

Adiabatic theorems in quantum mechanics

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Mathematical Challenges in Quantum Mechanics

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based on joint works with

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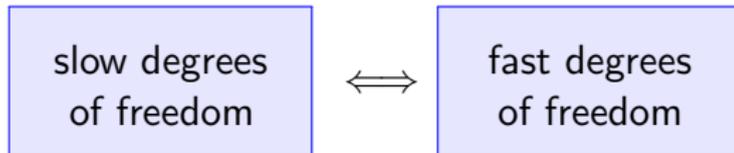
Disclaimer

These are the slides of a six hours course given at the winter school on “Mathematical Challenges in Quantum Mechanics” at La Sapienza, Rome, in February 2018.

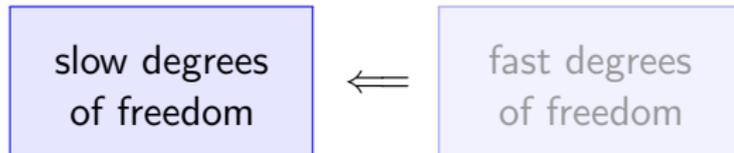
The course starts with an elementary introduction to basic ideas and concepts of adiabatic theorems in quantum mechanics, without trying to be historically accurate. In particular, the version of Kato's adiabatic theorem I present in section 1 is not really Kato's theorem, but includes ideas and aspects developed later on by many groups, including *Avron, Nenciu, Seiler, Simon* and many others. Also the super-adiabatic theorem of section 3 is a merger of different approaches and reflects my own view on the adiabatic problem today.

Apart from the extended introduction, the course is almost exclusively focussed on the time-adiabatic problem, i.e. the adiabatic limit of Hamiltonians depending slowly on time. The space-adiabatic problem is only touched upon in the very last section. There are also many further aspects of adiabatic theory that are mentioned only briefly or not at all and the list of references is certainly far from complete.

0. Basic principle: adiabatic decoupling



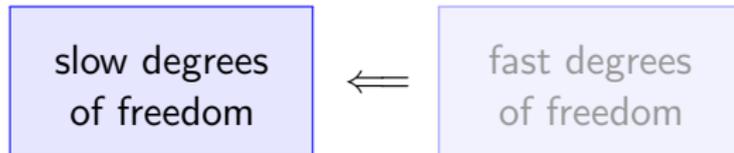
0. Basic principle: adiabatic decoupling



Goal: Effective equations of motion only for the slow variables

- ⇒ Reduction of complexity in large systems.
- ⇒ Simple and explicit formulas for certain quantities.

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Example: Spinning top

Slow degree of freedom = rotation axis

Fast degree of freedom = rotation angle

0. Basic principle: adiabatic decoupling

▶ **Spins in an external field:**

slow variation of
the external field



fast spin
oscillations

▶ **Molecules:**

slow nuclei \Leftrightarrow fast electrons

▶ **Charged particles in the radiation field:**

slow particles \Leftrightarrow fast photons

▶ **Electrons in a crystal:**

slow macroscopic
dynamics



fast dynamics on the
scale of the lattice

▶ **Strong constraining forces:**

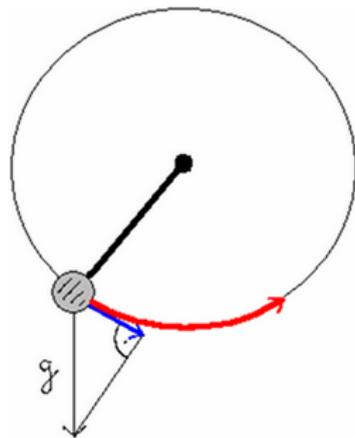
slow motion tangent to
the constraint manifold



fast motion normal to
the constraint manifold

0. Example: Realising constraints

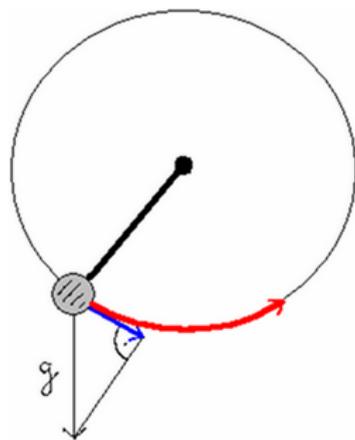
Stiff pendulum



configuration space = circle

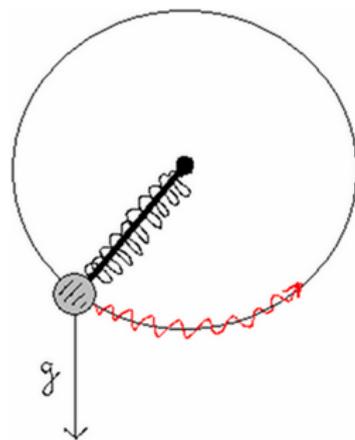
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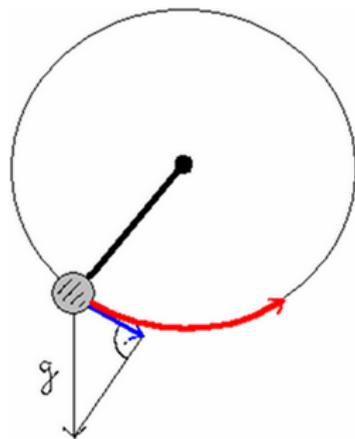
spring pendulum



configuration space = \mathbb{R}^2

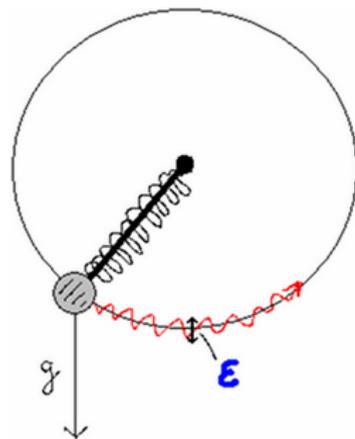
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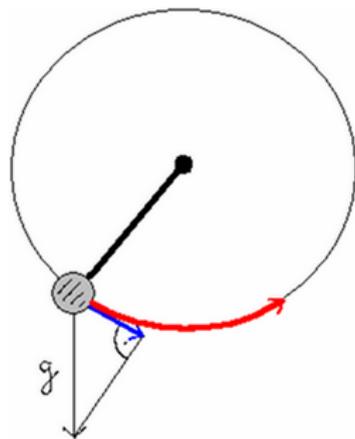
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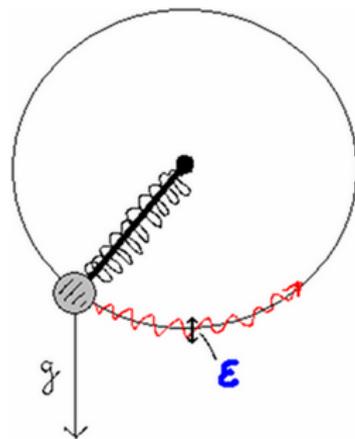
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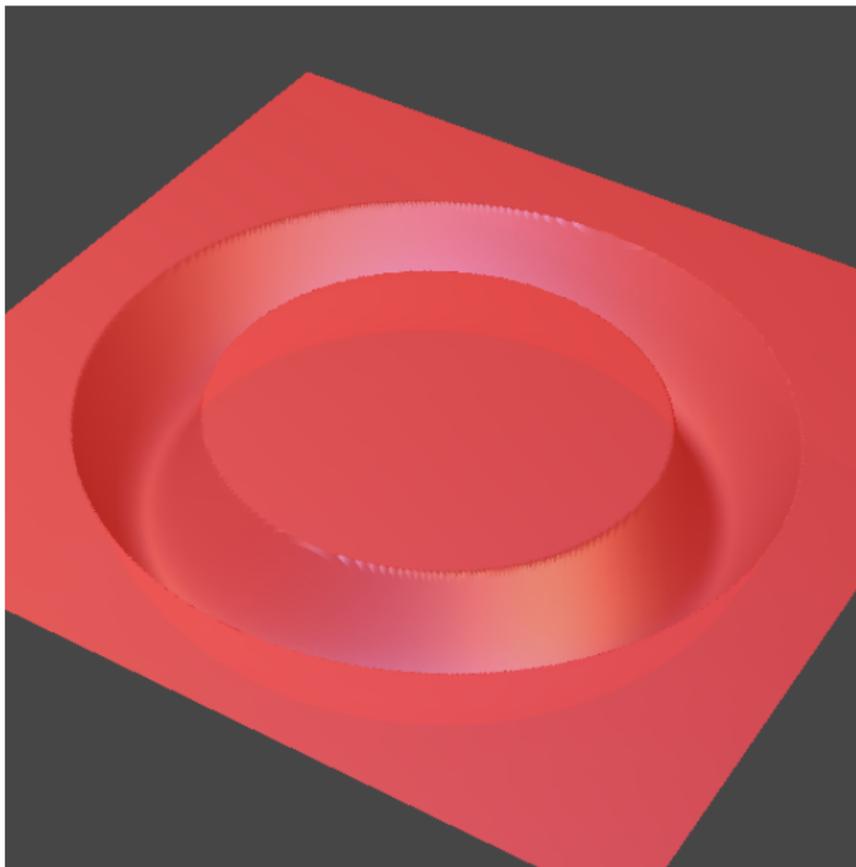
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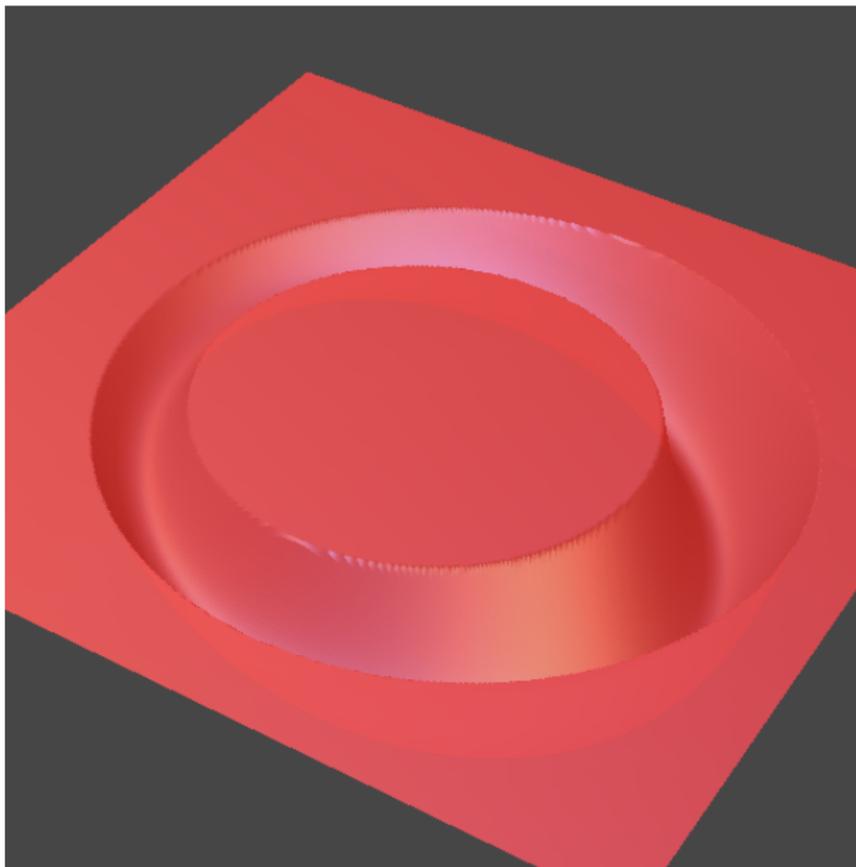
configuration space = \mathbb{R}^2

$\epsilon \rightarrow 0$
?

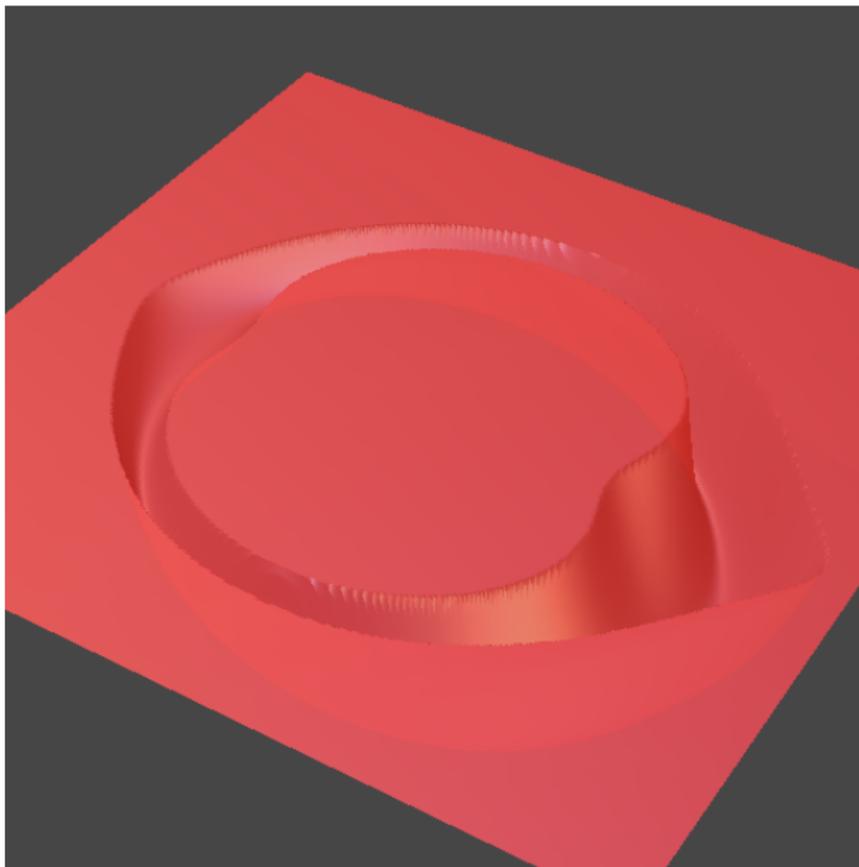
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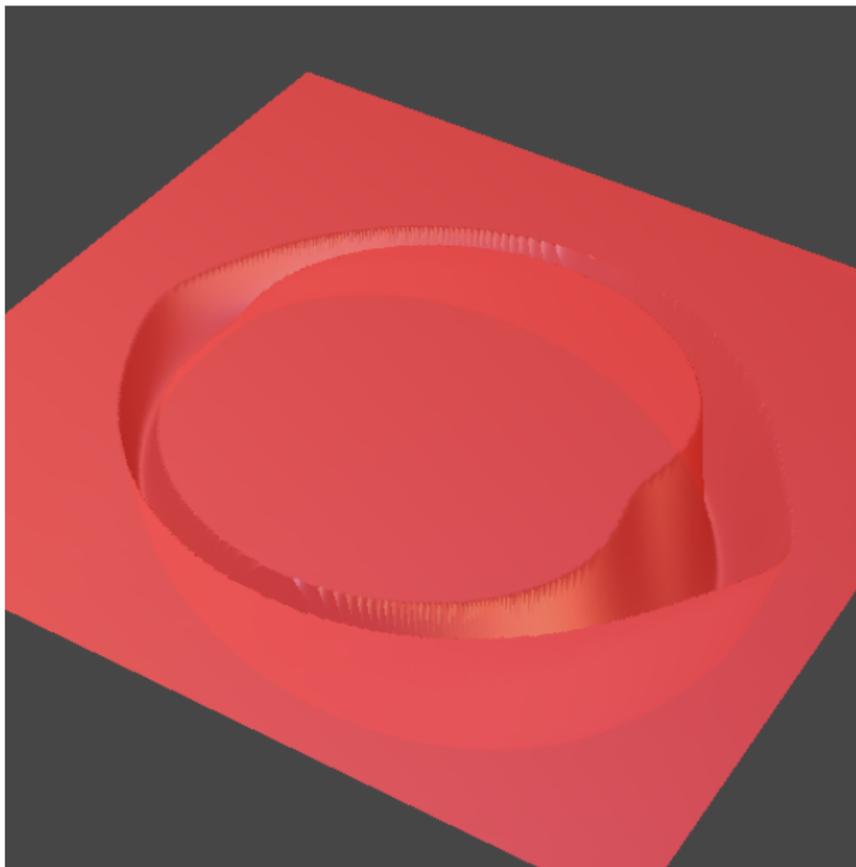
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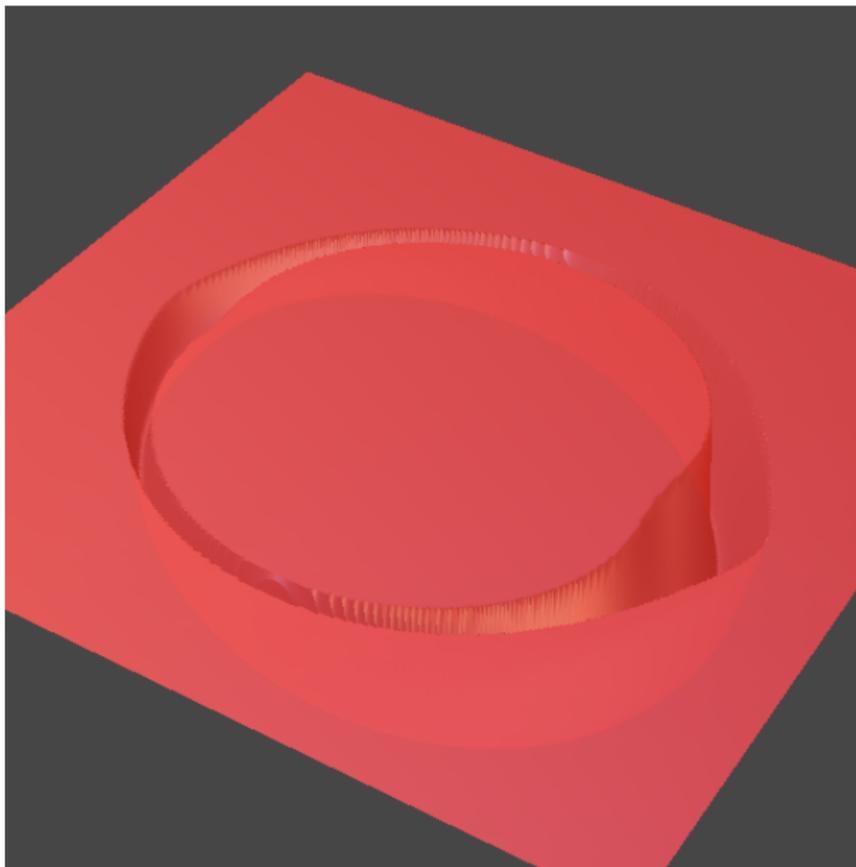
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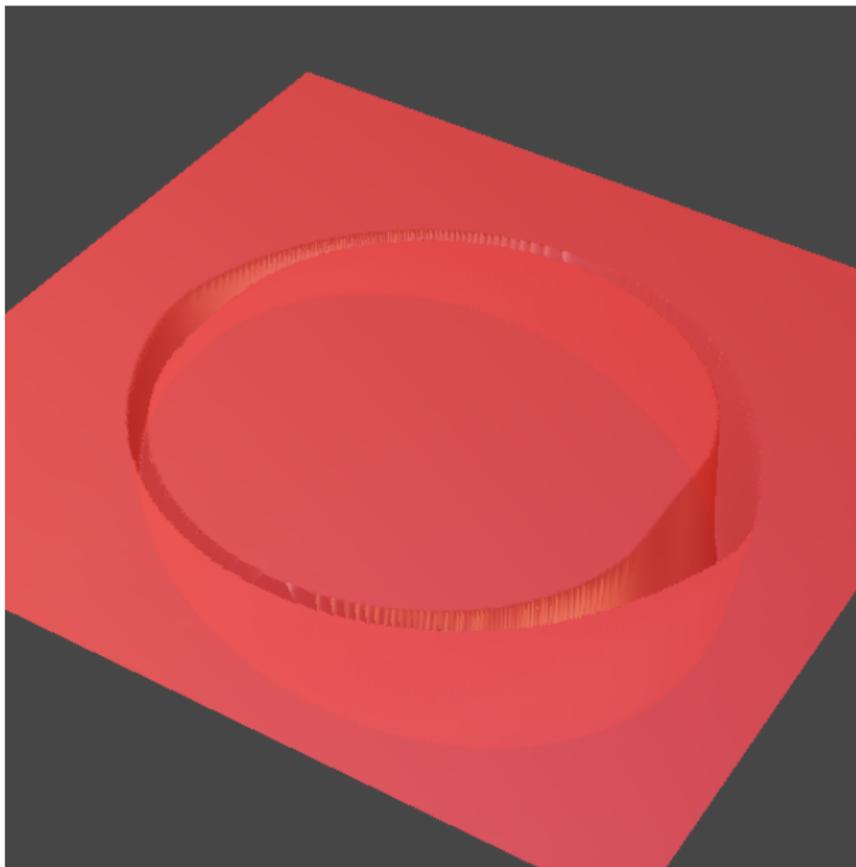
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In the following we look at the **model problem**

