

# **Adiabatic decoupling and the partial classical limit**

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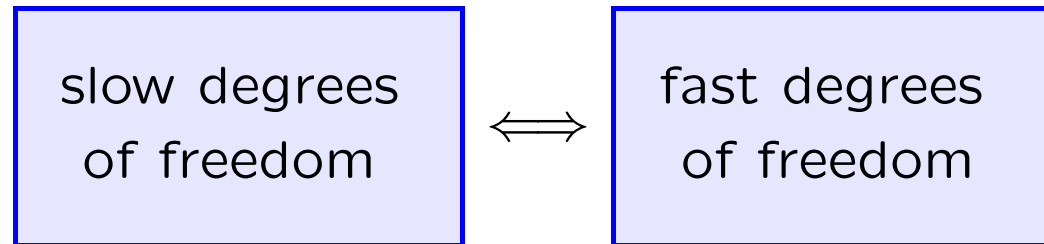
IMA Tutorial:

Fundamentals of chemical dynamics simulations

11. January 2009

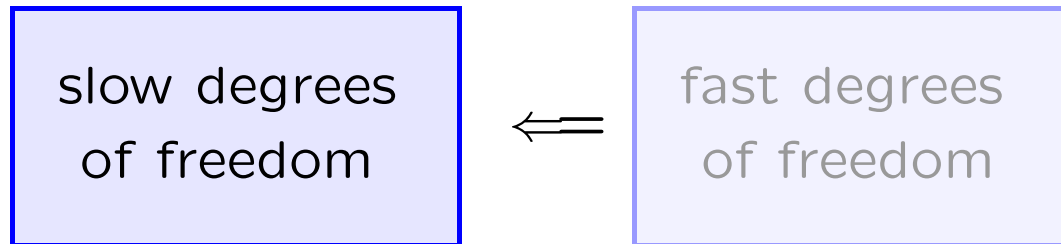
## *0. Basic principle: adiabatic decoupling*

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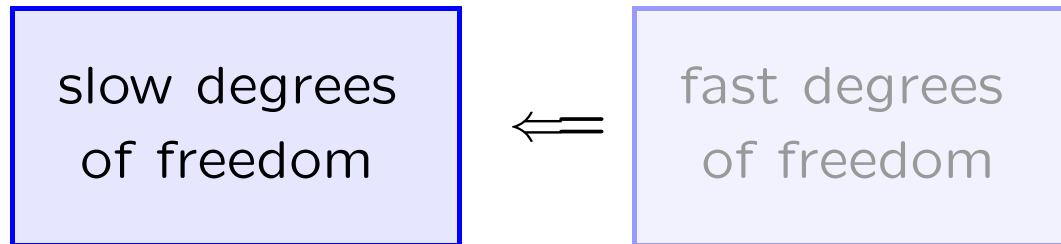


**Goal: Effective equations of motion only for the slow variables**

⇒ Reduction of complexity in large systems.

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⇒ Reduction of complexity in large systems.



Example: Spinning top

Slow degree of freedom = rotation axis

Fast degree of freedom = rotation angle

## *0. Examples in quantum dynamics*

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- **Molecules:**

slow nuclei  $\Leftrightarrow$  fast electrons

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- **Strong constraining forces:**

slow motion tangent to  
the constraint manifold

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fast motion normal to  
the constraint manifold

## *0. Contents of my lectures*

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### **1. Time-dependent quantum mechanics:**

A crash course and some remarks on composite systems

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### **2. Adiabatic decoupling and the partial semiclassical limit:**

The time-dependent Born-Oppenheimer approximation

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### **1. Time-dependent quantum mechanics:**

A crash course and some remarks on composite systems

### **2. Adiabatic decoupling and the partial semiclassical limit:**

The time-dependent Born-Oppenheimer approximation

### **3. Adiabatic perturbation theory:**

General slow-fast systems

## 1. Time-dependent quantum mechanics

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### 1. State space:

