p \cdot \nabla_q \chi_n(q) \Big\rangle_{\mathcal{H}_{\mathrm{el}}}.
\end{aligned}$$

Different **quantization rules** for the symbol (=function)

$$\mathcal{M} : X \times X^* \longrightarrow \mathbb{C}$$

$$\mathcal{M}(q,p) = \big\langle\, p\cdot\nabla\chi_n(q), (H_{\rm el}(q) - E_n(q))^{-1}(1-P_n(q))\, p\cdot\nabla\chi_n(q)\big\rangle_{\mathcal{H}_{\rm el}}$$

differ by terms of order $\mathcal{O}(\varepsilon)$.

The simplest symmetric choice for $\widehat{\mathcal{M}}$ is presumably

$$(\widehat{\mathcal{M}}\psi)(x) = \sum_{\ell,k=1}^{3K} \frac{1}{2}\Big(\mathfrak{m}_{\ell k}(x)(-{\rm i}\varepsilon\partial_{x_\ell})(-{\rm i}\varepsilon\partial_{x_k}) + (-{\rm i}\varepsilon\partial_{x_\ell})(-{\rm i}\varepsilon\partial_{x_k})\mathfrak{m}_{\ell k}(x)\Big)\psi(x)\,,$$

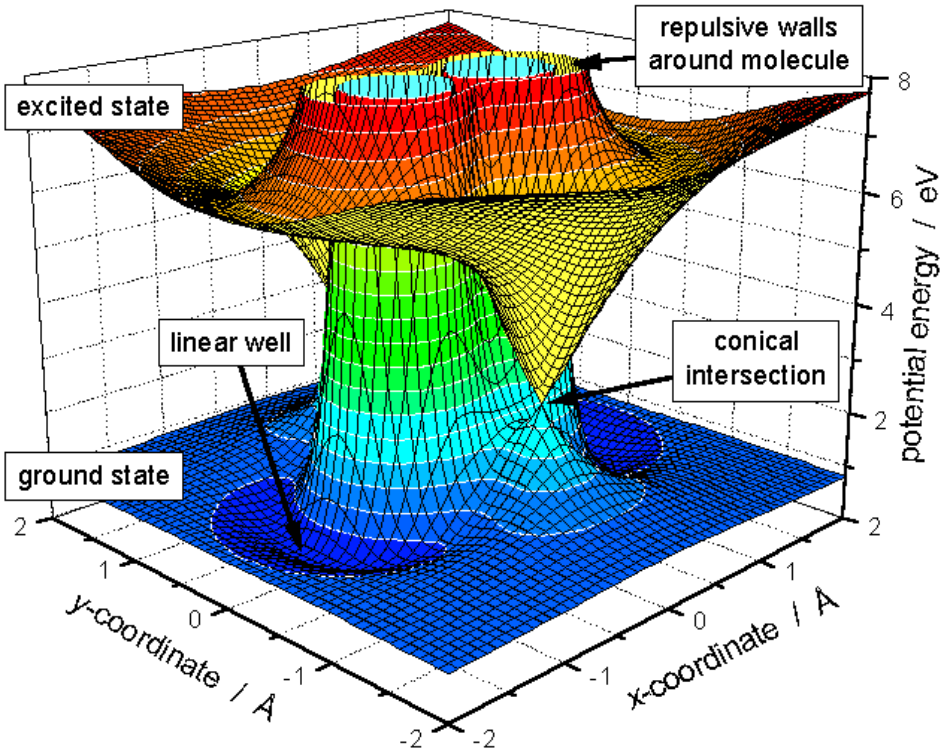
where $\mathfrak{m}$ is the x-dependent matrix

$$\mathfrak{m}_{\ell k}(x) = \big\langle\, \partial_\ell\chi_n(x), (H_{\rm e}(x) - E_n(x))^{-1}(1-P_n(x))\, \partial_k\chi_n(x)\big\rangle_{\mathcal{H}_{\rm el}}$$

Experimental relevance of higher-order terms

Scattering exchange reaction: $A + BC \longrightarrow AB + C$

Simplest example: $H + D_2 \longrightarrow HD + D$



Relation with the dynamics of the **Wigner function**

▷ Any wavefunction $\psi \in L^2(\mathbb{R}^d)$ can be uniquely represented (up to a global phase) by its **ε-Wigner function** $W_\varepsilon[\psi] \in L^2(\mathbb{R}^{2d})$ defined by

$$W_\varepsilon[\psi](q,p) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{ix\cdot p}\, \psi^*(q + \frac{\varepsilon}{2}x)\, \psi(q - \frac{\varepsilon}{2}x) dx.$$

The mapping $\psi \mapsto W_\varepsilon[\psi]$ is continuous from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^{2d})$.