$$V(x, \frac{y}{\varepsilon}) = -\frac{x^2}{2} + \frac{\omega(x)^2}{2} \left(\frac{y}{\varepsilon}\right)^2$$

for $\varepsilon = \frac{1}{5}$ with

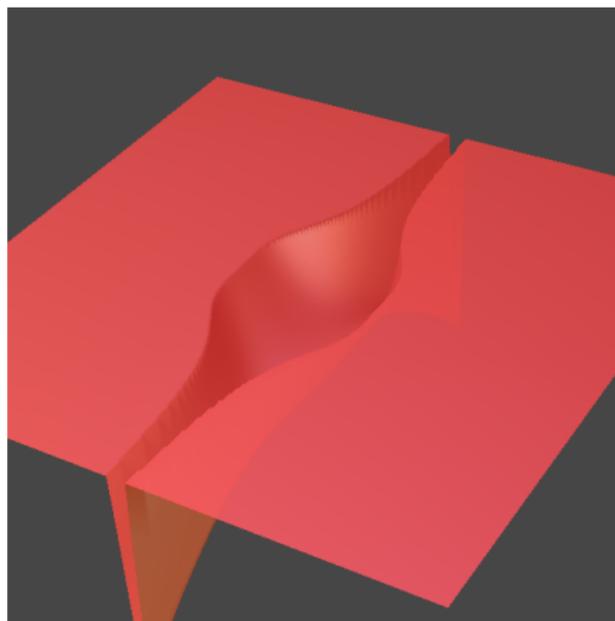
$$\omega(x) = \sqrt{2(1+x^4)}.$$

Newton's law

$$\ddot{q}(t) = -\nabla V(q(t))$$

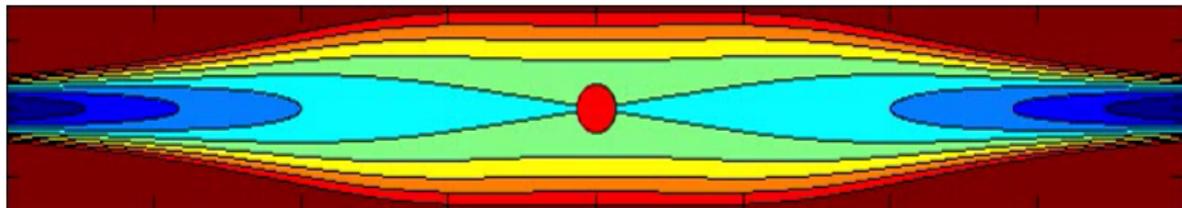
Schrödinger equation

$$i\partial_t\psi(t, q) = -\frac{1}{2}\Delta_q\psi(t, q) + V(q)\psi(t, q)$$



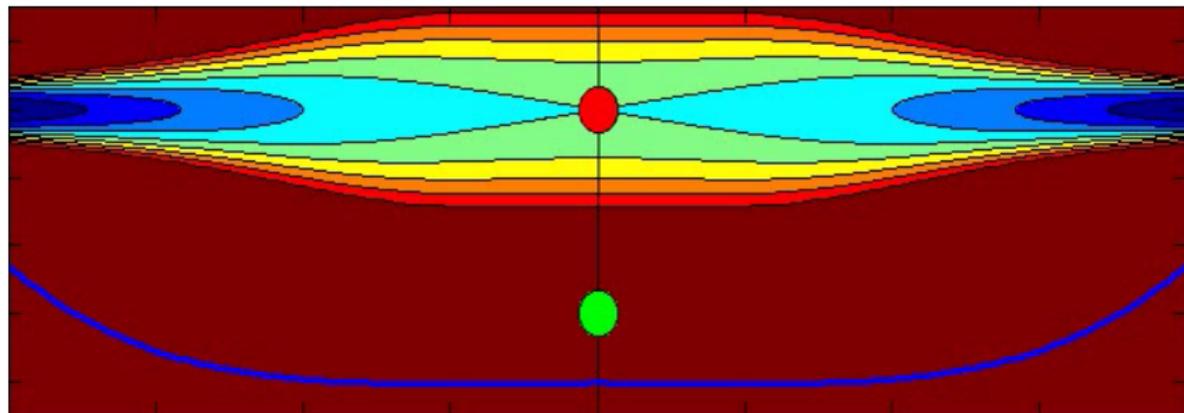
0. Example: Realising constraints

Classical motion in 2d-pot. $V(x, \frac{y}{\epsilon}) = -\frac{x^2}{2} + \frac{\omega(x)^2}{2} (\frac{y}{\epsilon})^2$ for $\epsilon = \frac{1}{5}$.



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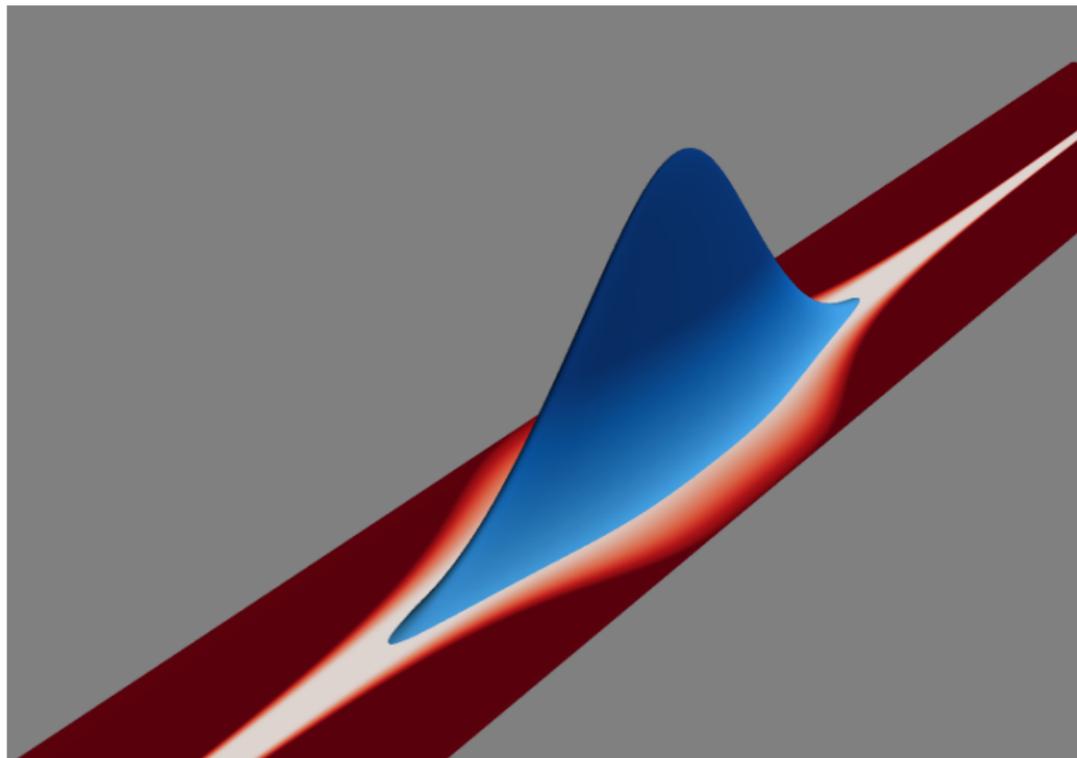
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Classical motion in the 1d-potential $V(x) = -\frac{x^2}{2} + I_0 \omega(x)$ obtained from “adiabatic invariance” of the action $\frac{E(x)}{\omega(x)}$ in the normal mode.

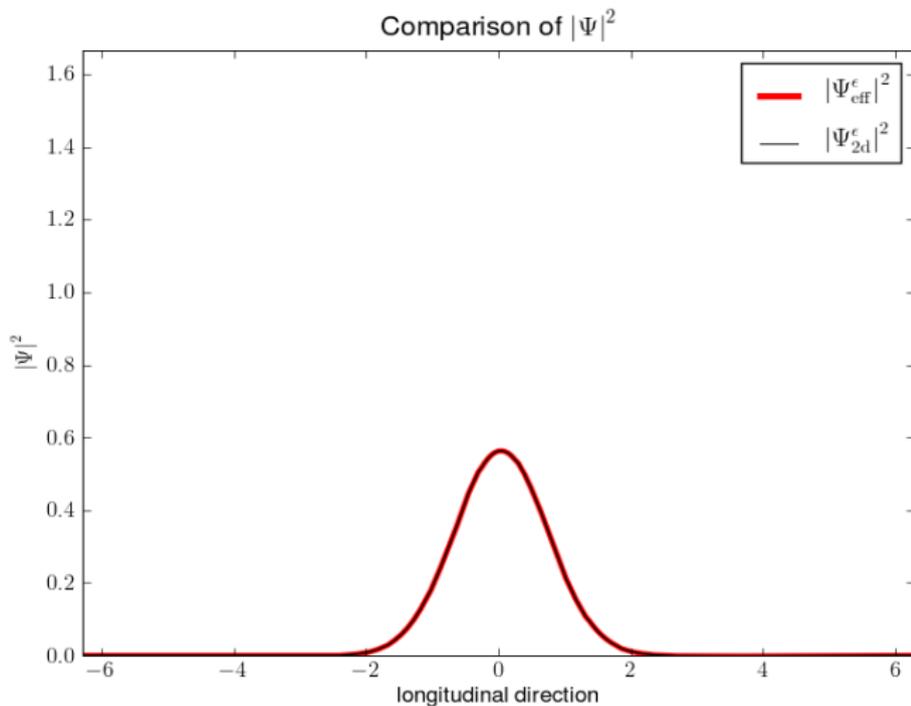
0. Example: Realising constraints

Schrödinger eq. in $2d$ -pot. $V(x, \frac{y}{\varepsilon}) = -\frac{x^2}{2} + \frac{\omega(x)^2}{2} (\frac{y}{\varepsilon})^2$ for $\varepsilon = \frac{1}{5}$.



0. Example: Realising constraints

Comparison with the solution of an effective 1d-Schrödinger equation with potential $V(x) = -\frac{x^2}{2} + \frac{\omega(x)}{2}$ obtained from the ground state energy $\frac{\omega(x)}{2}$ of the normal mode.



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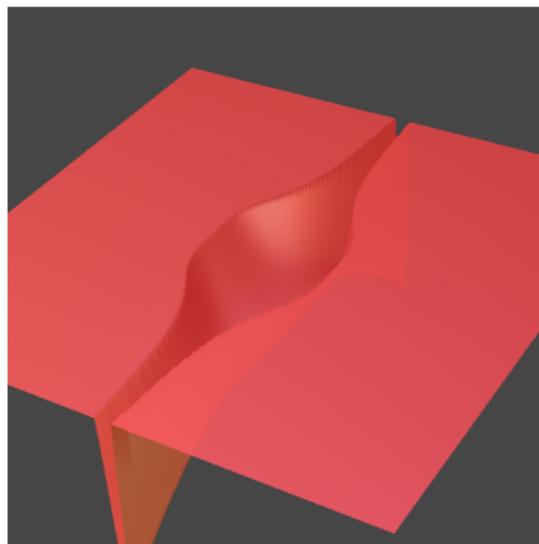
The Schrödinger operator on \mathbb{R}^2 with confining potential reads

$$H = -\frac{d^2}{dx^2} - \frac{d^2}{dy^2} + \frac{1}{\varepsilon^2} V\left(x, \frac{y}{\varepsilon}\right) \quad \text{on} \quad L^2(\mathbb{R}_{x,y}^2).$$

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Multiplying by ε^2 and substituting $\tilde{y} = y/\varepsilon$ the Hamiltonian becomes

$$H^\varepsilon = -\varepsilon^2 \frac{d^2}{dx^2} - \frac{d^2}{d\tilde{y}^2} + V(x, \tilde{y}) =: -\varepsilon^2 \frac{d^2}{dx^2} + H_f(x).$$

Here

$$H_f(x) = -\frac{d^2}{d\tilde{y}^2} + V(x, \tilde{y}) \quad \text{on} \quad L^2(\mathbb{R}_{\tilde{y}})$$

is the Hamiltonian for the fast degree of freedom \tilde{y} at fixed slow configuration x .

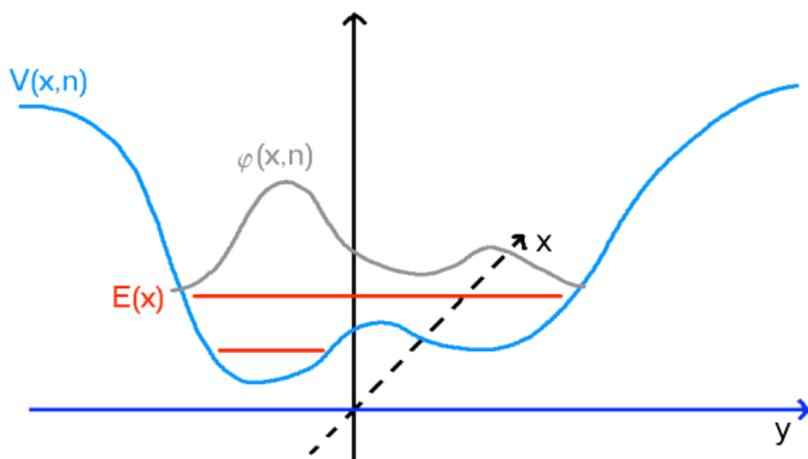
0. Example: Realising constraints

$$H_f(x) = -\frac{d^2}{d\tilde{y}^2} + V(x, \tilde{y}) \quad \text{on } L^2(\mathbb{R}_{\tilde{y}})$$

Assume that $H_f(x)$ has a normalized eigenfunction $\varphi_E(x, \tilde{y})$,

$$H_f(x) \varphi_E(x, \cdot) = E(x) \varphi_E(x, \cdot),$$

corresponding to an eigenvalue $E(x)$.



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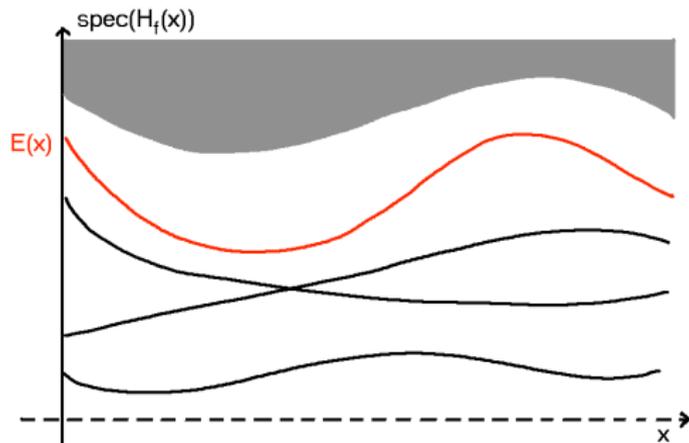
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Assume that $E(x)$ satisfies a **global gap condition**:



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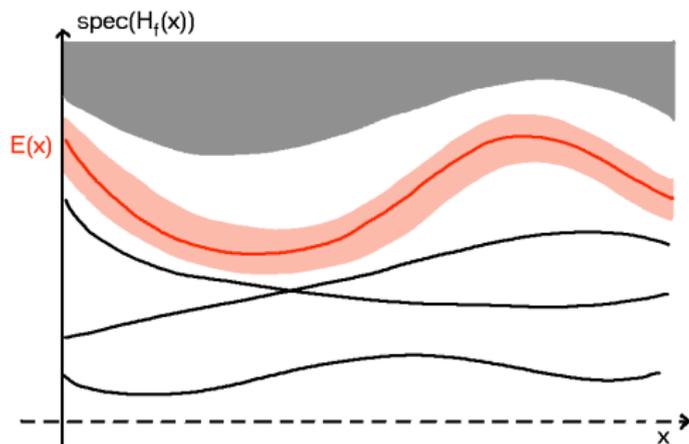
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0. Example: Realising constraints

Since for $\Psi(x, y) := \psi(x)\varphi_E(x, y)$

$$(H^\varepsilon \Psi)(x, y) = \left(-\varepsilon^2 \frac{d^2}{dx^2} + H_f(x) \right) \psi(x)\varphi_E(x, y)$$

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one expects that the subspace

$$\mathcal{P}_E := \{\psi(x)\varphi_E(x, y) \mid \psi \in L^2(\mathbb{R}_x)\} \subset L^2(\mathbb{R}_{x,y}^2)$$

is approximately invariant under the dynamics of H^ε and that for initial data $\Psi_0^\varepsilon = \psi_0^\varepsilon \varphi_E$ in \mathcal{P}_E the solution satisfies

$$\Psi^\varepsilon(t, x, y) = \left(e^{-iH^\varepsilon t} \Psi_0^\varepsilon\right)(x, y) \approx \left(e^{-iH_{\text{eff}}^\varepsilon t} \psi_0^\varepsilon\right)(t, x) \varphi_E(x, y).$$

0. Example: Realising constraints

To determine $H_{\text{eff}}^\varepsilon$ we project in

$$\begin{aligned} (H^\varepsilon \psi^\varepsilon \varphi_E)(x, y) &= \left[\left(-\varepsilon^2 \frac{d^2}{dx^2} + E(x) \right) \psi^\varepsilon(x) \right] \varphi_E(x, y) \\ &\quad - 2\varepsilon \left(\varepsilon \frac{d}{dx} \psi^\varepsilon(x) \right) \left(\frac{d}{dx} \varphi_E(x, y) \right) - \varepsilon^2 \psi^\varepsilon(x) \left(\frac{d^2}{dx^2} \varphi_E(x, y) \right), \end{aligned}$$

back onto \mathcal{P}_E ,

$$\begin{aligned} \langle \varphi(x), H^\varepsilon \psi^\varepsilon \varphi(x) \rangle_{L^2(\mathbb{R}_y)} &= \left(-\varepsilon^2 \frac{d^2}{dx^2} + E(x) \right) \psi^\varepsilon(x) \\ &\quad - 2\varepsilon \left(\varepsilon \frac{d}{dx} \psi^\varepsilon(x) \right) \langle \varphi(x), \varphi'(x) \rangle - \varepsilon^2 \psi^\varepsilon(x) \langle \varphi(x), \varphi''(x) \rangle \\ &=: \left(\left(i\varepsilon \frac{d}{dx} + \varepsilon A(x) \right)^2 + E(x) + \varepsilon^2 V(x) \right) \psi^\varepsilon(x) \\ &=: H_{\text{eff}}^\varepsilon \psi^\varepsilon(x). \end{aligned}$$

0. Example: Realising constraints

Hence,

$$H_{\text{eff}}^{\varepsilon} = \left(i\varepsilon \frac{d}{dx} + \varepsilon A(x) \right)^2 + E(x) + \varepsilon^2 V(x)$$

with the connection coefficient of the Berry connection

$$A(x) = i \langle \varphi(x), \varphi'(x) \rangle$$

and a potential term

$$V(x) = \langle \varphi'(x), (1 - P_E) \varphi'(x) \rangle,$$

which in the context of the Born-Oppenheimer approximation is called the Born-Huang potential.