The state space of a quantum system is a complex

Hilbert space  $\mathcal{H}$ ,

i.e., a complex vector space with an inner product  $\langle \cdot, \cdot \rangle$ . The inner product induces a norm

$$\|\psi\| = \sqrt{\langle \psi, \psi \rangle}.$$

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### **Examples:**

For a single spinless particle moving in  $\mathbb{R}^3$  the state space is

$$\mathcal{H} = L^2(\mathbb{R}^3) := \left\{ \psi : \mathbb{R}^3 \rightarrow \mathbb{C} \mid \|\psi\|^2 = \int_{\mathbb{R}^3} |\psi(x)|^2 dx < \infty \right\}$$

with inner product

$$\langle \psi, \phi \rangle = \int_{\mathbb{R}^3} \psi(x)^* \phi(x) dx.$$

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### **Examples:**

For  $N$  distinguishable spinless particles moving in  $\mathbb{R}^3$  the state space is

$$\mathcal{H} = L^2(\mathbb{R}^{3N}) := \left\{ \psi : \mathbb{R}^{3N} \rightarrow \mathbb{C} \mid \|\psi\|^2 = \int_{\mathbb{R}^{3N}} |\psi(x)|^2 dx < \infty \right\}$$

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For a single spin- $\frac{1}{2}$  degree of freedom the state space is

$$\mathcal{H} = \mathbb{C}^2 = \{ \psi = (\psi_1, \psi_2) \mid \psi_1, \psi_2 \in \mathbb{C} \}$$

with the inner product

$$\langle \psi, \phi \rangle = \sum_{j=1}^2 \psi_j^* \phi_j.$$

## 1. Time-dependent quantum mechanics

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For composite systems the Hilbert space of the full system is obtained as the **tensor product** denoted by “ $\otimes$ ” of the subsystem Hilbert spaces.

### Examples:

Two single particles  $\Rightarrow$

$$\psi(x) \text{ “+” } \phi(y)$$

System of two particles

$$(\psi \otimes \phi)(x, y) = \psi(x)\phi(y)$$

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$$L^2(\mathbb{R}^3) \text{ “+” } L^2(\mathbb{R}^3)$$

$$L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) \cong L^2(\mathbb{R}^6) \cong L^2(\mathbb{R}^3, L^2(\mathbb{R}^3))$$

A generic function in  $L^2(\mathbb{R}^6)$  is just a square integrable function  $\Psi(x, y)$  of two variables in  $\mathbb{R}^3$ .

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A generic function in  $L^2(\mathbb{R}^6)$  is just a square integrable function  $\Psi(x, y)$  of two variables in  $\mathbb{R}^3$ .

Hence not all functions in  $L^2(\mathbb{R}^6)$  are given by products  $\Psi(x, y) = \psi(x)\phi(y)$ . But they can always be approximated by linear combinations of products.

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$$\Psi(x) = \begin{pmatrix} \Psi_1(x) \\ \Psi_2(x) \end{pmatrix}.$$

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Sometimes it is convenient to write

$$\Psi(j, x) = \Psi_j(x),$$

where  $j = 1, 2$ .

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For composite systems the Hilbert space of the full system is obtained as the **tensor product** denoted by “ $\otimes$ ” of the subsystem Hilbert spaces.

### Examples:

$N$  single spin- $\frac{1}{2}$  particles  $\Rightarrow$  System of  $N$  spin- $\frac{1}{2}$  particles

$$L^2(\mathbb{R}^3, \mathbb{C}^2)^{\otimes N} \cong L^2(\mathbb{R}^3)^{\otimes N} \otimes (\mathbb{C}^2)^{\otimes N} \cong L^2(\mathbb{R}^{3N}) \otimes \mathbb{C}^{2^N} \cong L^2(\mathbb{R}^{3N}, \mathbb{C}^{2^N})$$

A generic function in  $L^2(\mathbb{R}^{3N}, \mathbb{C}^{2^N})$  is of the form

$$\Psi(x) = \begin{pmatrix} \Psi_1(x_1, \dots, x_N) \\ \vdots \\ \Psi_{2^N}(x_1, \dots, x_N) \end{pmatrix},$$

where again it is convenient to write

$$\Psi_j(x) = \Psi(j_1, \dots, j_N, x_1, \dots, x_N)$$

with  $j_k = 1, 2$  and  $x_k \in \mathbb{R}^3$ .

## 1. Time-dependent quantum mechanics

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### 2. Physical interpretation:

If the state of the  $N$ -particle system is  $\Psi(j, x)$ , then the **probability** that the particles have a configuration  $X = (X_1, \dots, X_N)$  in a region  $\Lambda \subset \mathbb{R}^{3N}$  of configuration space  $\mathbb{R}^{3N}$  is

$$\mathcal{P}(X \in \Lambda) = \sum_{j=1}^{2^N} \int_{\Lambda} |\Psi(j, x)|^2 dx .$$

This is called **Born's statistical interpretation** or postulate.