It is tempting to interpret $W_\varepsilon[\psi]$ as a **probability distribution over the classical phase space**, but **sign oscillations** appear.

▷ The advantage of the Wigner function is its relation with the **expectation values of semiclassical observables**, *i. e.* observables which are the ε-Weyl quantization of "smooth" functions

$$a \in C^\infty_{\rm b}(\mathbb{R}^{2d}) \qquad \|a(x, -i\varepsilon\nabla_x)\|_{\mathcal{B}(L^2)} \leq C \sum_{|\alpha|\leq 2d+1} \|\partial_x^\alpha a\|_\infty =: \|a\|_{\rm CW}$$

Indeed for any $a \in C^\infty_{\rm b}(\mathbb{R}^{2d})$ and any $\psi \in L^2(\mathbb{R}^d)$ one has

$$\langle \psi \,|\, a(x, -i\varepsilon\nabla_x)\psi \rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} a(q,p)\, W_\varepsilon[\psi](q,p)\, dqdp.$$

▷**Semiclassical dynamics in a band** Consider the Hamiltonian dynamical system

$$\begin{cases} \dot q = \nabla_p\, h_0(q,p) \\ \dot p = -\nabla_q\, h_0(q,p) \end{cases}$$

and let $\Phi^t : \mathbb{R}^{2d} \longrightarrow \mathbb{R}^{2d}$ be the corresponding dynamical flow.

Then for any bounded time interval I and for any $a \in C^\infty_{\rm b}(\mathbb{R}^{2d})$ one has

$$\left| \int_{\mathbb{R}^{2d}} a(q,p)\, \left(W_\varepsilon[\psi_t] - W_\varepsilon[\psi_0] \circ \Phi^{-t} \right)(q,p)\, dqdp \right| \leq C_I\, \varepsilon\, \|a\|_{\rm CW}\, \|\psi_0\|^2$$

for any $t \in I$.

Indeed for any $a \in C^\infty_{\rm b}(\mathbb{R}^{2d})$ and any $\psi \in L^2(\mathbb{R}^d)$ one has

$$\langle \psi \,|\, a(x, -i\varepsilon\nabla_x)\psi \rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} a(q,p)\, W_\varepsilon[\psi](q,p)\, dqdp.$$

▷**Semiclassical dynamics in a band** Consider the ε-dependent Hamiltonian dynamical system

$$\begin{cases} \dot q = \nabla_p \left(h_0(q,p) + \ \varepsilon h_1(q,p) \right) \\ \dot p = -\nabla_q \left(h_0(q,p) + \ \varepsilon h_1(q,p) \right) \end{cases}$$

and let $\Phi^t_\varepsilon : \mathbb{R}^{2d} \longrightarrow \mathbb{R}^{2d}$ be the corresponding dynamical flow.

Then for any bounded time interval I and for any $a \in C^\infty_{\rm b}(\mathbb{R}^{2d})$ one has

$$\left| \int_{\mathbb{R}^{2d}} a(q,p) \, \left(W_\varepsilon[\psi_t] - W_\varepsilon[\psi_0] \circ \Phi^{-t}_\varepsilon \right)(q,p)\, dqdp \right| \leq \tilde C\, \varepsilon^2 \, \|a\|_{\rm CW} \, \|\psi_0\|^2$$

for any $t \in I$.

Part II

Possible application to Quantum Control Theory

The intra-band dynamics with external controls

The original problem is now replaced by

$$i\varepsilon\frac{\partial}{\partial t}\Psi_t = \left(-\frac{\varepsilon^2}{2}\Delta_x + H_{\rm el}(x) + U(x,t)1_{\mathcal{H}_{\rm el}}\right)\Psi_t, \qquad \Psi_{t=0} = \Psi_0$$

where $U(x,t)$ is an **external control** and t is the **macroscopic time**. For example

$$U(x,t) = u_1(t)\,W_1(x) + \cdots + u_N(t)\,W_N(x).$$

Then the **semiclassical dynamics** is described by the effective Hamiltonian

$$H_{{\rm eff},\varepsilon}(q,p) = h_0(q,p) + \varepsilon h_1(q,p) + \varepsilon^2 h_2(q,p) + \mathcal{O}(\varepsilon^3)$$