0. Example: Realising constraints

Let

$$\mathcal{U}_E : \mathcal{P}_E \rightarrow L^2(\mathbb{R}_x), \quad \psi(x)\varphi_E(x, y) \mapsto \psi(x)$$

the bijective identification operator.

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$$H_{\text{diag}}^\varepsilon := P_E H^\varepsilon P_E = \mathcal{U}_E^* H_{\text{eff}}^\varepsilon \mathcal{U}_E.$$

In what sense and on which timescale is it true that

$$\left(e^{-iH^\varepsilon t} - \mathcal{U}_E^* e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}_E \right) P_E \xrightarrow{\varepsilon \rightarrow 0} 0 \quad ?$$

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Looking at

$$H_{\text{eff}}^\varepsilon = \left(i\varepsilon \frac{d}{dx} + \varepsilon A(x) \right)^2 + E(x) + \varepsilon^2 V(x)$$

suggests to look at solutions ψ^ε such that the kinetic energy

$$\left\| \varepsilon \frac{d}{dx} \psi^\varepsilon \right\|^2 = \mathcal{O}(1)$$

instead of

$$\left\| \varepsilon \frac{d}{dx} \psi^\varepsilon \right\|^2 = \mathcal{O}(\varepsilon^2).$$

0. Example: Realising constraints

Since $\varepsilon = m^{-1/2}$, such solutions propagate at a speed of order ε .

To see propagation over distances of order one, we have to wait for times of order $1/\varepsilon$, or look at the problem

$$\left(e^{-iH^\varepsilon t/\varepsilon} - \mathcal{U}_E^* e^{-iH_{\text{eff}}^\varepsilon t/\varepsilon} \mathcal{U}_E \right) P_E \xrightarrow{\varepsilon \rightarrow 0} 0 \quad ?$$

for finite times t .

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A simple Duhamel expansion shows that

$$\left(e^{-iH^\varepsilon \frac{t}{\varepsilon}} - e^{-iH_{\text{diag}}^\varepsilon \frac{t}{\varepsilon}} \right) P_E = -\frac{i}{\varepsilon} e^{-iH^\varepsilon \frac{t}{\varepsilon}} \int_0^t e^{iH^\varepsilon \frac{s}{\varepsilon}} (H^\varepsilon - H_{\text{diag}}^\varepsilon) P_E e^{-iH_{\text{diag}}^\varepsilon \frac{s}{\varepsilon}} ds$$

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Hence, there is something to prove in order to establish the validity of adiabatic approximations on relevant time-scales.

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$$\begin{aligned} \left(e^{-iH^\varepsilon \frac{t}{\varepsilon}} - e^{-iH_{\text{diag}}^\varepsilon \frac{t}{\varepsilon}} \right) P_E &= \\ &= -\frac{i}{\varepsilon} e^{-iH^\varepsilon \frac{t}{\varepsilon}} \int_0^t e^{iH^\varepsilon \frac{s}{\varepsilon}} \underbrace{\left[-\varepsilon^2 \frac{d^2}{dx^2}, P_E(x) \right]}_{\mathcal{O}(\varepsilon)} P_E e^{-iH_{\text{diag}}^\varepsilon \frac{s}{\varepsilon}} ds = \mathcal{O}(1). \end{aligned}$$

Hence, there is something to prove in order to establish the validity of adiabatic approximations on relevant time-scales.

In this course we will focus on the **time-adiabatic problem** and consider time-dependent Hamiltonians for the fast degrees of freedom only.

The time-dependence is slow and can be thought of as originating from a prescribed time-dependent configuration of the slow degree of freedom or just from slowly varying external fields/parameters in the Hamiltonian.

0. Plan of the course

1. A modern version of Kato's adiabatic theorem
2. Adiabatic theorems without spectral gap
3. Super-adiabatic approximations
4. Adiabatic currents in non-interacting fermion systems
5. Adiabatic theorems for extended interacting fermion systems on the lattice
6. The Kubo formula for the Hall conductance in interacting fermion systems on the lattice
7. Non-equilibrium almost stationary states for interacting fermion systems on the lattice

1. Kato's adiabatic theorem

Consider the time dependent Schrödinger equation

$$i \frac{d}{dt} \psi(t) = H \psi(t), \quad \psi(0) = \psi_0 \in \mathcal{H},$$

where H is a self-adjoint operator on \mathcal{H} with domain $D(H) \subset \mathcal{H}$.

Let P be a spectral projection of H , e.g. the orthogonal projection on the eigenspace of an eigenvalue E , then

$$[P, H] = 0.$$

Hence $\text{Ran}P \subset \mathcal{H}$ is an invariant subspace for H , i.e.

$$\psi_0 \in \text{Ran}P \quad \Rightarrow \quad \psi(t) = e^{-iEt} \psi_0 \in \text{Ran}P \quad \text{for all } t \in \mathbb{R},$$

or more compactly

$$[P, e^{-iHt}] = 0 \quad \text{for all } t \in \mathbb{R}.$$

What happens, if H and thus also P and E depend on t ?

1. Kato's adiabatic theorem

Now consider the time dependent Schrödinger equation

$$i \frac{d}{dt} \psi(t) = H(t) \psi(t), \quad \psi(0) = \psi_0 \in \mathcal{H},$$

with a time-dependent Hamiltonian $H(t)$ and $U(t, 0)$ the corresponding unitary evolution family, i.e.

$$i \frac{d}{dt} U(t, 0) = H(t) U(t, 0), \quad U(0, 0) = \mathbf{1}_{\mathcal{H}}.$$

Let $P(t)$ be the spectral projection of $H(t)$ corresponding to the eigenvalue $E(t)$, then again

$$[P(t), H(t)] = 0 \quad \text{for all } t \in \mathbb{R}.$$

Is it still true that

$$\psi_0 \in \text{Ran} P(0) \quad \Rightarrow \quad \psi(t) \in \text{Ran} P(t) \quad \text{for all } t \in \mathbb{R}$$

or, put differently, that

$$U(t, 0)^* P(t) U(t, 0) = P(0) \quad ?$$

No!

1. Kato's adiabatic theorem

Is it true that

$$U(t)^* P(t) U(t) = P(0) \quad ?$$

No! To see this, just take derivatives on both sides!

$$\begin{aligned} \frac{d}{dt} (U(t)^* P(t) U(t)) &= iU(t)^* [H(t), P(t)] U(t) + U(t)^* \dot{P}(t) U(t) \\ &= U(t)^* \dot{P}(t) U(t) \neq 0. \end{aligned}$$

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Idea: If $\dot{P}(t)$ is small, the equality should hold at least approximately.

Adiabatic limit: Mathematically we implement the slow variation by introducing the small **adiabatic parameter** $\varepsilon \ll 1$ in the time-dependence of the Hamiltonian.

On the **fast time-scale** the Schrödinger equation reads

$$i \frac{d}{ds} U_f^\varepsilon(s) = H(\varepsilon s) U_f^\varepsilon(s), \quad U_f(0) = \mathbf{1}_{\mathcal{H}}.$$

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Now we have

$$\begin{aligned} \frac{d}{ds} (U_f^*(s) P(\varepsilon s) U_f(s)) &= i U_f^*(s) [H(\varepsilon s), P(\varepsilon s)] U_f(s) + U_f^*(s) \varepsilon \dot{P}(\varepsilon s) U_f(s) \\ &= \varepsilon U_f^*(s) \dot{P}(\varepsilon s) U_f(s) = \mathcal{O}(\varepsilon). \end{aligned}$$

However, in order to see variations of H of order one, we consider times s of order ε^{-1} , e.g. $s \in [0, \varepsilon^{-1} T]$ for some fixed $T \in \mathbb{R}$. But then we are back to

$$\begin{aligned} \|U_f(s)^* P(\varepsilon s) U_f(s) - P(0)\| &= \left\| \int_0^{T/\varepsilon} ds \frac{d}{ds} (U_f(s)^* P(\varepsilon s) U_f(s)) \right\| \\ &\leq \frac{T}{\varepsilon} \cdot C\varepsilon = T \cdot C. \end{aligned}$$

1. Kato's adiabatic theorem

On the **fast time-scale** the Schrödinger equation reads

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1. Kato's adiabatic theorem

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A change of variable $t = \varepsilon s$ to the **slow time-scale** yields

$$i \varepsilon \frac{d}{dt} U^\varepsilon(t) = H(t) U^\varepsilon(t), \quad U^\varepsilon(0) = \mathbf{1}_{\mathcal{H}}.$$

for

$$U^\varepsilon(t) = U_f^\varepsilon\left(\frac{t}{\varepsilon}\right).$$

From now on we always use the **slow or macroscopic time-scale**. Note that now $H(t)$ and $P(t)$ are independent of ε , but the solution $U^\varepsilon(t)$ depends on ε .

1. Kato's adiabatic theorem

The gap condition

Let

$$H : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{D}, \mathcal{H}), \quad t \mapsto H(t)$$

be a continuous family of self-adjoint operators defined on a common dense domain $\mathcal{D} \subset \mathcal{H}$ and

$$\sigma_*(t) \subset \sigma(t)$$

a subset of the spectrum $\sigma(t)$ of $H(t)$ with spectral projection $P(t)$.

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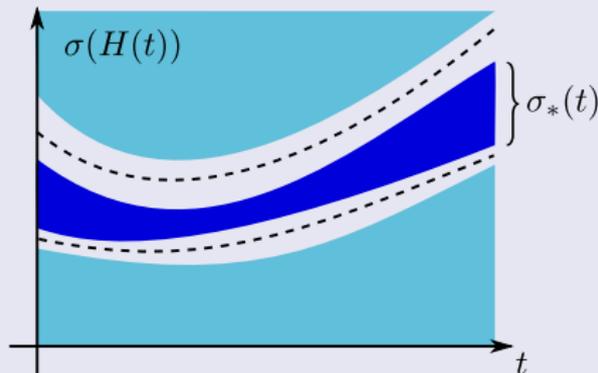
a subset of the spectrum $\sigma(t)$ of $H(t)$ with spectral projection $P(t)$.

We say that $\sigma_*(t)$ is separated by a uniform gap g if there are two bounded continuous functions $f_{\pm} \in C_b(\mathbb{R}, \mathbb{R})$ defining an interval $I(t) = [f_-(t), f_+(t)]$ such that

$$\sigma_*(t) = \sigma(t) \cap I(t)$$

and

$$\inf_{t \in \mathbb{R}} \text{dist}(f_{\pm}(t), \sigma(t)) \geq g/2.$$



1. Kato's adiabatic theorem

The Adiabatic Theorem (popular version):

Adiabatic invariance of gapped spectral subspaces

Let $H \in C_b^2(\mathbb{R}, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ and let $\sigma_*(t) \subset \sigma(t)$ satisfy the gap condition.

Then $P \in C_b^2(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$ and there exists $C < \infty$ such that for all $t \in \mathbb{R}$

$$\begin{aligned} \|P(t)U^\varepsilon(t) - U^\varepsilon(t)P(0)\| &= \|U^\varepsilon(t)^*P(t)U^\varepsilon(t) - P(0)\| \\ &\leq \varepsilon C(1 + |t|). \end{aligned}$$

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Consequently, the solution of

$$i\varepsilon \frac{d}{dt} \psi(t) = H(t) \psi(t), \quad \psi(0) = \psi_0 \in P(0)\mathcal{H},$$

remains within the subspace $P(t)\mathcal{H}$ up to terms of order ε ,

$$\|P(t)^\perp \psi(t)\| \leq \varepsilon C(1 + |t|) \|\psi_0\|.$$

1. Kato's adiabatic theorem

The Adiabatic Theorem: Kato's adiabatic evolution '50

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Define the **adiabatic Hamiltonian**

$$H_a(t) := H(t) + \varepsilon i[\dot{P}(t), P(t)] =: H(t) + \varepsilon K(t)$$

and the **adiabatic evolution** U_a^ε as the solution to

$$i\varepsilon \frac{d}{dt} U_a^\varepsilon(t) = H_a(t) U_a^\varepsilon(t), \quad U_a^\varepsilon(0) = \mathbf{1}_{\mathcal{H}}.$$

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Then

$$U_a^\varepsilon(t)^* P(t) U_a^\varepsilon(t) = P(0)$$

and there exists a constant $C < \infty$ such that for all $t \in \mathbb{R}$

$$\|U^\varepsilon(t) - U_a^\varepsilon(t)\| \leq \varepsilon C(1 + |t|).$$

1. Kato's adiabatic theorem

Note that

$$\| U^\varepsilon(t) - U_a^\varepsilon(t) \| \leq \varepsilon C (1 + |t|)$$

together with

$$P(t) U_a^\varepsilon(t) = U_a^\varepsilon(t) P(0)$$

implies immediately the adiabatic invariance of the spectral subspaces $P(t)$:

$$\begin{aligned} \| P(t)U^\varepsilon(t) - U^\varepsilon(t)P(0) \| &\leq \| P(t)U^\varepsilon(t) - P(t)U_a^\varepsilon(t) \| \\ &\quad + \| P(t)U_a^\varepsilon(t) - U^\varepsilon(t)P(0) \| \end{aligned}$$

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1. Kato's adiabatic theorem (proof)

Step 1: Regularity of the spectral projection $P(t)$

Riesz' formula reads

$$P(t) = \frac{i}{2\pi} \oint_{\gamma(t)} d\zeta (H(t) - \zeta)^{-1},$$

where $\gamma(t) \subset \mathbb{C}$ is a positively oriented closed curve encircling $\sigma_*(t)$ once such that

$$\inf_{t \in \mathbb{R}} \text{dist}(\gamma(t), \sigma(t)) = g/2.$$

Such curves $\gamma(t)$ exist because of the gap condition!

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Such curves $\gamma(t)$ exist because of the gap condition!

The continuity of f_{\pm} implies that for $|h|$ small enough $\gamma(t+h)$ is homotopic to $\gamma(t)$ in the resolvent set of $H(t+h)$. Thus for $|h|$ small enough

$$P(t+h) = \frac{i}{2\pi} \oint_{\gamma(t+h)} d\zeta (H(t+h) - \zeta)^{-1} = \frac{i}{2\pi} \oint_{\gamma(t)} d\zeta (H(t+h) - \zeta)^{-1}.$$

1. Kato's adiabatic theorem (proof)

Hence,

$$(*) \quad \frac{d}{dt} P(t) = \frac{i}{2\pi} \oint_{\gamma(t)} d\zeta \frac{d}{dt} (H(t) - \zeta)^{-1},$$

provided that the resolvent $R(\zeta, t) := (H(t) - \zeta)^{-1}$ is differentiable.

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But this follows from differentiating the identity

$$\mathbf{1}_{\mathcal{H}} = (H(t) - \zeta) R(\zeta, t)$$

with respect to t ,

$$\dot{R}(\zeta, t) = -R(\zeta, t) \dot{H}(t) R(\zeta, t).$$

This shows that $H \in C^n(\mathbb{R}, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ implies that also $R(\zeta) \in C^n(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$ for any ζ in the resolvent set.

With $(*)$ it follows that $P \in C^2(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$.

1. Kato's adiabatic theorem (proof)

Step 2: The adiabatic evolution

Recall the adiabatic Hamiltonian

$$H_a(t) := H(t) + \varepsilon K(t)$$

and the adiabatic evolution

$$i \varepsilon \frac{d}{dt} U_a^\varepsilon(t) = H_a(t) U_a^\varepsilon(t), \quad U_a^\varepsilon(0) = \mathbf{1}_{\mathcal{H}}.$$

As before we prove the claim that

$$U_a^\varepsilon(t)^* P(t) U_a^\varepsilon(t) - P(0) = 0$$

by noting that it holds at time $t = 0$ and by differentiating:

$$\begin{aligned} \frac{d}{dt} U_a^\varepsilon(t)^* P(t) U_a^\varepsilon(t) &= \\ &= U_a^\varepsilon(t)^* \dot{P}(t) U_a^\varepsilon(t) + \frac{i}{\varepsilon} (U_a^\varepsilon(t)^* [H_a(t), P(t)] U_a^\varepsilon(t)) \\ &= U_a^\varepsilon(t)^* \left(\dot{P}(t) + i [K(t), P(t)] \right) U_a^\varepsilon(t) \end{aligned}$$

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$$\frac{d}{dt} U_a^\varepsilon(t)^* P(t) U_a^\varepsilon(t) = U_a^\varepsilon(t)^* \left(\dot{P}(t) + i[K(t), P(t)] \right) U_a^\varepsilon(t)$$

Parallel transport lemma

$$\dot{P}(t) = [[\dot{P}(t), P(t)], P(t)]$$

and thus

$$i \frac{d}{dt} P(t) = [K(t), P(t)],$$

where $K(t) = i[\dot{P}(t), P(t)]$.

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Proof. $\dot{P}(t)$ is **block off-diagonal** with respect to $P(t)$, i.e.

$$\dot{P}(t) = \frac{d}{dt} P(t)^2 = \dot{P}(t) P(t) + P(t) \dot{P}(t)$$

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and thus

$$[[\dot{P}(t), P(t)], P(t)] = \dot{P}_{\text{od}}(t) = \dot{P}(t). \quad \square$$

1. Kato's adiabatic theorem (proof)

Step 3: Comparison of $U^\varepsilon(t)$ and $U_a^\varepsilon(t)$

By the fundamental theorem of calculus we have

$$U^\varepsilon(t) - U_a^\varepsilon(t) = U^\varepsilon(t)(\mathbf{1} - U^\varepsilon(t)^* U_a^\varepsilon(t))$$

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To show that this integral is small one uses that the integrand is oscillatory, more precisely, that it is the time derivative of a small oscillatory function, e.g. as in

$$\int_0^t \underbrace{e^{it'/\varepsilon}}_{=\mathcal{O}(1)} dt' = -i\varepsilon e^{it/\varepsilon}.$$

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To do so, we first write $K(t)$ as a commutator

$$K(t) = [H(t), F(t)]$$

for some operator-valued function $F(t)$.