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Everything else (other observables etc.) follows from this postulate, the collapse postulate and an analysis of the dynamics.

## 1. Time-dependent quantum mechanics

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### 3. Dynamics of states:

In general the state of a system changes with time. The dynamics for the time-dependent state  $\Psi(t)$  is determined by the **time-dependent Schrödinger equation**

$$i\frac{d}{dt}\Psi(t) = H\Psi(t).$$

Here  $H$  is a linear mapping

$$H : \mathcal{H} \supset D \rightarrow \mathcal{H}$$

the so called Hamilton operator or **Hamiltonian**.

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The exponential  $e^{-itH}$  of the Hamiltonian is called the **propagator** and defines a unitary evolution group

$$\|e^{-itH}\psi\| = \|\psi\|.$$

## 1. Time-dependent quantum mechanics

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### Examples:

- For a spin- $\frac{1}{2}$  in a magnetic field  $B$  the Hamiltonian  $H : \mathbb{C}^2 \rightarrow \mathbb{C}^2$  is the complex  $2 \times 2$ -matrix

$$H = B \cdot \sigma = B_x \sigma_x + B_y \sigma_y + B_z \sigma_z,$$

where  $\sigma = (\sigma_x, \sigma_y, \sigma_z)$  is the vector of Pauli matrices.

The propagator is given by the convergent power series

$$e^{-itH} = \sum_{n=0}^{\infty} \frac{(-itH)^n}{n!}.$$

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- For a single non-relativistic charged particle of mass  $m$  moving in a potential  $V : \mathbb{R}^3 \rightarrow \mathbb{R}$  the Hamiltonian  $H : L^2(\mathbb{R}^3) \supset D \rightarrow L^2(\mathbb{R}^3)$  is the differential operator

$$H = -\frac{1}{2m} \Delta + V(x, y, z)$$

with the Laplace operator  $\Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ .

## 1. Time-dependent quantum mechanics

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### Example: Molecules

$N_n$  nuclei, each with mass  $M$

( $N_n = 3$  for  $\text{CO}_2$ )

$N_e$  electrons, mass  $m$

( $N_e = 22$  for  $\text{CO}_2$ )

The Hamiltonian is

$$H_{\text{mol}} = \sum_{j=1}^{N_n} \left( -\frac{1}{2M} \Delta_{x_j} \right) + \sum_{k=1}^{N_e} \left( -\frac{1}{2m} \Delta_{y_k} \right) + \\ + \sum_{i < j=1}^{N_n} \frac{Z_j Z_i}{|x_i - x_j|} + \sum_{k < l=1}^{N_e} \frac{1}{|y_k - y_l|} - \sum_{j=1}^{N_n} \sum_{k=1}^{N_e} \frac{Z_j}{|y_k - x_j|}$$

acting on

$$\mathcal{H} = L^2(\mathbb{R}^{3(N_n+N_e)}) \cong L^2(\mathbb{R}_x^{3N_n}) \otimes \underbrace{L^2(\mathbb{R}_y^{3N_e})}_{\mathcal{H}_e} \cong L^2(\mathbb{R}_x^{3N_n}, \mathcal{H}_e).$$

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## 1. Time-dependent quantum mechanics

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### Observation of Born and Oppenheimer (1928):

The small mass ratio

$$\frac{m}{M} \approx 10^{-4} \dots 10^{-5}$$

can be used as the parameter for an asymptotic expansion of the eigenvalues

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$$\varepsilon = \sqrt{\frac{m}{M}}$$

In atomic units ( $m = 1$ ) we have

$$H_{\text{mol}} = -\frac{\varepsilon^2}{2} \Delta_x + H_e(x) \quad \text{on} \quad \mathcal{H} = L^2(\mathbb{R}_x^{N_n}, \mathcal{H}_e)$$

with

$$H_e(x) = -\frac{1}{2} \Delta_y + V(x, y) \quad \text{on} \quad \mathcal{H}_e = L^2(\mathbb{R}_y^{3N_e}).$$

## 2. The time-dependent Born-Oppenheimer approximation

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If  $H_e(x)$  was real-valued instead of operator valued, then the limit  $\varepsilon \rightarrow 0$  for

$$i\varepsilon \frac{\partial}{\partial t} \Psi(t, x) = \left( -\frac{\varepsilon^2}{2} \Delta_x + H_e(x) \right) \Psi(t, x)$$

would just be the standard semiclassical limit.