$$h_0(q,p) \;=\; \tfrac{1}{2}p^2 + E_n(q) + U(t,q)$$

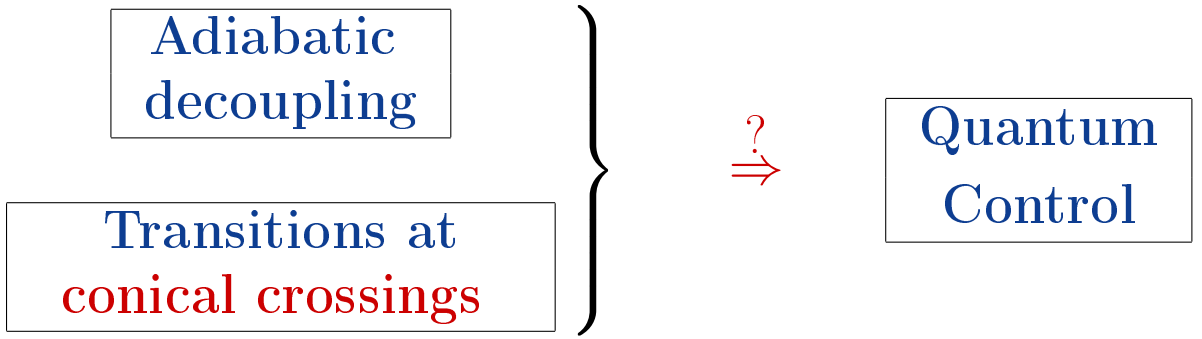
and **higher-order corrections** can be computed algorithmically.

In the adiabatic approximation **isolated bands are approximately decoupled**, *i. e.* **different bands cannot be connected by the dynamics**.

Adiabatic decoupling $\not\Rightarrow$ **Quantum Control**

In the adiabatic approximation **isolated bands are approximately decoupled**, *i. e.* **different bands cannot be connected by the dynamics**.

One can exploit the existence of **eigenvalue crossings**, where transitions to other bands are possible!



Outline of a general strategy

(i) Use the **external controls** to **drive the system** to a selected conical intersection with prescribed **focusing**

- ▷ **Tool:** adiabatic theory, in particular **space-adiabatic theorems**, see [Panati Spohn Teufel 03] or [Teufel book].
- ▷ **Advantages:** small errors, uniform estimates in the initial datum

(ii) Use detailed information about the **transition probability at the crossing point**

- ▷ **Tools:** multiscale Wigner functions, surface-hopping algoritms
- ▷ **Trick:** **optimize the incoming wavefunction** to obtain the desired transition probability, up to reasonable errors

The standard model for the conical intersection

If the **other bands are separated by a gap**, by adiabatic decoupling and linearization of the energy bands, one is reduced to consider $\psi(t) \in L^2(\mathbb{R}^2, \mathbb{C}^2)$ satisfying

$$i\varepsilon\partial_t\psi(q,t) = -\frac{\varepsilon^2}{2}\Delta_q + \begin{pmatrix} q_1 & q_2 \\ q_2 & -q_1 \end{pmatrix}\psi(q,t).$$

The matrix $V(q)$ is analytic in q, with eigenvalues $E_\pm(q) = \pm\sqrt{q_1^2+q_2^2}$.

▷**Dynamics at a conical intersection:** an accurate description of the dynamics, as an approximated evolution group for $\varepsilon \ll 1$, is nowadays available [Hagedorn & Joye] [Fermannian & Gerard] [Lasser & Teufel].

References

(i) Literature about dynamics at conical intersections theorems

- ▷ [Hagedorn 94][Hagedorn Joye 99]: propagation of **gaussian wavepackets**
- ▷ [Colin de Verdiere, Lombardi Pollet 99]: **microlocal Landau-Zener formula**
- ▷ [Fermannian Gerard 02][Fermannian Lasser 02]: **two-scales Wigner functions**
- ▷ [Lasser Teufel 05 & 07]: **surface hopping algorithm** and asymptotic $\varepsilon \longrightarrow 0$ evolution semigroup

(ii) Quantum Control using this general strategy (in simpler models)

- ▷ Adami & Boscain 2005, *Controllability of the Schrödinger Equation via Intersection of Eigenvalues*: **simple one-dimensional models**
- ▷ Boscain, Chittaro, Mason, Sigalotti 2010 *Quantum Control via Adiabatic Theory*: more general systems, **talk at this workshop, on Saturday**.

Thank you
for your attention!!