1. The inverse of the commutator $\text{ad}_H(\cdot) = [H, \cdot]$

Let P be a gapped spectral projection of H and let

$$\mathcal{L}_{\text{dia}}(\mathcal{H}) := \{A \in \mathcal{L}(\mathcal{H}) \mid A = PAP + P^\perp AP^\perp\}$$

$$\mathcal{L}_{\text{od}}(\mathcal{H}) := \{A \in \mathcal{L}(\mathcal{H}) \mid A = PAP^\perp + P^\perp AP\}.$$

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Then for $A \in \ker \text{ad}_H$, i.e. $\text{ad}_H(A) = [H, A] = 0$ we have also $[P, A] = 0$ and hence $A \in \mathcal{L}_{\text{dia}}(\mathcal{H})$. Therefore

$$\text{ad}_H : \mathcal{L}_{\text{od}}(\mathcal{H}) \rightarrow \mathcal{L}_{\text{od}}(\mathcal{H}), \quad A \mapsto [H, A]$$

is **injective**.

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Then for $A \in \ker \text{ad}_H$, i.e. $\text{ad}_H(A) = [H, A] = 0$ we have also $[P, A] = 0$ and hence $A \in \mathcal{L}_{\text{dia}}(\mathcal{H})$. Therefore

$$\text{ad}_H : \mathcal{L}_{\text{od}}(\mathcal{H}) \rightarrow \mathcal{L}_{\text{od}}(\mathcal{H}), \quad A \mapsto [H, A]$$

is **injective**. It is also **surjective**, as can be seen by writing the unique solution of $[H, A] = B$ as follows,

$$A = \frac{1}{2\pi i} \int_{\gamma} (H - z)^{-1} [B, P] (H - z)^{-1} dz,$$

where γ is a closed curve in the resolvent set encircling σ_* once in the positive direction.

1. The inverse of the commutator $\text{ad}_H(\cdot) = [H, \cdot]$

If $\sigma_* = \{E\}$ is an eigenvalue, then

$$A = (H - E)^{-1}P^\perp BP - PBP^\perp(H - E)^{-1},$$

where the **reduced resolvent**

$$\|(H - E)^{-1}P^\perp\| \leq \frac{1}{g}$$

is well defined, since

$$\sigma(H|_{\text{ran}P^\perp}) = \sigma(H) \setminus \{E\}.$$

1. Kato's adiabatic theorem (proof)

Since $K(t) = i[\dot{P}(t), P(t)]$ is clearly off-diagonal,

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With

$$G(t) := i\varepsilon U^\varepsilon(t)^* F(t) U^\varepsilon(t) = \mathcal{O}(\varepsilon)$$

we have

$$\begin{aligned} \frac{d}{dt} G(t) &= U^\varepsilon(t)^* [H(t), F(t)] U^\varepsilon(t) + i\varepsilon U^\varepsilon(t)^* \dot{F}(t) U^\varepsilon(t) \\ &= U^\varepsilon(t)^* K(t) U^\varepsilon(t) + i\varepsilon U^\varepsilon(t)^* \dot{F}(t) U^\varepsilon(t) \end{aligned}$$

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Now we can do the integration by parts:

$$\|U^\varepsilon(t) - U_a^\varepsilon(t)\| = \left\| \int_0^t dt' U^\varepsilon(t')^* K(t') U^\varepsilon(t') U^\varepsilon(t')^* U_a^\varepsilon(t') \right\|$$

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□

1. Kato's adiabatic theorem (proof)

The proof yields **explicit error bounds**: for an isolated eigenvalue $\sigma_*(t) = \{E(t)\}$ with gap $g(t) := \text{dist}(E(t), \sigma(H(t)) \setminus \{E(t)\})$ it holds that

$$\|U^\varepsilon(t) - U_a^\varepsilon(t)\| \leq 2\varepsilon \left\{ \frac{\|\dot{P}(t)\|}{g(t)} + \frac{\|\dot{P}(0)\|}{g(0)} + \int_0^t \left(\frac{2\|\dot{P}(s)\|^2}{g(s)} + \frac{\|\ddot{P}(s)\|}{g(s)} + \frac{\|\dot{P}(s)\| \|\dot{H}(s)\|}{g(s)^2} \right) ds \right\}$$

1. First remarks on the Berry connection

The cartesian product $\mathcal{E}^{\mathcal{H}} := \mathbb{R} \times \mathcal{H}$ can be seen as a **trivial vector bundle** with base space \mathbb{R} and fibres $\mathcal{E}_t^{\mathcal{H}} = \mathcal{H}$.

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The spectral projections $P(t)$ define a subbundle

$$\mathcal{E}^P := \{ (t, \psi) \in \mathbb{R} \times \mathcal{H} \mid \psi \in P(t)\mathcal{H} \},$$

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A section $\psi \in \Gamma(\mathcal{E}^{\mathcal{H}})$ of the trivial bundle $\mathcal{E}^{\mathcal{H}} = \mathbb{R} \times \mathcal{H}$ is just a map

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A **connection** D on a vector bundle \mathcal{E} over \mathbb{R} is a “derivative”, i.e. a \mathbb{C} -linear map

$$D : \Gamma(\mathcal{E}) \rightarrow \Gamma(\mathcal{E})$$

satisfying the Leibniz rule

$$D(f\psi) = \dot{f}\psi + f D\psi \quad \text{for all } f \in C^\infty(\mathbb{R}).$$

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Given $\psi_0 \in \mathcal{E}_{t_0}$, there exists a unique parallel section $\psi \in \Gamma(\mathcal{E})$ such that $\psi(t_0) = \psi_0$. The map $T(t, t_0) : \mathcal{E}_{t_0} \rightarrow \mathcal{E}_t$, $\psi_0 \mapsto \psi(t)$, is called the **parallel transport map** of the connection D .

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The parallel transport map of the Berry connection on the eigenspace bundle \mathcal{E}^P is given by the solution to

$$i\frac{d}{dt}T(t, t_0) = K(t)T(t, t_0) \quad \text{with} \quad T(t_0, t_0) = \text{id}_{\mathcal{H}},$$

where $K(t) = i[\dot{P}(t), P(t)]$ is Kato's generator of the adiabatic evolution.

1. First remarks on the Berry connection

Hence, if $\sigma_*(t) = \{E(t)\}$ is an isolated eigenvalue, then the adiabatic evolution $U_a^\varepsilon(t, t_0)$ generated by

$$H_a(t) = H(t) + \varepsilon K(t)$$

acts on initial data $\psi \in \text{ran}P(t_0)$ as

$$U_a^\varepsilon(t, t_0)\psi = e^{-\frac{i}{\varepsilon} \int_{t_0}^t E(s) ds} T(t, t_0)\psi,$$

i.e. by parallel transport and a so called dynamical phase.

1. Kato's adiabatic theorem

Generalizations and variants of the adiabatic theorem:

- ▶ Adiabatic theorems **without spectral gap** condition
- ▶ Higher order adiabatic theorems, i.e. with $\mathcal{O}(\varepsilon^N)$ error bounds for $N > 1$, so called **super-adiabatic theorems**
- ▶ Adiabatic theorems for systems with slow degrees of freedom, so called **space-adiabatic theorems**

2. Adiabatic theorem without spectral gap

Bornemann '98 and *Avron, Elgart '99* realized independently that under certain conditions an adiabatic theorem can also hold in absence of a spectral gap.

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An adiabatic theorem without gap condition (T. '01)

Let $H \in C^1(\mathbb{R}, \mathcal{L}(\mathcal{D}, \mathcal{H}))$, let $E \in C(\mathbb{R})$ and $P \in C^2(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ such that

$$H(t)P(t) = E(t)P(t) \quad \text{for all } t \in \mathbb{R}$$

and such that $P(t)$ is the finite rank spectral projection onto the eigenspace of the eigenvalue $E(t)$ of $H(t)$ for almost all $t \in \mathbb{R}$.

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and such that $P(t)$ is the finite rank spectral projection onto the eigenspace of the eigenvalue $E(t)$ of $H(t)$ for almost all $t \in \mathbb{R}$.

Then

$$U_a^\varepsilon(t)^* P(t) U_a^\varepsilon(t) = P(0)$$

and

$$\lim_{\varepsilon \rightarrow 0} \| U^\varepsilon(t) - U_a^\varepsilon(t) \| = 0$$

uniformly on bounded intervals in time.

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In Kato's proof of the adiabatic theorem we used the gap condition at two places:

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In absence of a spectral gap, the reduced resolvent $(H - E)^{-1} P^\perp$ is not a bounded operator!

Idea: Replace F by

$$F^\delta = (H - E + i\delta)^{-1} P^\perp K P - P K P^\perp (H - E + i\delta)^{-1},$$

proceed as in the previous proof, and take $\delta = \delta(\varepsilon) \rightarrow 0$ when $\varepsilon \rightarrow 0$.

2. Adiabatic theorem without spectral gap (proof)

With

$$F^\delta = (H - E + i\delta)^{-1} P^\perp K P - P K P^\perp (H - E + i\delta)^{-1},$$

we have

$$\begin{aligned} [H, F^\delta] &= [H - E + i\delta, F^\delta] \\ &= K - i\delta \left(P K P^\perp (H - E + i\delta)^{-1} + (H - E + i\delta)^{-1} P^\perp K P \right) \end{aligned}$$

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Proceeding exactly as in the previous proof, we find that

$$\|U^\varepsilon(t) - U_a^\varepsilon(t)\| \leq C(1 + |t|) \times \sup_{s \in [0, t]} \left(\varepsilon \|F^\delta(s)\| + \varepsilon \|\dot{F}^\delta(s)\| + \int_0^t \|\delta(H - E + i\delta)^{-1} P^\perp K P\| ds \right)$$

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where in the last inequality we used

$$\|(H - z)^{-1}\| = \frac{1}{\text{dist}(z, \sigma(H))}.$$

2. Adiabatic theorem without spectral gap (proof)

Lemma

Let H be a self-adjoint operator on some Hilbert space \mathcal{H} . Let E an eigenvalue of H with spectral projection P . Then for all $\psi \in P^\perp \mathcal{H}$

$$\lim_{\delta \rightarrow 0} \|\delta(H - E + i\delta)^{-1}\psi\| = 0.$$

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Proof.

By dominated convergence

$$\lim_{\delta \rightarrow 0} \delta^2 \|(H - E + i\delta)^{-1}\psi\|^2 = \lim_{\delta \rightarrow 0} \int_{\sigma(H)} \frac{\delta^2}{(\lambda - E)^2 + \delta^2} d\mu^\psi(\lambda) = \mu^\psi(\{E\}),$$

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where μ^ψ denotes the spectral measure of H for ψ . Since ψ is orthogonal to the spectral subspace of E , $\mu^\psi(\{E\}) = 0$. □

2. Adiabatic theorem without spectral gap (proof)

Hence, since the range of $P(s)$ is finite dimensional,

$$\lim_{\delta \rightarrow 0} \|\delta(H(s) - E(s) + i\delta)^{-1} P^\perp(s) K(s) P(s)\| = 0 \quad (*)$$

for almost all $s \in \mathbb{R}$.

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Choosing $\delta(\varepsilon) = \varepsilon^{\frac{1}{4}}$, we find by dominated convergence that

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \|U^\varepsilon(t) - U_a^\varepsilon(t)\| &\leq \\ &\leq \lim_{\varepsilon \rightarrow 0} C(1 + |t|) \left(\frac{\varepsilon}{\delta} + \frac{\varepsilon}{\delta^2} + \int_0^t \|\delta(H - E + i\delta)^{-1} P^\perp K P\| ds \right) = 0. \end{aligned}$$

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□

In concrete models one can obtain also a rate of convergence by analysing the rate of convergence in (*) and optimizing $\delta(\varepsilon)$.

2. Adiabatic theorem without spectral gap

Applications and extensions:

- ▶ *T.* '02: Effective dynamics in the massless Nelson model
- ▶ *Abou-Salem, Fröhlich* '05: Adiabatic theorems and reversible isothermal processes
- ▶ *Tenuta, T.* '08: Effective dynamics for particles coupled to a quantized scalar field
- ▶ *Tenuta* '08: Quasi-static limits in nonrelativistic quantum electrodynamics
- ▶ *von Keler, T.* '12: Non-adiabatic transitions in a massless scalar field

2. Adiabatic theorem: Further extensions

Adiabatic theorems for resonances

- ▶ *Abou-Salem, Fröhlich '07*: Adiabatic theorems for quantum resonances
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Adiabatic theorems for non-self-adjoint generators

Nenciu, Rasche '92; Abou-Salem '07; Joye '07; Schmid '12; Avron, Fraas, Graf, Grech '12

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Adiabatic pair creation

Nenciu '87; Dürr, Pickl '08; Cornean, Jensen, Knörr, Nenciu '17

3. Super-adiabatic approximations

Can one improve the order of the error in the presence of a spectral gap ?

Not in a naive way, since due to the **boundary terms** indeed

$$\left\| P(t)^\perp U^\varepsilon(t) P(0) \right\| = \mathcal{O}(\varepsilon)$$

but not smaller.

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but not smaller.

Variant of the Adiabatic Theorem by Avron, Seiler, Yaffe '84

Let $H \in C^\infty(\mathbb{R}, \mathcal{L}_{\text{sa}}(\mathcal{H}))$ such that

$$\text{supp } \dot{H} \subset [0, T].$$

Then for any $N \in \mathbb{N}$ there is a constant $C_N < \infty$ such that for all $t \notin (0, T)$

$$\| U^\varepsilon(t) - U_a^\varepsilon(t) \| \leq C_N \varepsilon^N$$

and, in particular,

$$\| U^\varepsilon(t)^* P(t) U^\varepsilon(t) - P(0) \| \leq C_N \varepsilon^N.$$

3. Super-adiabatic approximations

As was realized for example by *Lenard (1959)*, *Garrido (1964)*, *Nenciu (1981)*, and *Berry (1990)*, under the same conditions there exist slightly tilted **super-adiabatic subspaces**

$$P_N^\varepsilon(t) = P(t) + \mathcal{O}(\varepsilon)$$

such that

$$\|U^\varepsilon(t, s)^* P_N^\varepsilon(t) U^\varepsilon(t, s) - P_N^\varepsilon(s)\| \leq C_N \varepsilon^N |t - s|$$

for all $t, s \in \mathbb{R}$ and such that

$$P_N^\varepsilon(t) = P(t)$$

for $t \notin \text{supp } \dot{H}$.

3. Super-adiabatic approximations

Super-Adiabatic Theorem

Let $H \in C_b^{N+1}(\mathbb{R}, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ and let $\sigma_*(t) \subset \sigma(t)$ satisfy the gap condition. There exist operator-valued functions $V^\varepsilon, K^\varepsilon \in C_b^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ such that $V^\varepsilon(t)$ is **unitary** and $K^\varepsilon(t)$ is **self-adjoint** for all $t \in \mathbb{R}$. Let

$$H_a^\varepsilon(t) := H(t) + \varepsilon K^\varepsilon(t).$$

3. Super-adiabatic approximations

Super-Adiabatic Theorem

Let $H \in C_b^{N+1}(\mathbb{R}, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ and let $\sigma_*(t) \subset \sigma(t)$ satisfy the gap condition. There exist operator-valued functions $V^\varepsilon, K^\varepsilon \in C_b^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ such that $V^\varepsilon(t)$ is **unitary** and $K^\varepsilon(t)$ is **self-adjoint** for all $t \in \mathbb{R}$. Let

$$H_a^\varepsilon(t) := H(t) + \varepsilon K^\varepsilon(t).$$

Then the solution to

$$i \varepsilon \frac{d}{dt} U_a^\varepsilon(t, s) = H_a^\varepsilon(t) U_a^\varepsilon(t, s), \quad U_a^\varepsilon(s) = \mathbf{1}_{\mathcal{H}}$$

satisfies

$$U_a^\varepsilon(t, s)^* P(t) U_a^\varepsilon(t, s) = P(s)$$

and there exists a constant $C < \infty$ such that for all $t \in \mathbb{R}$

$$\left\| U^\varepsilon(t, s) - \underbrace{V^\varepsilon(t) U_a^\varepsilon(t, s) V^\varepsilon(s)^*}_{=: U_{sa}^\varepsilon(t)} \right\| \leq \varepsilon^N C |t - s|.$$

3. Super-adiabatic approximations

Thm continued

If $\frac{d^n}{dt^n} H(t') = 0$ for some $t' \in \mathbb{R}$ and all $n = 1, \dots, N$, then

$$V^\varepsilon(t') = \text{id} \quad \text{and} \quad K^\varepsilon(t') = 0.$$

3. Super-adiabatic approximations

Thm continued

If $\frac{d^n}{dt^n} H(t') = 0$ for some $t' \in \mathbb{R}$ and all $n = 1, \dots, N$, then

$$V^\varepsilon(t') = \text{id} \quad \text{and} \quad K^\varepsilon(t') = 0.$$

Corollary: super-adiabatic projection

The **super-adiabatic projection**

$$P^\varepsilon(t) := V^\varepsilon(t) P(t) V^\varepsilon(t)^*$$

satisfies

$$\|U^\varepsilon(t, s)^* P^\varepsilon(t) U^\varepsilon(t, s) - P^\varepsilon(s)\| \leq C \varepsilon^N |t - s|$$

for all $t, s \in \mathbb{R}$.

If $\frac{d^n}{dt^n} H(t') = 0$ for some $t' \in \mathbb{R}$ and all $n = 1, \dots, N$, then

$$P^\varepsilon(t') = P(t').$$

3. Super-adiabatic approximations (proof)

Again by the fundamental theorem of calculus we have

$$\begin{aligned}U^\varepsilon(t, s) - U_{\text{sa}}^\varepsilon(t, s) &= U^\varepsilon(t, s) (\mathbf{1} - U^\varepsilon(t, s)^* U_{\text{sa}}^\varepsilon(t, s)) \\ &= -U^\varepsilon(t, s) \int_0^t dt' \frac{d}{dt'} \left(U^\varepsilon(t', s)^* U_{\text{sa}}^\varepsilon(t', s) \right)\end{aligned}$$

and the claim follows if we can show that

$$\left\| \frac{d}{dt} \left(U^\varepsilon(t, s)^* U_{\text{sa}}^\varepsilon(t, s) \right) \right\| = \mathcal{O}(\varepsilon^N).$$

3. Super-adiabatic approximations (proof)

$$\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) = \frac{d}{dt} \left(U(t, s)^* V(t) U_a(t, s) V(s)^* \right)$$

3. Super-adiabatic approximations (proof)

$$\begin{aligned}\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) &= \frac{d}{dt} \left(U(t, s)^* V(t) U_{\text{a}}(t, s) V(s)^* \right) \\ &= \frac{i}{\epsilon} \left(U(t, s)^* H(t) U_{\text{sa}}(t, s) - U(t, s)^* V(t) H_{\text{a}}(t) U_{\text{a}}(t, s) V(s)^* \right) \\ &\quad + U(t, s)^* \dot{V}(t) U_{\text{a}}(t, s) V(s)^*\end{aligned}$$

3. Super-adiabatic approximations (proof)

$$\begin{aligned}\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) &= \frac{d}{dt} \left(U(t, s)^* V(t) U_a(t, s) V(s)^* \right) \\ &= \frac{i}{\epsilon} \left(U(t, s)^* H(t) U_{\text{sa}}(t, s) - U(t, s)^* V(t) H_a(t) U_a(t, s) V(s)^* \right) \\ &\quad + U(t, s)^* \dot{V}(t) U_a(t, s) V(s)^* \\ &= \frac{i}{\epsilon} \left(U^* V V^* H V U_a V^* - U^* V H_a U_a V^* \right) \\ &\quad + U^* \dot{V} V^* V U_a V^*\end{aligned}$$

3. Super-adiabatic approximations (proof)

$$\begin{aligned}\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) &= \frac{d}{dt} \left(U(t, s)^* V(t) U_a(t, s) V(s)^* \right) \\ &= \frac{i}{\epsilon} \left(U(t, s)^* H(t) U_{\text{sa}}(t, s) - U(t, s)^* V(t) H_a(t) U_a(t, s) V(s)^* \right) \\ &\quad + U(t, s)^* \dot{V}(t) U_a(t, s) V(s)^* \\ &= \frac{i}{\epsilon} \left(U^* V V^* H V U_a V^* - U^* V H_a U_a V^* \right) \\ &\quad + U^* \dot{V} V^* V U_a V^* \\ &= \frac{i}{\epsilon} U^* V \left(V^* H V - H_a + i\epsilon \dot{V}^* V \right) V^* V U_a V^*\end{aligned}$$

3. Super-adiabatic approximations (proof)

$$\begin{aligned}\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) &= \frac{d}{dt} \left(U(t, s)^* V(t) U_a(t, s) V(s)^* \right) \\ &= \frac{i}{\epsilon} \left(U(t, s)^* H(t) U_{\text{sa}}(t, s) - U(t, s)^* V(t) H_a(t) U_a(t, s) V(s)^* \right) \\ &\quad + U(t, s)^* \dot{V}(t) U_a(t, s) V(s)^* \\ &= \frac{i}{\epsilon} \left(U^* V V^* H V U_a V^* - U^* V H_a U_a V^* \right) \\ &\quad + U^* \dot{V} V^* V U_a V^* \\ &= \frac{i}{\epsilon} U^* V \left(V^* H V - H_a + i\epsilon \dot{V}^* V \right) V^* V U_a V^* \\ &=: U(t, s)^* R(t) U_{\text{sa}}(t, s),\end{aligned}$$

where we used $0 = \frac{d}{dt}(V V^*) = \dot{V} V^* + V \dot{V}^*$.