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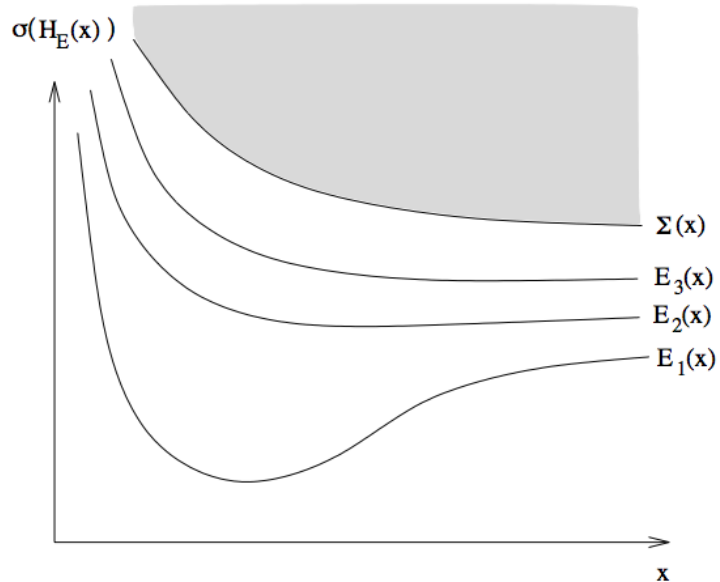
However, on eigenstates  $H_e(x)$  acts as a real-valued multiplication operator

$$H_e(x)\chi(x) = E(x)\chi(x).$$

## 2. The time-dependent Born-Oppenheimer approximation

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For a diatomic molecule a schematic picture of the spectral surfaces is



We consider an isolated eigenvalue surface  $E(x)$  with

$$H_e(x) \chi(x, y) = E(x) \chi(x, y)$$

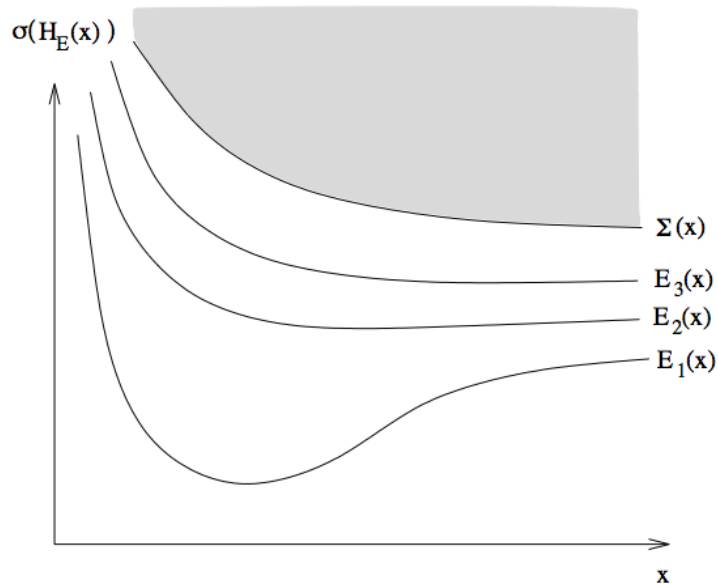
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Let  $P_E \mathcal{H} \subset \mathcal{H}$  be the subspace of functions of the form

$$\psi(x, y) = \phi(x) \chi(x, y), \quad \text{where } \phi \in L^2(\mathbb{R}^{3N_n}).$$

Then

$$H_e(x) P_E = E(x) P_E.$$

## 2. The time-dependent Born-Oppenheimer approximation

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The full Hamiltonian

$$H_{\text{mol}} = -\frac{\varepsilon^2}{2} \Delta_x + H_e(x)$$

acts on functions in  $P_E \mathcal{H}$  as

$$H_{\text{mol}} \phi(x) \chi(x, y) = \underbrace{\left[ \left( -\frac{\varepsilon^2}{2} \Delta_x + E(x) \right) \phi(x) \right]}_{\in P_E} \chi(x, y) + R^\varepsilon$$

with

$$R^\varepsilon = -\varepsilon (\varepsilon \nabla_x \phi(x)) \cdot \nabla_x \chi(x, y) + \frac{\varepsilon^2}{2} \phi(x) \Delta_x \chi(x, y) = \mathcal{O}(\varepsilon).$$

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Let

$$H_{\text{BO}} \phi(x) \chi(x, y) = \left[ \left( -\frac{\varepsilon^2}{2} \Delta_x + E(x) \right) \phi(x) \right] \chi(x, y)$$

be the effective “Born-Oppenheimer” Hamiltonian for the nuclei corresponding to the energy surface  $E(x)$  on the **adiabatic subspace**  $P_E \mathcal{H}$ .