3. Super-adiabatic approximations (proof)

$$\begin{aligned}\frac{d}{dt} \left(U(t, s)^* U_{\text{sa}}(t, s) \right) &= \frac{d}{dt} \left(U(t, s)^* V(t) U_a(t, s) V(s)^* \right) \\ &= \frac{i}{\varepsilon} \left(U(t, s)^* H(t) U_{\text{sa}}(t, s) - U(t, s)^* V(t) H_a(t) U_a(t, s) V(s)^* \right) \\ &\quad + U(t, s)^* \dot{V}(t) U_a(t, s) V(s)^* \\ &= \frac{i}{\varepsilon} \left(U^* V V^* H V U_a V^* - U^* V H_a U_a V^* \right) \\ &\quad + U^* \dot{V} V^* V U_a V^* \\ &= \frac{i}{\varepsilon} U^* V \left(V^* H V - H_a + i\varepsilon \dot{V}^* V \right) V^* V U_a V^* \\ &=: U(t, s)^* R(t) U_{\text{sa}}(t, s),\end{aligned}$$

where we used $0 = \frac{d}{dt}(V V^*) = \dot{V} V^* + V \dot{V}^*$.

Hence, we need to choose V and H_a such that

$$\|V^*(t) H(t) V(t) - H_a(t) + i\varepsilon \dot{V}^*(t) V(t)\| = \mathcal{O}(\varepsilon^{N+1})$$

for all $t \in \mathbb{R}$.

3. Super-adiabatic approximations (proof)

We construct inductively smooth operator-valued functions $A_n, K_n \in C^{N+1-n}(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$, $n = 1, \dots, N$, such that with

$$S^\varepsilon(t) := \sum_{n=1}^N \varepsilon^{n-1} A_n(t)$$

the operators

$$V^\varepsilon(t) := e^{i\varepsilon S^\varepsilon(t)}$$

and

$$K^\varepsilon(t) := \sum_{n=1}^N \varepsilon^n K_n(t)$$

satisfy

$$\|V^* H V - H_a + i\varepsilon \dot{V}^* V\| = \|V^* H V - H - \varepsilon K + i\varepsilon \dot{V}^* V\| = \mathcal{O}(\varepsilon^{N+1}).$$

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satisfy

$$\|V^* H V - H_a + i\varepsilon \dot{V}^* V\| = \|V^* H V - H - \varepsilon K + i\varepsilon \dot{V}^* V\| = \mathcal{O}(\varepsilon^{N+1}).$$

For K_1 we already know that we should choose Kato's generator of the adiabatic evolution,

$$K_1 = K = i[\dot{P}, P].$$

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

Expanding V^*HV yields

$$\begin{aligned} V^*HV &= e^{-i\varepsilon S} H e^{i\varepsilon S} \\ &= \sum_{n=0}^N \frac{(-i\varepsilon)^n}{n!} \text{ad}_S^n(H) + \frac{(-i\varepsilon)^{N+1}}{(N+1)!} e^{-i\tilde{\varepsilon}S} \text{ad}_S^{N+1}(H) e^{i\tilde{\varepsilon}S} \\ &=: \sum_{\mu=0}^N \varepsilon^\mu H_\mu + \varepsilon^{N+1} h_N(\varepsilon), \end{aligned}$$

where $\tilde{\varepsilon} \in [0, \varepsilon]$ and

$$\text{ad}_S^n(H) := \underbrace{[S, [\dots, [S, [S, H]] \dots]]}_{n \text{ copies of } S}.$$

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

Expanding V^*HV yields

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where $\tilde{\varepsilon} \in [0, \varepsilon]$ and

$$\text{ad}_S^n(H) := \underbrace{[S, [\dots, [S, [S, H]] \dots]]}_{n \text{ copies of } S}.$$

Recalling that $S = \sum_{n=1}^N \varepsilon^{n-1} A_n$, we observe that

$$H_0 = H, \quad H_1 = i \text{ad}_H(A_1), \quad \text{and} \quad H_\mu = \text{ad}_H(A_\mu) + L_\mu \quad \text{for } \mu \geq 2,$$

where L_μ depends only on $A_1, \dots, A_{\mu-1}$.

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

In order to expand $i\varepsilon \dot{V}^*V$, one uses Duhamel's formula

$$i\varepsilon \dot{V}^*V = \varepsilon^2 \int_0^1 e^{-i\lambda\varepsilon S} \dot{S} e^{i\lambda\varepsilon S} d\lambda,$$

expands the integrand as a series of nested commutators, and integrates term by term to find

$$\begin{aligned} i\varepsilon \dot{V}^*V &= \varepsilon^2 \sum_{n=0}^{N-2} \frac{(-i\varepsilon)^n}{(n+1)!} \text{ad}_S^n(\dot{S}) + \frac{(-i\varepsilon)^{N+1}}{(N-1)!} \int_0^1 e^{-i\lambda\varepsilon S} \text{ad}_S^{N-1}(\dot{S}) e^{i\lambda\varepsilon S} d\lambda \\ &= \sum_{\mu=2}^N \varepsilon^\mu Q_\mu + \varepsilon^{N+1} q_N(\varepsilon), \end{aligned}$$

where Q_μ depends only on $A_1, \dots, A_{\mu-1}$ and $\dot{A}_1, \dots, \dot{A}_{\mu-1}$.

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

In summary we have that

$$V^*HV - H_N + i\varepsilon \dot{V}^*V = \sum_{\mu=0}^N \varepsilon^\mu (H_\mu - K_\mu + Q_\mu) + \varepsilon^{N+1} (h_N(\varepsilon) + q_N(\varepsilon))$$

and now pick A_μ and K_μ inductively starting at $\mu = 0$ in such a way that

$$H_\mu - K_\mu + Q_\mu = 0$$

for $\mu = 0, \dots, N$.

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In summary we have that

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for $\mu = 0, \dots, N$.

$\mu = 0$: $H_0 - K_0 + Q_0 = H - H + 0 = 0 \quad \checkmark$

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

In summary we have that

$$V^*HV - H_N + i\varepsilon \dot{V}^*V = \sum_{\mu=0}^N \varepsilon^\mu (H_\mu - K_\mu + Q_\mu) + \varepsilon^{N+1} (h_N(\varepsilon) + q_N(\varepsilon))$$

and now pick A_μ and K_μ inductively starting at $\mu = 0$ in such a way that

$$H_\mu - K_\mu + Q_\mu = 0$$

for $\mu = 0, \dots, N$.

$$\underline{\mu = 0}: H_0 - K_0 + Q_0 = H - H + 0 = 0 \quad \checkmark$$

$$\underline{\mu = 1}: H_1 - K_1 + Q_1 = i \operatorname{ad}_H(A_1) - K_1 = i[H, A_1] - K \stackrel{!}{=} 0$$

Since $K = i[\dot{P}, P]$ is off-diagonal,

$$i[H, A_1] = K$$

has a unique off-diagonal solution $A_1 \in C^N(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$.

3. Expanding $V^*HV - H_a + i\varepsilon \dot{V}^*V$ up to ε^{N+1}

$\mu \geq 2$: Now assume that we constructed $A_1, \dots, A_{\mu-1}$. Then we need to specify A_μ and K_μ such that

$$H_\mu - K_\mu + Q_\mu = i[H, A_\mu] + L_\mu - K_\mu + Q_\mu \stackrel{!}{=} 0. \quad (*)$$

Recall that L_μ and Q_μ depend only on $A_1, \dots, A_{\mu-1}$ and are thus given at this stage. Putting

$$K_\mu := (L_\mu + Q_\mu)_{\text{dia}} := P(L_\mu + Q_\mu)P + P^\perp(L_\mu + Q_\mu)P^\perp$$

and $A_\mu \in C^{N+1-\mu}(\mathbb{R}, \mathcal{L}(\mathcal{H}, \mathcal{D}))$ equal to the unique off-diagonal solution of

$$i[H, A_\mu] = -(L_\mu + Q_\mu)_{\text{od}}$$

provides a solution of (*).



3. Super-adiabatic approximations: Exponential estimates

Exponential bounds

Joye, Pfister '91; Nenciu '93; Sjöstrand '93; Jung '00

For $t \mapsto H(t)$ analytic one can replace $\mathcal{O}(\varepsilon^N)$ by $\mathcal{O}(e^{-\frac{\gamma}{\varepsilon}})$.

3. Super-adiabatic approximations: Exponential estimates

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For $t \mapsto H(t)$ analytic one can replace $\mathcal{O}(\varepsilon^N)$ by $\mathcal{O}(e^{-\frac{\gamma}{\varepsilon}})$.

More than bounds: transition probabilities

Zener '32; ...; Berry '90; Joye, Kunz, Pfister '91; ...

Let $t \mapsto H(t)$ be analytic and matrix-valued, let $\sigma_*(t) = \{E(t)\}$ be a simple eigenvalue and let $\lim_{t \rightarrow \pm\infty} \|\dot{H}(t)\| = 0$. Then

$$\lim_{t \rightarrow \infty} \left\| P^\perp(t) U^\varepsilon(t, -t) P(-t) \right\|^2 = 4 \sin^2 \left(\frac{\pi\gamma}{2} \right) e^{-\frac{2\tau_c}{\varepsilon}} (1 + o(1)) .$$

“Landau-Zener formula”

3. Super-adiabatic approximations: Transition histories

More than bounds: adiabatic transition histories

Berry '90; Hagedorn, Joye '04; Betz, T. '05

Let $t \mapsto H(t)$ be analytic and 2×2 -matrix-valued, let

$\sigma_*(t) = \{E(t)\}$ be a simple eigenvalue and let $\lim_{t \rightarrow \pm\infty} \|\dot{H}(t)\| = 0$.

Then

$$\lim_{t_0 \rightarrow -\infty} \left\| P^{\varepsilon\perp}(t) U^\varepsilon(t, t_0) P^\varepsilon(t_0) \right\|^2 = 4 \sin^2 \left(\frac{\pi\gamma}{2} \right) e^{-\frac{2\tau_c}{\varepsilon}} \left(\operatorname{erf} \left(\frac{t}{\sqrt{2\varepsilon\tau_c}} \right) - 1 \right)^2$$

where $P^\varepsilon(t)$ are the optimal superadiabatic projections.

3. Super-adiabatic approximations: Transition histories

More than bounds: adiabatic transition histories

Berry '90; Hagedorn, Joye '04; Betz, T. '05

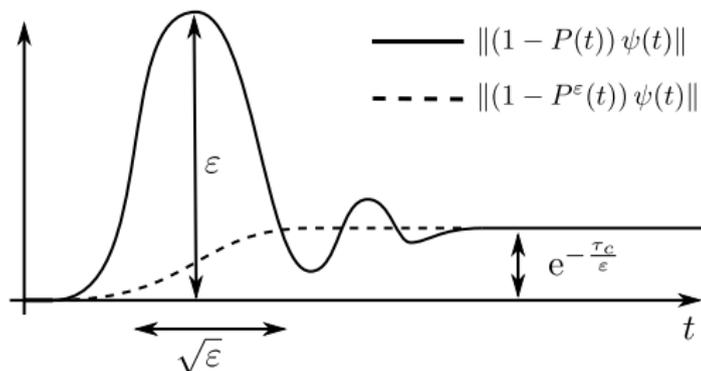
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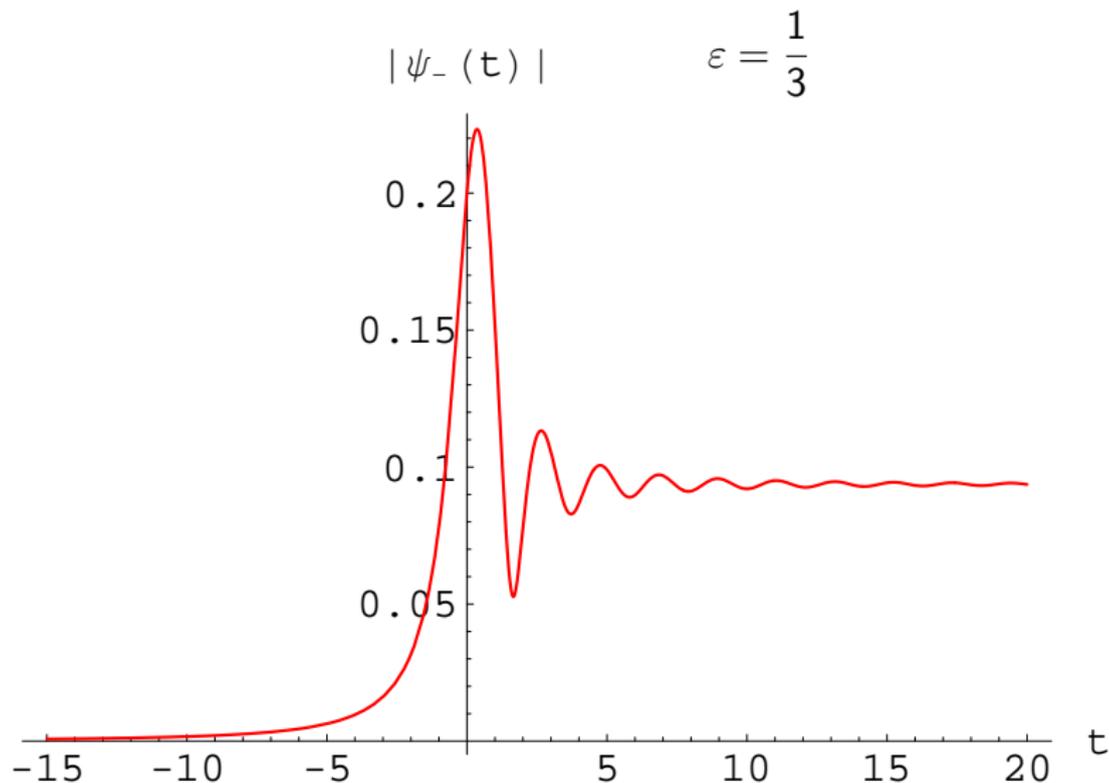
Then

$$\lim_{t_0 \rightarrow -\infty} \left\| P^{\varepsilon\perp}(t) U^\varepsilon(t, t_0) P^\varepsilon(t_0) \right\|^2 = 4 \sin^2 \left(\frac{\pi\gamma}{2} \right) e^{-\frac{2\tau_c}{\varepsilon}} \left(\operatorname{erf} \left(\frac{t}{\sqrt{2\varepsilon\tau_c}} \right) - 1 \right)^2$$

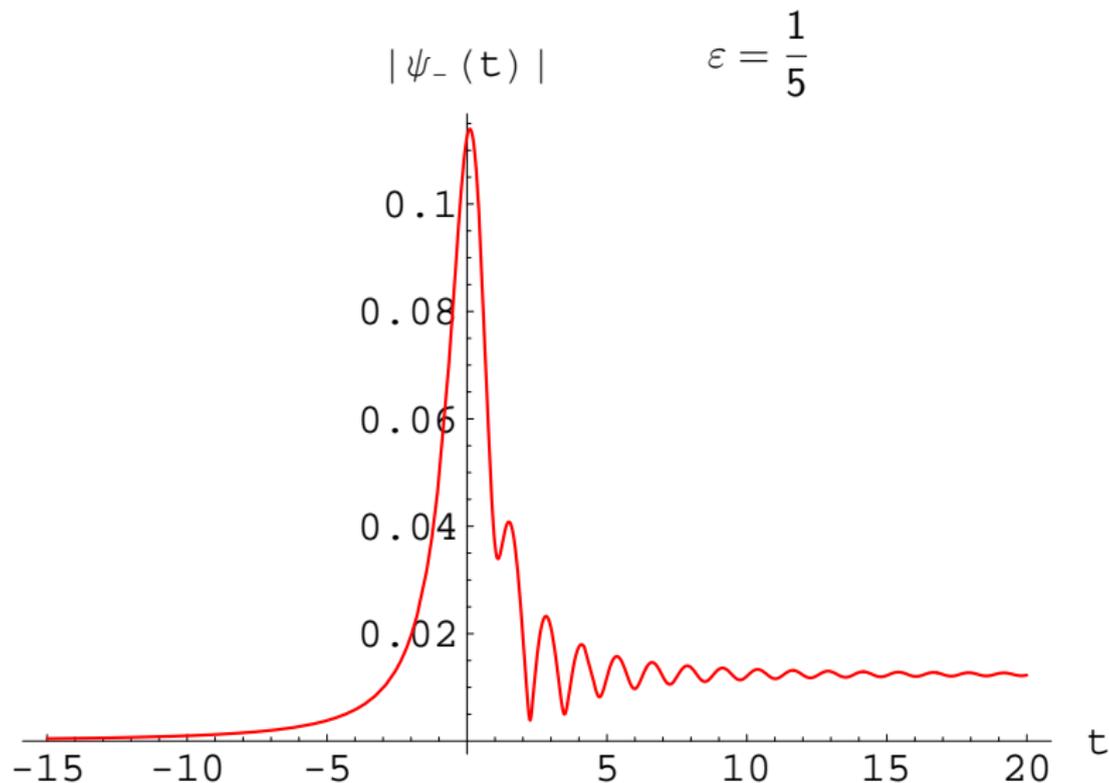
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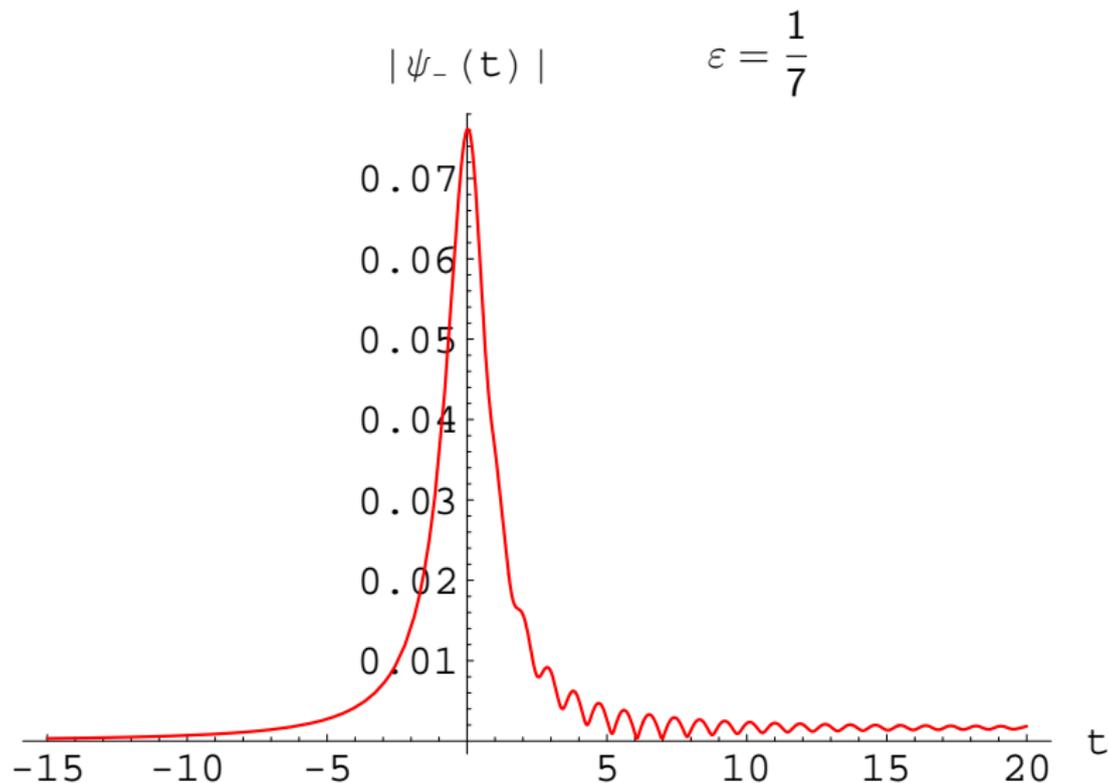
3. Super-adiabatic approximations: Transition histories



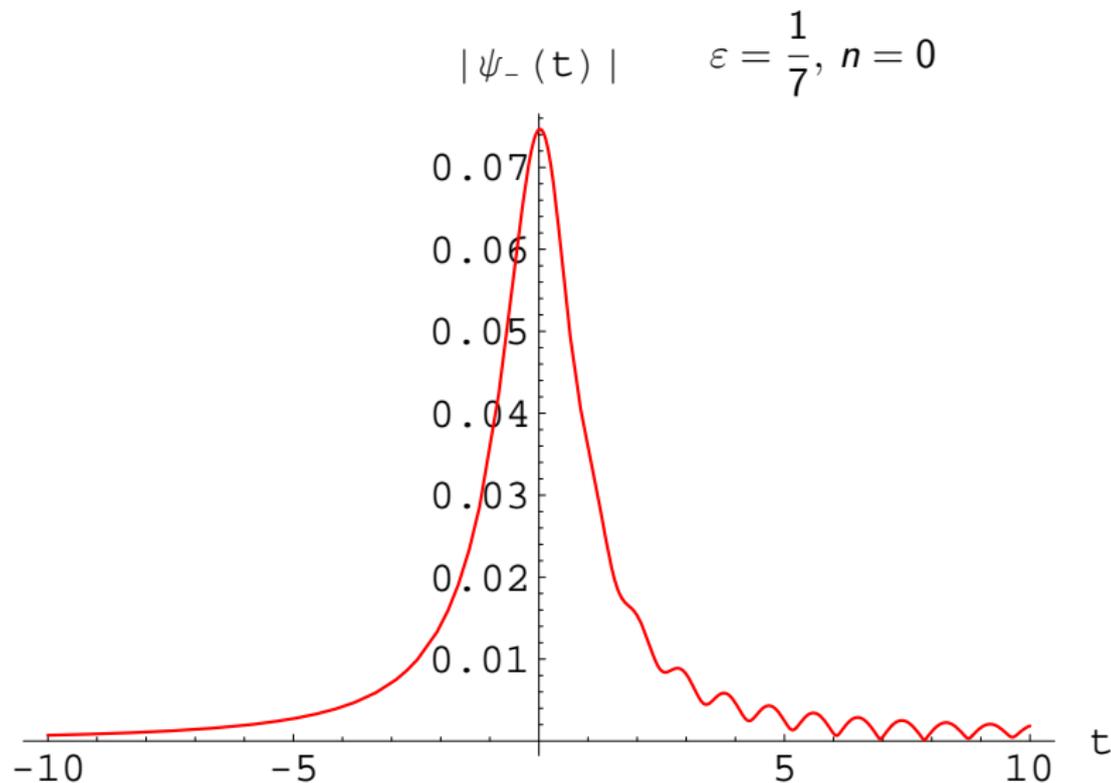
3. Super-adiabatic approximations: Transition histories



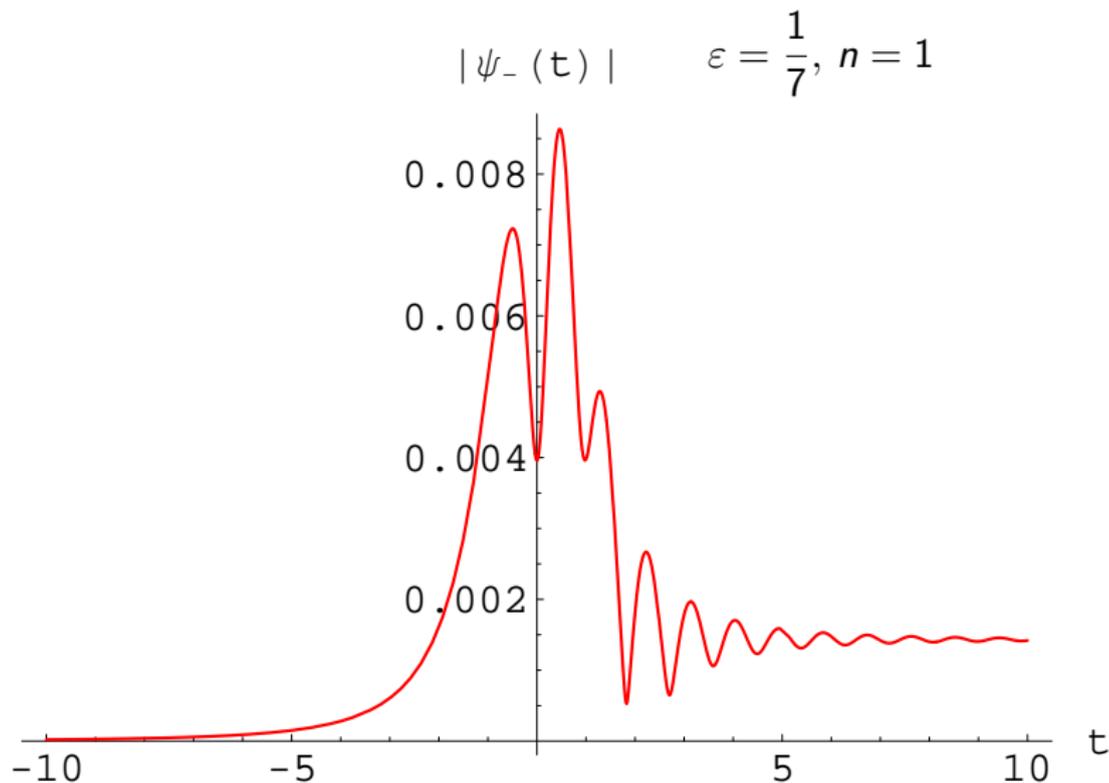
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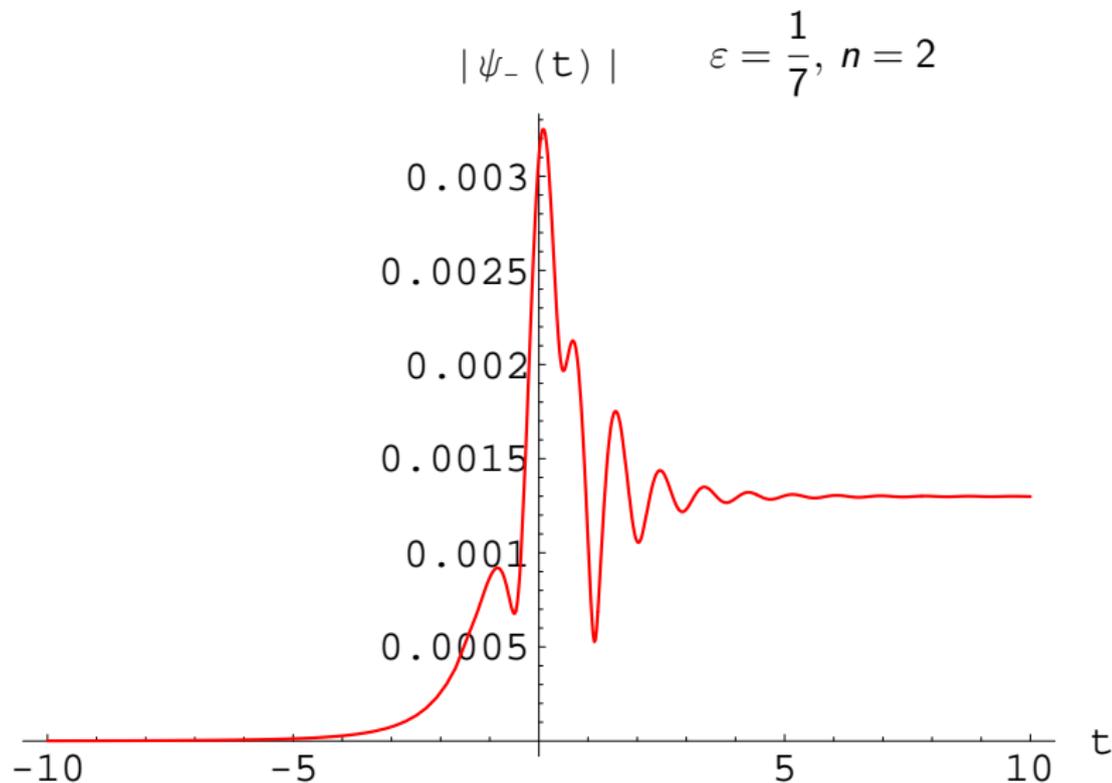
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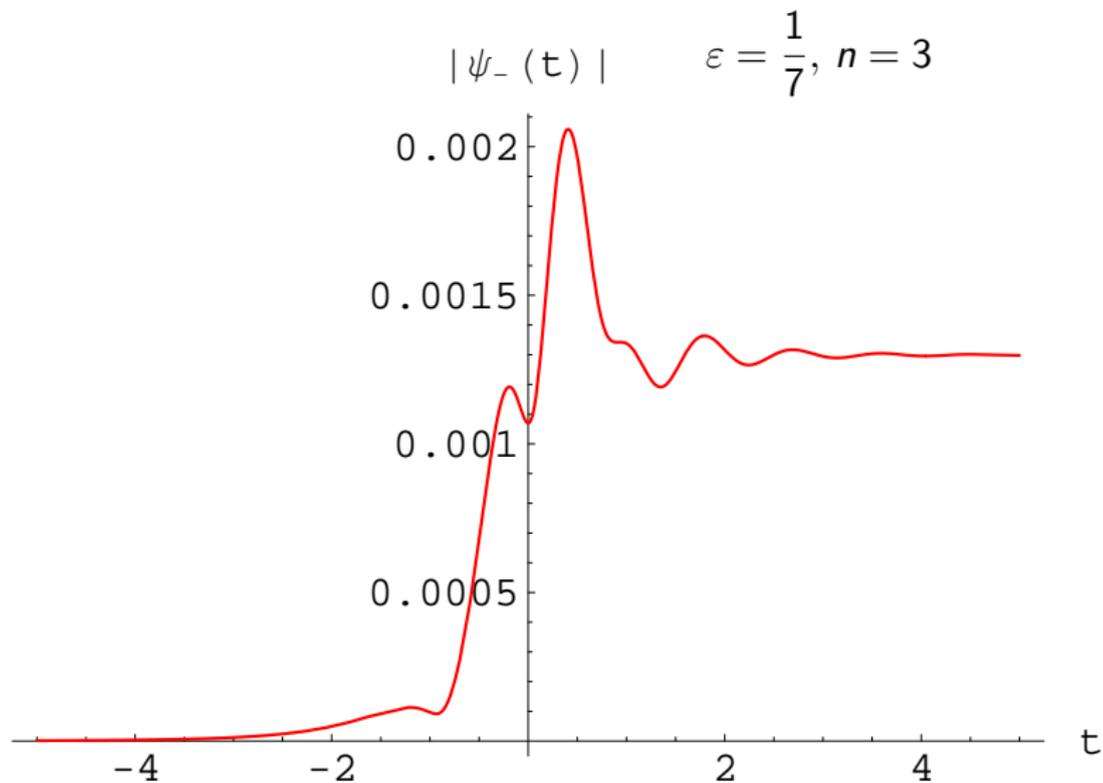
3. Super-adiabatic approximations: Transition histories



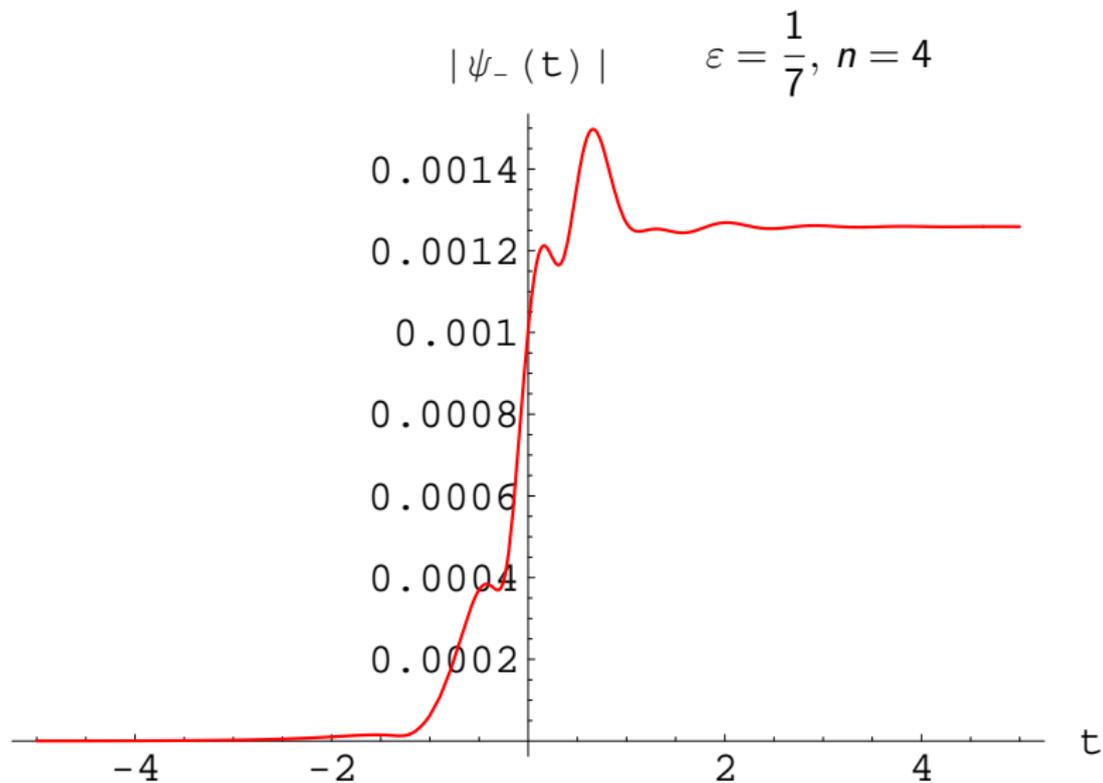
3. Super-adiabatic approximations: Transition histories



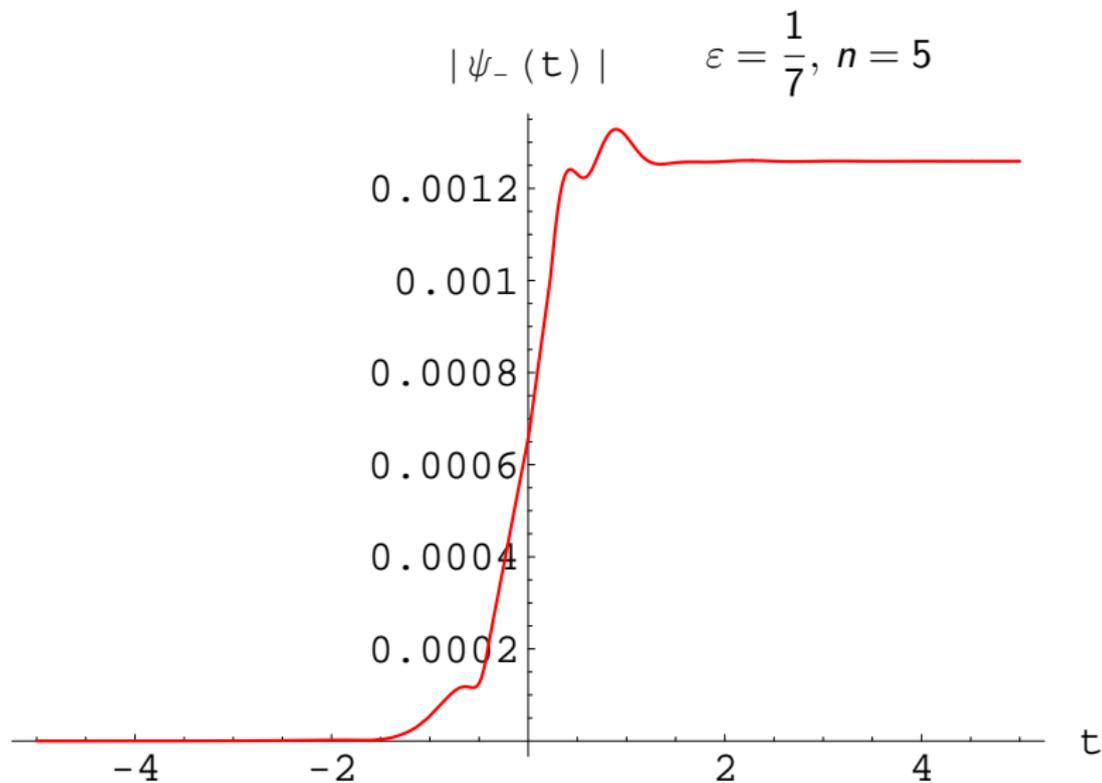
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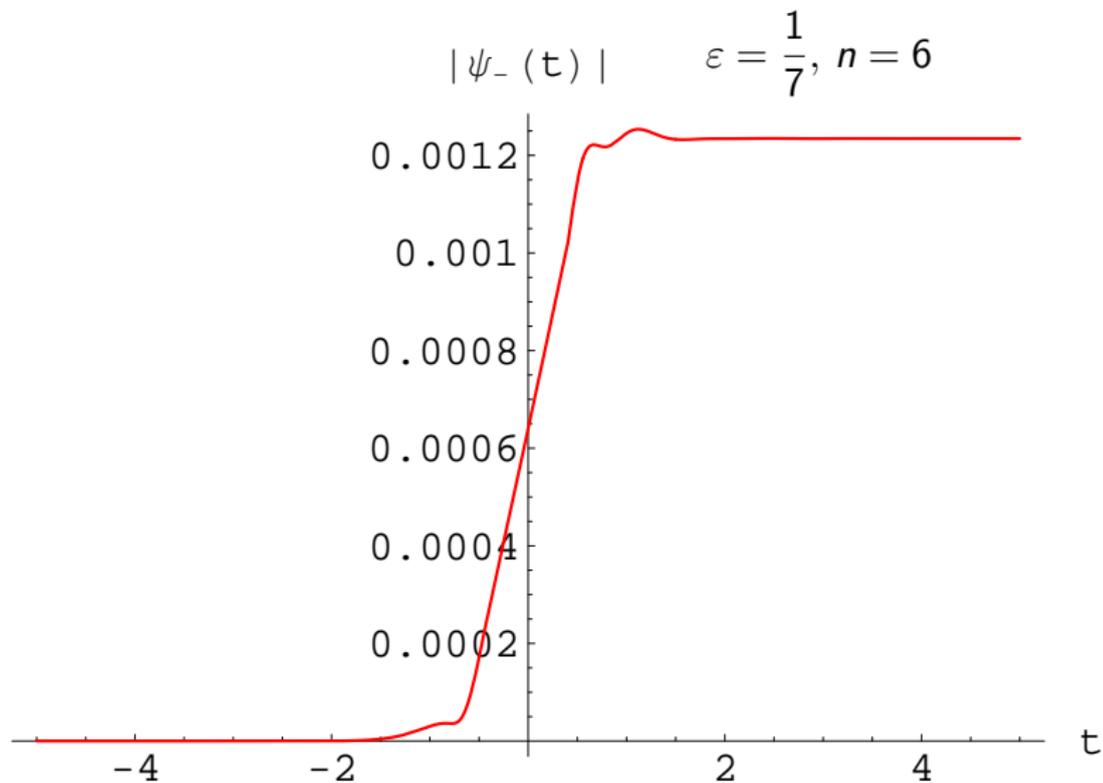
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4. Adiabatic currents in non-interacting fermion systems