## 2. The time-dependent Born-Oppenheimer approximation

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### The time-dependent Born-Oppenheimer approximation

For an initial wave function  $\Psi_0(x, y) = \phi_0(x)\chi(x, y) \in P_E$  solve the **effective Schrödinger equation** for the nucleonic wave function

$$i\varepsilon \frac{\partial}{\partial t} \phi(t, x) = \left( -\frac{\varepsilon^2}{2} \Delta_x + E(x) \right) \phi(t, x)$$

with initial value  $\phi(0, x) = \phi_0(x)$ .

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Now one expects that

$$\Psi_{\text{BO}}(t, x, y) = \phi(t, x)\chi(x, y)$$

is an approximate solution of the full Schrödinger equation

$$i\varepsilon \frac{\partial}{\partial t} \Psi(t, x, y) = \left( -\frac{\varepsilon^2}{2} \Delta_x + H_e(x) \right) \Psi(t, x, y).$$

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**Is this really correct?**

## 2. The time-dependent Born-Oppenheimer approximation

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Is this really correct? We checked that

$$(H - H_{\text{BO}})P_E = \mathcal{O}(\varepsilon),$$

but we don't know whether the true solution remains in the range of  $P_E$ .

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$$\|\Psi(t) - \Psi_{\text{BO}}(t)\| = \left\| \left( e^{-iH\frac{t}{\varepsilon}} - e^{-iH_{\text{BO}}\frac{t}{\varepsilon}} \right) \phi\chi \right\|$$

## 2. The time-dependent Born-Oppenheimer approximation

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## 2. The time-dependent Born-Oppenheimer approximation

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So a direct computation suggest that while  $H - H_{\text{BO}}$  is of order  $\varepsilon$  on  $P_E$  might add up to difference of order one over times of order  $1/\varepsilon$ .

## 2. The time-dependent Born-Oppenheimer approximation

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$$\begin{aligned}\|\Psi(t) - \Psi_{\text{BO}}(t)\| &= \frac{1}{\varepsilon} \left\| \int_0^t e^{iH\frac{s}{\varepsilon}} (H - H_{\text{BO}}) e^{-iH_{\text{BO}}\frac{s}{\varepsilon}} \phi_\chi \, ds \right\| \\ &= \frac{1}{\varepsilon} \left\| \int_0^t e^{iH\frac{s}{\varepsilon}} (P_E + P_E^\perp) (H - H_{\text{BO}}) e^{-iH_{\text{BO}}\frac{s}{\varepsilon}} \phi_\chi \, ds \right\| \\ &\leq \frac{1}{\varepsilon} \left\| \int_0^t e^{iH\frac{s}{\varepsilon}} (P_E H P_E - H_{\text{BO}}) e^{-iH_{\text{BO}}\frac{s}{\varepsilon}} \phi_\chi \, ds \right\| \\ &\quad + \frac{1}{\varepsilon} \left\| \int_0^t e^{iH\frac{s}{\varepsilon}} P_E^\perp H P_E e^{-iH_{\text{BO}}\frac{s}{\varepsilon}} \phi_\chi \, ds \right\|\end{aligned}$$

So we have to define  $H_{\text{BO}}$  such that

$$P_E H P_E - H_{\text{BO}} = \mathcal{O}(\varepsilon^2)$$

and to show that

$$\int_0^t e^{iH\frac{s}{\varepsilon}} P_E^\perp H P_E e^{-iH_{\text{BO}}\frac{s}{\varepsilon}} \phi_\chi \, ds = \mathcal{O}(\varepsilon).$$

## 2. The time-dependent Born-Oppenheimer approximation

---

If one includes  $P_E R^\varepsilon P_E$  in the effective Hamiltonian and defines

$$H_{\text{BO}} = \frac{\varepsilon^2}{2} \left( -i\nabla_x + A_{\text{B}}(x) \right)^2 + E(x)$$

with the Berry connection coefficient

$$A_{\text{B}}(x) = i \langle \chi(x), \nabla_x \chi(x) \rangle_{\mathcal{H}_e},$$

the following statement is true:

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the following statement is true:

### **Theorem:**

There is a constant  $C < \infty$  such that for all  $t \in \mathbb{R}$  and for all  $\phi(0) \in L^2(\mathbb{R}^{3N_n})$  with  $\Psi(0) = \phi(0)\chi \in \text{Ran } P_E \mathbf{1}(H \leq \mathcal{E})$  it holds that

$$\left\| \Psi^\varepsilon(t) - \Psi_{\text{BO}}^\varepsilon(t) \right\| \leq C \varepsilon (1 + \mathcal{E})(1 + |t|) \|\phi(0)\|.$$

[Spohn, Teufel; Commun. Math. Phys. **224** (2001)]

## 2. The time-dependent Born-Oppenheimer approximation

---

In particular this implies:

- Initial data in the subspace  $P_E\mathcal{H}$  will approximately remain in this subspace under the time evolution.  
⇒ One says that the subspace is adiabatically decoupled from the rest.

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- Within the decoupled subspace  $P_E\mathcal{H}$  the dynamics is much simpler: an approximate solution to the full Schrödinger equation for  $\Psi(0) = \phi(0)\chi$  is obtained by solving the effective equation for the nuclei

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- The effective equation is of the standard semiclassical form for  $\varepsilon \rightarrow 0$ . Thus one can use **standard semiclassical methods** to find approximate solutions of this effective equation.

## 2. The time-dependent Born-Oppenheimer approximation

---

Can one improve the result by choosing a better  $H_{\text{BO}}$ ? E.g. by adding the  $\mathcal{O}(\varepsilon^2)$  term from the expansion of  $P_E H P_E$  ?

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No, since the piece of the solution leaving  $P_E \mathcal{H}$  is of order  $\mathcal{O}(\varepsilon)$ , i.e.,

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Can one improve the adiabatic approximation at all?

Yes, by approximating the solution not on the adiabatic subspace  $P_E \mathcal{H}$ , but on suitable super-adiabatic subspaces!

### 3. *General structure of adiabatic problems*

---

#### 1. Hilbert space

$$\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_f = L^2(M) \otimes \mathcal{H}_f \cong L^2(M, \mathcal{H}_f)$$

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#### 2. Hamiltonian

$$H^\varepsilon = H(x, -i\varepsilon \nabla_x) := \text{Op}^W H$$

$H^\varepsilon$  is the Weyl-quantization of an operator-valued symbol

$$H : T^*M \rightarrow \mathcal{L}_{\text{sa}}(\mathcal{H}_f).$$

The symbol  $H(q, p)$  is the Hamiltonian for the fast system, when the slow system has configuration  $q$  and momentum  $p$ .

### 3. General structure of adiabatic problems

---

For molecular dynamics we had

**Hamiltonian:**

$$H_{\text{mol}}^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x + H_e(x) \quad \text{on} \quad L^2(\mathbb{R}_x^{3N_n}, L^2(\mathbb{R}_y^{3N_e}))$$