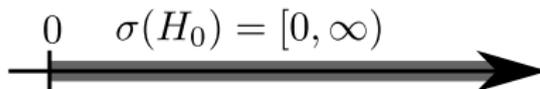
► $H_0 = -\Delta_x$ on $L^2(\mathbb{R}_x^2)$

0 $\sigma(H_0) = [0, \infty)$

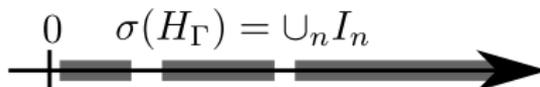


4. Adiabatic currents in non-interacting fermion systems

▶ $H_0 = -\Delta_x$ on $L^2(\mathbb{R}_x^2)$



▶ $H_\Gamma = -\Delta_x + V_\Gamma(x)$

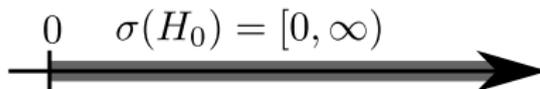


Bloch bands

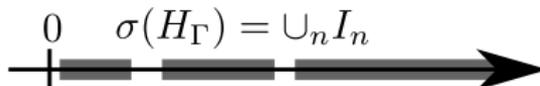
with $V_\Gamma(x + \gamma) = V_\Gamma(x)$ for all $x \in \mathbb{R}^2$, $\gamma \in \Gamma \sim \mathbb{Z}^2$

4. Adiabatic currents in non-interacting fermion systems

▶ $H_0 = -\Delta_x$ on $L^2(\mathbb{R}_x^2)$



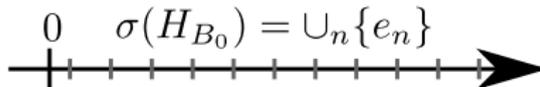
▶ $H_\Gamma = -\Delta_x + V_\Gamma(x)$



Block bands

with $V_\Gamma(x + \gamma) = V_\Gamma(x)$ for all $x \in \mathbb{R}^2$, $\gamma \in \Gamma \sim \mathbb{Z}^2$

▶ $H_{B_0} = (-i\nabla_x + A_0(x))^2$

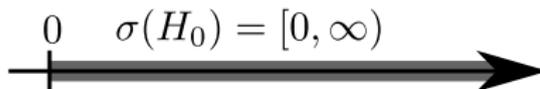


Landau levels

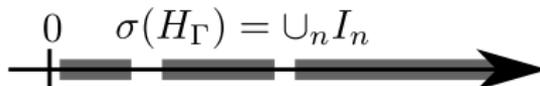
with $dA_0 = B_0 = \text{const.}$

4. Adiabatic currents in non-interacting fermion systems

▶ $H_0 = -\Delta_x$ on $L^2(\mathbb{R}_x^2)$



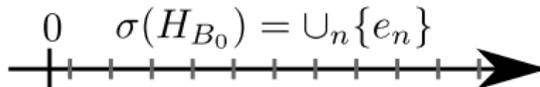
▶ $H_\Gamma = -\Delta_x + V_\Gamma(x)$



Bloch bands

with $V_\Gamma(x + \gamma) = V_\Gamma(x)$ for all $x \in \mathbb{R}^2$, $\gamma \in \Gamma \sim \mathbb{Z}^2$

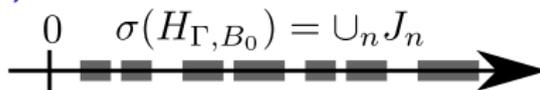
▶ $H_{B_0} = (-i\nabla_x + A_0(x))^2$



Landau levels

with $dA_0 = B_0 = \text{const.}$

▶ $H_{\Gamma, B_0} = (-i\nabla_x + A_0(x))^2 + V_\Gamma(x)$



Magnetic Bloch bands

with Γ and B_0 commensurable

4. Adiabatic currents in non-interacting fermion systems

If the chemical potential μ lies in a gap of the spectrum of such a one-body Hamiltonian H , then the **one-body density matrix** of the ground state of a system of infinitely many non-interacting fermions is given by the gapped spectral projection $P = \chi_{(-\infty, \mu]}(H)$.

4. Adiabatic currents in non-interacting fermion systems

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If the Hamiltonian $H = H(t)$ varies slowly in time, e.g. because of changes in the lattice structure (**piezoelectric effect**) or because of time-dependent external fields, then the time-dependent one-body density matrix, i.e. the solution of the Liouville equation

$$i\epsilon \frac{d}{dt} \rho^\epsilon(t) = [H(t), \rho^\epsilon(t)], \quad \rho^\epsilon(0) = \chi_{(-\infty, \mu]}(H(0)),$$

can be approximated using (super)adiabatic approximations as long as the gap in which the chemical potential μ was initially located doesn't close.

4. Adiabatic currents in non-interacting fermion systems

For the following somewhat informal discussion we assume that $t \mapsto H(t)$ is a C^{N+2} family of Hamiltonians such that

- ▶ for fixed t the Hamiltonian $H(t)$ is a periodic operator or a covariant family of operators in such a way that the current operator

$$J^\varepsilon(t) := \frac{i}{\varepsilon} [H(t), X]$$

is well defined (and then itself periodic resp. covariant) and the **trace per unit volume**

$$\tau(\rho^\varepsilon(t) J^\varepsilon(t)) := \lim_{\Lambda \rightarrow \mathbb{R}^d} \frac{1}{|\Lambda|} \text{tr}(\chi_\Lambda \rho^\varepsilon(t) J^\varepsilon(t) \chi_\Lambda)$$

is well defined.

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- ▶ $t \mapsto \mu(t) \in \mathbb{R}$ is continuous and lies in a gap of the spectrum of $H(t)$ for all $t \in \mathbb{R}$
- ▶ either H changes only on a compact interval, $\text{supp} \dot{H} \subset [0, T]$, or changes periodically, $H(t + T) = H(t)$.

4. Adiabatic currents in non-interacting fermion systems

We are interested in the **transported charge**, i.e. the integrated adiabatic current density, **during one cycle**,

$$\Delta Q := \int_0^T \tau(\rho^\varepsilon(t) J^\varepsilon(t)) dt$$

when starting initially in the ground state

$$\rho^\varepsilon(0) = \chi_{(-\infty, \mu]}(H(0)) =: P(0)$$

for a compactly supported change of the Hamiltonian, or in the superadiabatic state

$$\rho^\varepsilon(0) = P^\varepsilon(0)$$

for a periodic driving.

4. Adiabatic currents in non-interacting fermion systems

Theorem: Adiabatic charge transport

It holds that

$$\Delta Q = \int_0^T \tau (P(t) \left[\frac{d}{dt} P(t), [X, P(t)] \right]) dt + \mathcal{O}(\varepsilon^N).$$

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Moreover, the transported charge is a **diffeotopy invariant**: let $H_1(t)$ be another family of gapped Hamiltonians that is diffeotopic to $H(t) =: H_0(t)$, i.e. there exists a smooth gapped family of Hamiltonians $H(t, \alpha)$ on $[0, T] \times [0, 1]$ such that $H(t, 0) = H_0(t)$ and $H(t, 1) = H_1(t)$ and

- ▶ either $H(0, \alpha) = H_0(0)$ and $H(1, \alpha) = H_0(1)$
- ▶ or $\frac{d^n}{dt^n} H(\cdot, \alpha)|_{t=0} = \frac{d^n}{dt^n} H(\cdot, \alpha)|_{t=T}$ for all $\alpha \in [0, 1]$ and $n = 1, \dots, N + 2$.

Then $|\Delta Q_1 - \Delta Q_0| = \mathcal{O}(\varepsilon^N)$.

- ▶ *Panati, Sparber, T. '09*: $H(t) = -\Delta + V_\Gamma(t)$ on $L^2(\mathbb{R}^d)$.
- ▶ *Schulz-Baldes, T. '12*: $H(t) = H_\omega(t)$ is a covariant family of random operators on $\ell^2(\mathbb{Z}^d)$.

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Piezoelectricity for Harper like models was also discussed by *Avron, Berger, Last '97*.

4. Adiabatic currents in non-interacting systems (proof)

Proposition

It holds that

$$\tau(\rho^\varepsilon(t) J^\varepsilon(t)) = \tau(\rho^\varepsilon(t) [\frac{d}{dt}\rho^\varepsilon(t), [X, \rho^\varepsilon(t)]]) .$$

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Proof.

Using $\rho^\varepsilon(t)^2 = \rho^\varepsilon(t)$ and cyclicity of the trace per unit volume we find that

$$\tau(\rho^\varepsilon(t) \left[\frac{d}{dt} \rho^\varepsilon(t), [X, \rho^\varepsilon(t)] \right]) =$$

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□

4. Adiabatic currents in non-interacting systems (proof)

According to the superadiabatic theorem we have that

$$\rho^\varepsilon(t) = P^\varepsilon(t) + \mathcal{O}(\varepsilon^N)$$

and thus (modulo proving the above statement in the right topology)

$$\tau(\rho^\varepsilon(t) J^\varepsilon(t)) = \tau(P^\varepsilon(t) \left[\frac{d}{dt} P^\varepsilon(t), [X, P^\varepsilon(t)] \right]) + \mathcal{O}(\varepsilon^N).$$

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Proposition

Let $\Pi : [0, T] \times [0, 1] \rightarrow \mathcal{L}(\mathcal{H})$ be a C^1 -family of orthogonal projections, such that

- ▶ either $\Pi(0, \alpha) \equiv \Pi_0$ and $\Pi(1, \alpha) \equiv \Pi_1$ for all $\alpha \in [0, 1]$
- ▶ or $\frac{d^n}{d\alpha^n} \Pi(0, \alpha) = \frac{d^n}{d\alpha^n} \Pi(T, \alpha)$ for all $\alpha \in [0, 1]$ and $n = 0, 1$.

Then

$$\frac{d}{d\alpha} \int_0^T \tau(\Pi(t, \alpha) \left[\frac{d}{dt} \Pi(t, \alpha), [X, \Pi(t, \alpha)] \right]) dt = 0.$$

4. Adiabatic currents in non-interacting systems (proof)

Proof.

$$\begin{aligned} & \frac{d}{d\alpha} \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}(t, \alpha), [X, \Pi(t, \alpha)] \right] \right) dt \\ &= \int_0^T \tau \left(\Pi'(t, \alpha) \left[\dot{\Pi}(t, \alpha), [X, \Pi(t, \alpha)] \right] \right) dt \\ &+ \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}'(t, \alpha), [X, \Pi(t, \alpha)] \right] \right) dt \\ &+ \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}(t, \alpha), [X, \Pi'(t, \alpha)] \right] \right) dt \end{aligned}$$

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$$\begin{aligned} & \frac{d}{d\alpha} \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}(t, \alpha), [\mathcal{X}, \Pi(t, \alpha)] \right] \right) dt \\ &= \int_0^T \tau \left(\Pi'(t, \alpha) \left[\dot{\Pi}(t, \alpha), [\mathcal{X}, \Pi(t, \alpha)] \right] \right) dt \\ & \quad + \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}'(t, \alpha), [\mathcal{X}, \Pi(t, \alpha)] \right] \right) dt \\ & \quad + \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}(t, \alpha), [\mathcal{X}, \Pi'(t, \alpha)] \right] \right) dt \\ &= \tau \left(\Pi(t, \alpha) \left[\Pi'(t, \alpha), [\mathcal{X}, \Pi(t, \alpha)] \right] \right) \Big|_0^T \\ & \quad - \int_0^T \tau \left(\Pi(t, \alpha) \left[\Pi'(t, \alpha), [\mathcal{X}, \dot{\Pi}(t, \alpha)] \right] \right) dt \\ & \quad + \int_0^T \tau \left(\Pi(t, \alpha) \left[\dot{\Pi}(t, \alpha), [\mathcal{X}, \Pi'(t, \alpha)] \right] \right) dt \end{aligned}$$

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4. Adiabatic currents in non-interacting systems (proof)

Hence we find in summary that

$$\begin{aligned}\int_0^T \tau(\rho^\varepsilon(t) J^\varepsilon(t)) dt &= \int_0^T \tau(P^\varepsilon(t) \left[\frac{d}{dt} P^\varepsilon(t), [X, P^\varepsilon(t)] \right]) dt + \mathcal{O}(\varepsilon^N) \\ &= \int_0^T \tau(P(t) \left[\frac{d}{dt} P(t), [X, P(t)] \right]) dt + \mathcal{O}(\varepsilon^N)\end{aligned}$$

since $\varepsilon \mapsto P^\varepsilon$ is indeed analytic. □

4. Adiabatic currents: Geometric aspects

For periodic operators the expression for the transported charge has a natural geometric meaning.

Let the one-body configuration space \mathcal{X}^d be either \mathbb{R}^d or \mathbb{Z}^d and the one-body Hilbert space $\mathcal{H} := L^2(\mathcal{X}^d; \mathbb{C}^m)$.

Let

$$T : \mathbb{Z}^d \rightarrow \mathcal{U}(\mathcal{H}), \quad \gamma \mapsto T_\gamma, \quad (T_\gamma \psi)(x) = c(\gamma, x) \psi(x - \gamma)$$

be a unitary representation of the group \mathbb{Z}^d by (magnetic) translations.

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Then an operator $A \in \mathcal{L}(\mathcal{H})$ is called **periodic**, if

$$[A, T_\gamma] = 0 \quad \text{for all } \gamma \in \mathbb{Z}^d.$$

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Periodic operators can be “diagonalized” by the **Bloch-Floquet transformation**

$$U_{\text{BF}} : L^2(\mathcal{X}^d; \mathbb{C}^m) \rightarrow L^2(\mathbb{T}^d; L^2(\mathcal{X}^d/\mathbb{Z}^d) \otimes \mathbb{C}^m),$$
$$(U_{\text{BF}} \psi)(k, x) := e^{-ik \cdot x} \sum_{\gamma \in \mathbb{Z}^d} e^{ik \cdot \gamma} (T_\gamma \psi)(x).$$

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$$(U_{\text{BF}}\psi)(k, y) := e^{-ik \cdot y} \sum_{\gamma \in \mathbb{Z}^d} e^{ik \cdot \gamma} (T_\gamma \psi)(y),$$

where $\mathbb{T}^d := [0, 2\pi)^d$.

A periodic operator A becomes an operator-valued multiplication operator in Bloch-Floquet representation:

$$(U_{\text{BF}} A U_{\text{BF}}^* \varphi)(k) = A(k) \varphi(k)$$

for an operator valued function

$$A : \mathbb{T}^d \rightarrow \mathcal{L}(\mathcal{H}_f), \quad \text{where} \quad \mathcal{H}_f := L^2(\mathcal{X}^d/\mathbb{Z}^d) \otimes \mathbb{C}^m.$$

4. Adiabatic currents: Geometric aspects

Note that if A is periodic, then

- ▶ the spectral projections P are periodic (obviously)
- ▶ the commutator $i[A, X]$ is periodic and has the Bloch-Floquet fibration

$$(U_{\text{BF}} i[A, X] U_{\text{BF}}^* \varphi)(k) = (\nabla_k A)(k) \varphi(k).$$

- ▶ its trace per unit volume, if it exists, is given by

$$\tau(A) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \text{tr}_{\mathcal{H}_f} A(k) dk.$$

4. Adiabatic currents: Geometric aspects

Hence for a periodic time-dependent Hamiltonian $H(t)$ the transported charge is given by

$$\begin{aligned}\Delta Q &= \int_0^T \tau (P(t) \left[\frac{d}{dt} P(t), [X, P(t)] \right]) dt + \mathcal{O}(\varepsilon^N) \\ &= \frac{i}{(2\pi)^d} \int_0^T \int_{\mathbb{T}^d} \text{tr}_{\mathcal{H}_f} \left(P(t, k) \left[\dot{P}(t, k), \nabla_k P(t, k) \right] \right) dk dt\end{aligned}$$

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Hence for a periodic time-dependent Hamiltonian $H(t)$ the transported charge is given by

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The operator valued function

$$(t, k) \mapsto P(t, k) \left[\dot{P}(t, k), \nabla_k P(t, k) \right]$$

is (a component of) the **curvature 2-form of the Berry connection** on the (extended) Bloch bundle.

4. Bloch bundle and the Berry connection

The cartesian product $\mathcal{E} := \mathbb{T}^d \times \mathcal{H}_f$ can be seen as a **trivial vector bundle** with base space \mathbb{T}^d and fibres $\mathcal{E}_k = \mathcal{H}_f$.

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The spectral projections $P(k)$ define a subbundle

$$\mathcal{E}^P := \{ (k, \psi) \in \mathbb{T}^d \times \mathcal{H}_f \mid \psi \in P(k)\mathcal{H}_f \},$$

called the **Bloch bundle**.

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A section $\psi \in \Gamma(\mathcal{E})$ of the trivial bundle $\mathcal{E} = \mathbb{T}^d \times \mathcal{H}_f$ is just a map

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A section $\psi \in \Gamma(\mathcal{E}^P)$ of the Bloch bundle \mathcal{E}^P is a map $\psi : \mathbb{T}^d \rightarrow \mathcal{H}_f$ with

$$P(k)\psi(k) = \psi(k) \quad \text{for all } k \in \mathbb{T}^d.$$

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$$\mathcal{E}^P := \{ (k, \psi) \in \mathbb{T}^d \times \mathcal{H}_f \mid \psi \in P(k)\mathcal{H}_f \},$$

called the **Bloch bundle**.