**Symbol:**

$$H_{\text{mol}}(q, p) = \frac{1}{2}p^2 + H_e(q)$$

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#### 3. Spectral gap

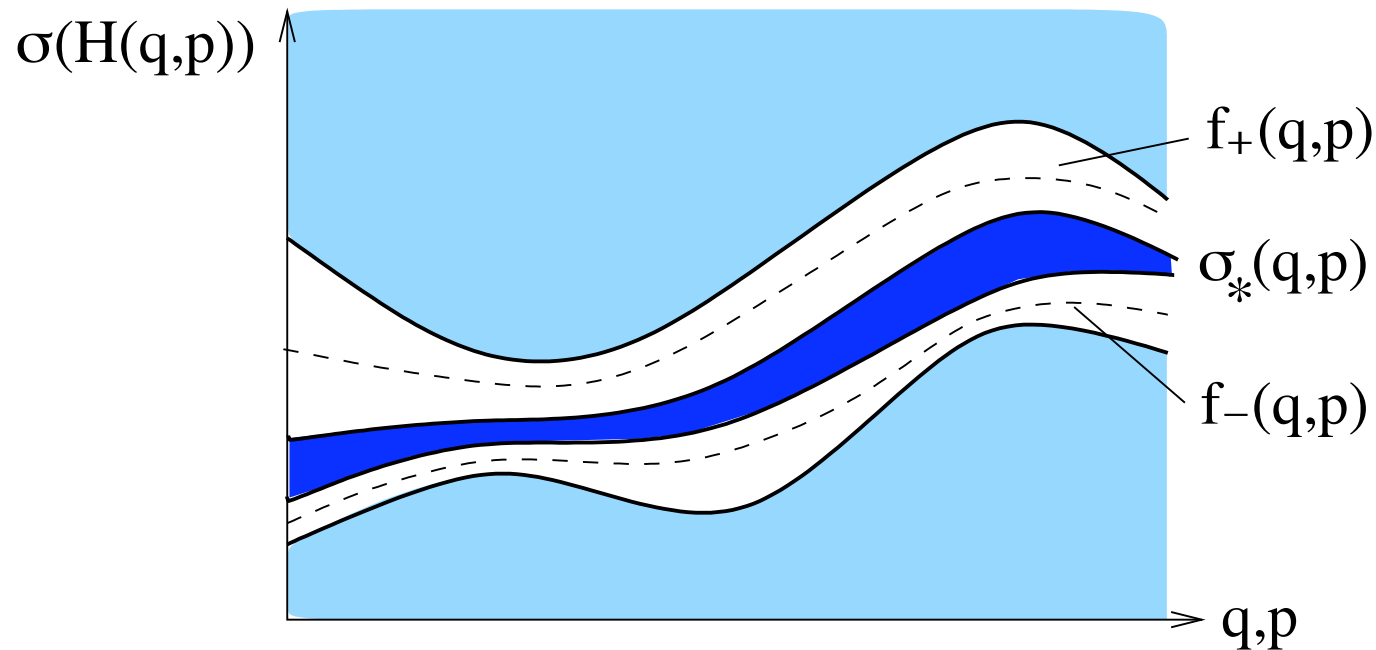
The spectrum  $\sigma(H(q, p))$  contains a subset  $\sigma_*(q, p)$ , which is separated by a **gap** from the remainder  $\sigma(H(q, p)) \setminus \sigma_*(q, p)$  for all  $(q, p) \in T^*M$ .

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### 3. Adiabatic perturbation theory: results

---

#### 1. Approximately invariant subspaces

Let  $P_*(q, p)$  be the spectral projection of  $H(q, p)$  corresponding to  $\sigma_*(q, p)$ . Then one can construct an orthogonal projection  $P_N^\varepsilon$  such that

$$\| [H^\varepsilon, P_N^\varepsilon] \| = \mathcal{O}(\varepsilon^{N+1})$$

and

$$\| P_N^\varepsilon - \text{Op}^W P_* \| = \mathcal{O}(\varepsilon).$$

Thus the subspace  $\text{Ran } P_N^\varepsilon \subset \mathcal{H}$  is invariant under the time-evolution up to  $\mathcal{O}(\varepsilon^N)$ .

[based on Emrlich, Weinstein '96 and Martinez, Nenciu, Sordani '01]

### 3. Adiabatic perturbation theory: results

---

## 2. Transformation to a simple representation space

The subspace  $P_N^\varepsilon \mathcal{H}$  of the big space  $\mathcal{H}$  depends on  $\varepsilon$  and its elements can not be easily characterized.

$\Rightarrow$  We construct a unitary operator  $U_N^\varepsilon$ , which maps the almost invariant subspace to a space appropriate for representing the slow degrees of freedom:

$$U_N^\varepsilon : P_N^\varepsilon \mathcal{H} \rightarrow \mathcal{K} = L^2(M, \mathcal{K}_f).$$

If  $\dim(\text{Ran} P_*(q, p)) = n < \infty$ , then  $\mathcal{K}_f = \mathbb{C}^n$ .

### *3. Adiabatic perturbation theory: results*

---

### 3. The effective Hamiltonian

$$H_{\text{eff}}^\varepsilon := H^\varepsilon$$

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#### 3. The effective Hamiltonian

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In summary we thus have

$$\left\| \left( e^{-iH^\varepsilon t/\varepsilon} - U_N^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t/\varepsilon} U_N^\varepsilon \right) P_N^\varepsilon \right\| = \mathcal{O}(\varepsilon^N |t|).$$

### 3. Adiabatic perturbation theory: results

---

#### 4. Asymptotic expansion of $H_{\text{eff}}^\varepsilon$

$$H_{\text{eff}}^\varepsilon = \text{Op}^W H_{\text{eff}}(\varepsilon)$$

with

$$H_{\text{eff}}(\varepsilon, q, p) \asymp \sum_{n=0}^{\infty} \varepsilon^n h_n(q, p).$$

The effective Hamiltonian  $H_{\text{eff}}^\varepsilon$  must be computed up to order  $\varepsilon^{N+1}$  to obtain an approximation to  $e^{-iH_{\text{eff}}^\varepsilon t/\varepsilon}$  up to order  $\varepsilon^N$ .

### 3. Adiabatic perturbation theory: results

---

#### 5. Important special case: isolated eigenvalue

Let  $\sigma_*(q, p) = \{E(q, p)\}$  be  $\ell$ -times degenerate.

Then the natural representation space is  $\mathcal{K} = L^2(M; \mathbb{C}^\ell)$ . One finds that

$$h_0(q, p) = E(q, p) \mathbf{1}_{\mathbb{C}^\ell},$$

which is known in physics as “Peierls substitution”.

### 3. Adiabatic perturbation theory: results

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which is known in physics as “Peierls substitution”.

The first correction to “Peierls’ substitution” is

$$h_1(q, p)_{\alpha\beta} = -\frac{i}{2} \left\langle \psi_\alpha(q, p), \{ (H(q, p) - E(q, p) \mathbf{1}_{\mathcal{H}_f}), \psi_\beta(q, p) \} \right\rangle_{\mathcal{H}_f},$$

where  $\{\psi_\alpha(q, p)\}_{\alpha=1}^\ell$  is an orthonormal basis of  $P_*(q, p)\mathcal{H}_f$ .

### 3. Adiabatic perturbation theory: results

---

For the **Born-Oppenheimer approximation** one finds

$$\begin{aligned} H_{\text{BO}}(q, p) &= \frac{1}{2} (p + \varepsilon A_{\text{B}}(q))^2 + E(q) \\ &+ \frac{\varepsilon^2}{2} \text{Tr}_{\mathcal{H}_e} \left( \nabla P_*(q) \cdot \nabla P_*(q) (1 - P_*(q)) \right) \\ &- \varepsilon^2 \text{Tr}_{\mathcal{H}_e} \left( (p \cdot \nabla P_*(q))^2 (H_e(q) - E(q))^{-1} (1 - P_*(q)) \right) \\ &+ \mathcal{O}(\varepsilon^3). \end{aligned}$$

### *3. Other applications*

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- **Solid State Physics:**

Peierls substitution and the semiclassical model of solids including new corrections, Piezo effect

(with G. Panati, H. Spohn, C. Sparber)

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Effective dynamics for slow charged particles ← no spectral gap

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(with L. Tenuta)

- **Constraints in Quantum Dynamics:**

Effective dynamics on constraint manifolds

(with J. Wachsmuth)

### *3. Beyond the adiabatic approximation*

---

- In the presence of (nontrivial) eigenvalue crossings, e.g. conical crossings, the adiabatic approximation breaks down.  
⇒ Quantitative description of transitions between adiabatic subspaces near crossings  
(with C. Lasser)

### 3. *Beyond the adiabatic approximation*

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- In the presence of (nontrivial) eigenvalue crossings, e.g. conical crossings, the adiabatic approximation breaks down.  
⇒ Quantitative description of transitions between adiabatic subspaces near crossings  
(with C. Lasser)
  
- Even in the presence of a spectral gap, the adiabatic subspaces are approximately but **not** exactly invariant.  
However, the transitions are exponentially small with respect to  $\varepsilon$ , i.e. of order  $e^{-c/\varepsilon}$  for some  $c > 0$ .  
⇒ beyond perturbation theory  
(with V. Betz)

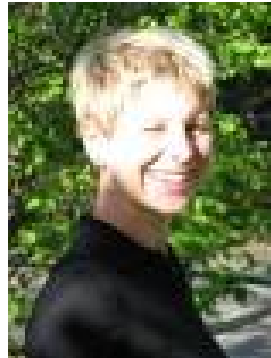
### 3. The end

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Thank you for listening and thanks to my collaborators



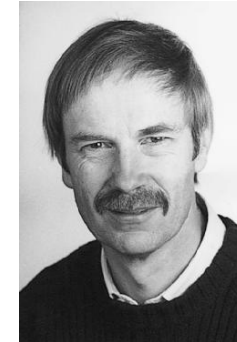
Volker Betz  
(Warwick)



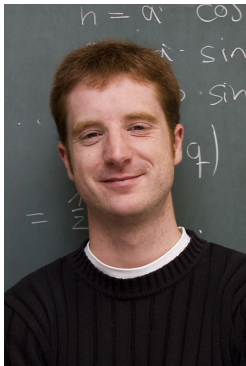
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