A section $\psi \in \Gamma(\mathcal{E})$ of the trivial bundle $\mathcal{E} = \mathbb{T}^d \times \mathcal{H}_f$ is just a map

$$\psi : \mathbb{T}^d \rightarrow \mathcal{H}_f.$$

A section $\psi \in \Gamma(\mathcal{E}^P)$ of the Bloch bundle \mathcal{E}^P is a map $\psi : \mathbb{T}^d \rightarrow \mathcal{H}_f$ with

$$P(k)\psi(k) = \psi(k) \quad \text{for all } k \in \mathbb{T}^d.$$

A **connection** ∇ on a vector bundle \mathcal{E} over \mathbb{T}^d is a “derivative”, i.e. a \mathbb{C} -linear map

$$\nabla : \Gamma(\mathcal{E}) \rightarrow \Gamma(T^*\mathbb{T}^d \otimes \mathcal{E})$$

satisfying the Leibniz rule

$$\nabla_{k_i}(f\psi) = \partial_{k_i} f \cdot \psi + f \nabla_{k_i} \psi \quad \text{for all } f \in C^\infty(\mathbb{T}^d).$$

4. Bloch bundle and the Berry connection

The **trivial connection** on $\mathbb{T}^d \times \mathcal{H}_f$ is

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The **curvature 2-form of a connection** is the endomorphism-valued 2-form

$$\Omega_{ij} \psi = \nabla_{k_i} \nabla_{k_j} \psi - \nabla_{k_j} \nabla_{k_i} \psi$$

4. Bloch bundle and the Berry connection

Proposition

The curvature 2-form of the Berry connection on the Bloch bundle is given by

$$\Omega_{ij}^{\mathbb{B}}(k) = P(k) [\partial_{k_i} P(k), \partial_{k_j} P(k)] .$$

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Proof.

For $\psi \in \Gamma(\mathcal{E}^P)$ we have that

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4. Adiabatic currents: Geometric aspects

Hence for a periodic time-dependent Hamiltonian $H(t)$ the transported charge in direction j is given by

$$\begin{aligned}\Delta Q_j &= \int_0^T \tau(P(t) \left[\frac{d}{dt} P(t), [X_j, P(t)] \right]) dt + \mathcal{O}(\varepsilon^N) \\ &= \frac{i}{(2\pi)^d} \int_0^T \int_{\mathbb{T}^d} \text{tr}_{\mathcal{H}_f} \left(P(t, k) \left[\dot{P}(t, k), \nabla_{k_j} P(t, k) \right] \right) dk dt + \mathcal{O}(\varepsilon^N) \\ &= \frac{i}{(2\pi)^d} \int_0^T \int_{\mathbb{T}^d} \text{tr}_{\mathcal{H}_f} \Omega_{0j}^B(t, k) dk dt + \mathcal{O}(\varepsilon^N),\end{aligned}$$

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where we identify $t = k_0$.

For $d = 1$ the curvature form is a volume form and for periodic driving the transported charge per cycle is quantized,

$$\frac{i}{2\pi} \int_0^T \int_{\mathbb{T}^1} \text{tr}_{\mathcal{H}_f} \Omega_{01}^B(t, k) dk dt \in \mathbb{Z} .$$

4. Adiabatic currents: Geometric aspects

Assume for simplicity that $P(t, k)$ has rank one, i.e. that

$$\mathcal{E}^P := \left\{ ((t, k), \psi) \in ([0, T] \times \mathbb{T}^d) \times \mathcal{H}_f \mid \psi \in P(t, k)\mathcal{H}_f \right\},$$

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$$\begin{aligned} (\nabla_{k_j}^B \psi)(t, k) &= |\varphi(t, k)\rangle \langle \varphi(t, k)| \partial_{k_j} (f\varphi)(t, k) \\ &= (\partial_{k_j} f(t, k) + \langle \varphi(t, k), \partial_{k_j} \varphi(t, k) \rangle f(t, k)) \varphi(t, k) \\ &=: \{(\partial_{k_j} - i\mathcal{A}_j(t, k)) f(t, k)\} \varphi(t, k) \end{aligned}$$

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and

$$\begin{aligned} (\nabla_t^B \psi)(t, k) &= (\partial_t f(t, k) + \langle \varphi(t, k), \partial_t \varphi(t, k) \rangle f(t, k)) \varphi(t, k) \\ &=: \{(\partial_t - i\Phi(t, k)) f(t, k)\} \varphi(t, k) \end{aligned}$$

4. Adiabatic currents: Geometric aspects

with

$$\mathcal{A}_j(t, k) = i\langle \varphi(t, k), \partial_{k_j} \varphi(t, k) \rangle \quad \text{and} \quad \Phi(t, k) = i\langle \varphi(t, k), \partial_t \varphi(t, k) \rangle.$$

Then the piezoelectric curvature can be written in the form

$$\begin{aligned} \Theta(t, k) &:= i \operatorname{tr}_{\mathcal{H}_f} \Omega_{0j}^{\mathbb{B}}(t, k) = i \operatorname{tr}_{\mathcal{H}_f} \left(P(t, k) \left[\dot{P}(t, k), \nabla_{k_j} P(t, k) \right] \right) \\ &= -\partial_t \mathcal{A}_j(t, k) - \partial_{k_j} \Phi(t, k) \end{aligned}$$

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and we obtain the **King-Smith and Vanderbilt formula**

$$\Delta Q_j = \frac{i}{(2\pi)^d} \int_0^T \int_{\mathbb{T}^d} \operatorname{tr}_{\mathcal{H}_f} \Omega_{0j}^B(t, k) dk dt$$

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4. Adiabatic currents: Geometric aspects

In the case $d = 1$ a trivializing section φ always exists and for a time-periodic Hamiltonian one has

$$\varphi(T, k) = e^{-i\theta(k)}\varphi(0, k)$$

with $\theta \in C^\infty([0, 2\pi], \mathbb{R})$ and $\theta(2\pi) - \theta(0) \in 2\pi\mathbb{Z}$.

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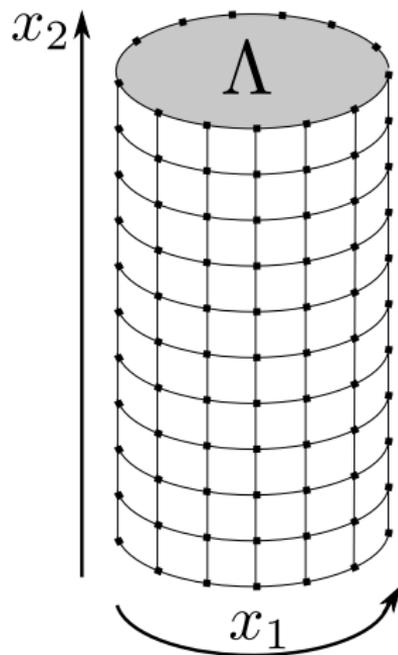
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5. Adiabatic theorems for extended interacting systems

Consider now a system of interacting fermions on the domain Λ , where $\Lambda \subset \mathbb{Z}^d$ is the centred cube of side-length L , possibly with some of the faces identified.

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A typical Hamiltonian could be of the form

$$\begin{aligned} H_0^\Lambda &= \sum_{(x,y) \in \Lambda^2} a_x^* T(x-y) a_y + \sum_{x \in \Lambda} a_x^* \phi(x) a_x \\ &+ \sum_{\{x,y\} \subset \Lambda} a_x^* a_x W(d^\Lambda(x,y)) a_y^* a_y - \mu \mathfrak{N}_\Lambda, \end{aligned}$$

where $a_{x,i}^*$ and $a_{x,i}$ are standard fermionic creation and annihilation operators of fermions with “spin” $i \in \{1, \dots, m\}$ at the sites $x \in \Lambda$.

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In the following by a “**local Hamiltonian**” we mean a family $A = \{A^\Lambda\}_\Lambda$ of self-adjoint operators A^Λ indexed by the system size Λ and possibly other parameters that is a “sum of local terms”.

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Typically

$$\|A^\Lambda\| \sim |\Lambda| = L^d.$$

5. Adiabatic theorems for extended interacting systems

Assume that $H_0 = \{H_0^\Lambda\}$ has a ground state that is gapped uniformly in the system size $|\Lambda|$, i.e.

$$\inf_{\Lambda} \text{dist} \left(E_0^\Lambda, \sigma(H_0^\Lambda) \setminus \{E_0^\Lambda\} \right) = g > 0.$$

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Examples

- ▶ Electrons of an insulating material, i.e. with the chemical potential μ in a band gap.
- ▶ The filled Dirac sea.

Proving stability of the gap under small perturbations by local Hamiltonians, i.e. the existence of a spectral gap for

$$H = H_0 + \varepsilon H_1$$

and ε small enough, is a highly nontrivial problem (e.g. *de Roeck, Salmhofer '17; Hastings '17* for perturbations of non-interacting H_0).

5. Adiabatic theorems for extended interacting systems

As observed by *Niu and Thouless '84* and by *Avron and Seiler '85*, one can apply the **adiabatic theorem** to a time-dependent family of such Hamiltonians with a gapped ground state in order to understand quantization of the Hall conductance for interacting fermions. (Their argument will be explained later.)

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The main difference to the previous section is that one now applies the adiabatic theorem to the **many-body evolution of the initial many-body ground state** of a large but finite system.

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The main difference to the previous section is that one now applies the adiabatic theorem to the **many-body evolution of the initial many-body ground state** of a large but finite system.

However, the constants in the error terms of the adiabatic theorem grow, as we saw in the proof of Kato's version, typically as

$$\|U^{\varepsilon, \Lambda}(t) - U_a^{\varepsilon, \Lambda}(t)\| \leq \varepsilon \left(\int_0^t \|\dot{H}^\Lambda(s)\| ds + \dots \right) \sim \varepsilon |\Lambda| = \varepsilon L^d.$$

Hence, the usual adiabatic theorem is of no use if one is interested in approximations that are uniform in the size of the system and that survive the thermodynamic limit.

5. Adiabatic theorems for extended interacting systems

This error bound can not be improved, since for N non-interacting particles in a product state $\psi_1 \wedge \cdots \wedge \psi_N$ one easily finds that

$$\begin{aligned} & \| (U^{\varepsilon, N}(t) - U_a^{\varepsilon, N}(t)) \psi \| = \\ &= \| U^{\varepsilon, 1}(t) \psi_1 \wedge \cdots \wedge U^{\varepsilon, 1}(t) \psi_N - U_a^{\varepsilon, 1}(t) \psi_1 \wedge \cdots \wedge U_a^{\varepsilon, 1}(t) \psi_N \| \\ &= \sum_{n=1}^N \| (U^{\varepsilon, 1}(t) - U_a^{\varepsilon, 1}(t)) \psi_n \| \sim N \varepsilon. \end{aligned}$$

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$$\begin{aligned} & \| (U^{\varepsilon, N}(t) - U_a^{\varepsilon, N}(t)) \psi \| = \\ &= \| U^{\varepsilon, 1}(t) \psi_1 \wedge \cdots \wedge U^{\varepsilon, 1}(t) \psi_N - U_a^{\varepsilon, 1}(t) \psi_1 \wedge \cdots \wedge U_a^{\varepsilon, 1}(t) \psi_N \| \\ &= \sum_{n=1}^N \| (U^{\varepsilon, 1}(t) - U_a^{\varepsilon, 1}(t)) \psi_n \| \sim N \varepsilon. \end{aligned}$$

In the previous section the way out was to consider the adiabatic evolution of the one-body density matrix.

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In the previous section the way out was to consider the adiabatic evolution of the one-body density matrix.

Recently, *Bachmann, De Roeck, and Fraas '17 (v4)* proved an adiabatic theorem for extended lattice systems showing

$$\left| \langle U^{\varepsilon, \Lambda}(t) \psi, O U^{\varepsilon, \Lambda}(t) \psi \rangle - \langle U_a^{\varepsilon, \Lambda}(t) \psi, O U_a^{\varepsilon, \Lambda}(t) \psi \rangle \right| \leq \varepsilon C \|O\| |\text{supp } O|^2$$

for $\psi \in \text{ran} P(0)$ and for local observables O with a constant C independent of the system size Λ .

5. Fermions on the lattice: mathematical formalism

To each finite subset $\Lambda \subset \mathbb{Z}^d$ one associates a corresponding

- ▶ **one-particle Hilbert space** $\mathfrak{h}_\Lambda = \ell^2(\Lambda, \mathbb{C}^\ell)$

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Let $a_{i,x}$ and $a_{i,x}^*$, $i = 1, \dots, \ell$, $x \in \Gamma$, be the standard fermionic annihilation and creation operators satisfying the canonical anti-commutation relations

$$\{a_{i,x}, a_{j,y}^*\} = \delta_{i,j} \delta_{x,y} \mathbf{1}_{\mathfrak{F}_\Lambda} \quad \text{and} \quad \{a_{i,x}, a_{j,y}\} = 0 = \{a_{i,x}^*, a_{j,y}^*\}.$$

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For a subset $X \subset \Lambda$ we denote by $\mathcal{A}_X \subset \mathcal{L}(\mathfrak{F}_\Lambda)$ the algebra of operators generated by the set

$$\{\mathbf{1}, a_{i,x}, a_{i,x}^* \mid x \in X, i = 1, \dots, \ell\}.$$

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$\{\mathbf{1}, a_{i,x}, a_{i,x}^* \mid x \in X, i = 1, \dots, \ell\}$. Those elements of \mathcal{A}_X commuting with the number operator

$$\mathfrak{N}_X := \sum_{x \in X} a_x^* a_x := \sum_{x \in X} \sum_{j=1}^{\ell} a_{j,x}^* a_{j,x}$$

form a subalgebra $\mathcal{A}_X^{\mathfrak{N}}$ of \mathcal{A}_X contained in the subalgebra \mathcal{A}_X^+ of even elements, i.e. $\mathcal{A}_X^{\mathfrak{N}} \subset \mathcal{A}_X^+ \subset \mathcal{A}_X$.

5. Fermions on the lattice: mathematical formalism

Let $\mathcal{F}(\Gamma) := \{X \subset \Gamma \mid |X| < \infty\}$ denote the set of all finite subsets of Γ , and define analogously also $\mathcal{F}(\Lambda) := \{X \subset \Lambda\}$.

An **interaction** $\Phi = \{\Phi^\Lambda\}_{\Lambda \in \mathcal{F}(\Gamma)}$ is a family of maps

$$\Phi^\Lambda : \mathcal{F}(\Lambda) \rightarrow \bigcup_{X \in \mathcal{F}(\Lambda)} \mathcal{A}_X^{\mathfrak{N}}, \quad X \mapsto \Phi^\Lambda(X) \in \mathcal{A}_X^{\mathfrak{N}}$$

taking values in the self-adjoint operators.

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The **Hamiltonian** $A = \{A^\Lambda\}_\Lambda$ associated with the interaction Φ is the family of self-adjoint operators

$$A^\Lambda \equiv A^\Lambda(\Phi) := \sum_{X \subset \Lambda} \Phi^\Lambda(X) \in \mathcal{A}_\Lambda^{\mathfrak{N}}.$$

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Since the norm of a Hamiltonian typically grows as

$$\|A^\Lambda\| \sim |\Lambda| = L^d$$

with the system size, one introduces normed spaces of interactions.

5. Fermions on the lattice: mathematical formalism

Define

$$F(r) := \frac{1}{(1+r)^{d+1}} \quad \text{and} \quad F_\zeta(r) := \frac{\zeta(r)}{(1+r)^{d+1}},$$

where

$$\zeta \in \mathcal{S} := \{ \zeta : [0, \infty) \rightarrow (0, \infty) \mid \zeta \text{ is bounded, non-increasing, satisfies} \\ \zeta(r+s) \geq \zeta(r)\zeta(s) \text{ for all } r, s \in [0, \infty) \text{ and} \\ \sup_{r \geq 0} r^n \zeta(r) < \infty \text{ for all } n \in \mathbb{N} \}.$$

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For each $\zeta \in \mathcal{S}$ and $n \in \mathbb{N}_0$ one defines a **norm on the vector space of interactions** by

$$\|\Phi\|_{\zeta, n} := \sup_{\Lambda} \sup_{x, y \in \Lambda} \sum_{\substack{X \subset \Lambda: \\ \{x, y\} \subset X}} |X|^n \frac{\|\Phi^\wedge(X)\|}{F_\zeta(d^\wedge(x, y))}$$

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The prime example for a function $\zeta \in \mathcal{S}$ is $\zeta(r) = e^{-ar}$ for some $a > 0$. For this specific choice of ζ we write F_a and $\|\Phi\|_{a, n}$ for the corresponding norm.

5. Fermions on the lattice: mathematical formalism

Let $\mathcal{B}_{\zeta,n}$ be the Banach space of interactions with finite $\|\cdot\|_{\zeta,n}$ -norm, and put

$$\mathcal{B}_{\mathcal{S},n} := \bigcup_{\zeta \in \mathcal{S}} \mathcal{B}_{\zeta,n}, \quad \mathcal{B}_{\mathcal{E},n} := \bigcup_{a>0} \mathcal{B}_{a,n},$$

and

$$\mathcal{B}_{\mathcal{S},\infty} := \bigcap_{n \in \mathbb{N}_0} \mathcal{B}_{\mathcal{S},n}, \quad \mathcal{B}_{\mathcal{E},\infty} := \bigcap_{n \in \mathbb{N}_0} \mathcal{B}_{\mathcal{E},n}.$$

The corresponding spaces of Hamiltonians are denoted by $\mathcal{L}_{\zeta,n}$, $\mathcal{L}_{\mathcal{E},n}$, $\mathcal{L}_{\mathcal{E},\infty}$, $\mathcal{L}_{\mathcal{S},n}$, and $\mathcal{L}_{\mathcal{S},\infty}$ respectively.

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Lemma

Let $H = \{H^\Lambda\} \in \mathcal{L}_{\zeta,0}$, then there is a constant C_ζ such that

$$\|H^\Lambda\| \leq C_\zeta |\Lambda| \|\Phi_H\|_{\zeta,0}.$$

5. Fermions on the lattice: mathematical formalism

Assumption: Regularity of the Hamiltonian:

Let $\Phi_H(t)$, $t \in \mathbb{R}$, be a time-dependent interaction with

$$\|\Phi_H\|_{a,n,T} := \sup_{t \in [-T, T]} \|\Phi_H\|_{a,n} < \infty$$

for some $a > 0$ and all $T > 0$ and $n \in \mathbb{N}_0$.

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Let $N \in \mathbb{N}$ and assume that each map $[0, \infty) \rightarrow \mathcal{A}_X^{\mathfrak{M}}$, $t \mapsto \Phi_H^\wedge(t, X)$ is $(N + d)$ -times differentiable.

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Let $\{(\Phi_H^\wedge)^{(k)}(t)\}_\Lambda$ be the time-dependent interactions defined by their k -th derivatives, for $1 \leq k \leq N + d$. Assume that

$$\sup_{1 \leq k \leq N+d} \|(\Phi_H^\wedge)^{(k)}\|_{a,n,T} < \infty \quad \text{for any } T > 0 \text{ and } n \in \mathbb{N}_0.$$

5. Fermions on the lattice: mathematical formalism

Assumption: Gapped part of the spectrum

We assume that there exists $L_0 \in \mathbb{N}$ such that for all $L \geq L_0$ and corresponding $\Lambda = \Lambda(L)$ the operator $H^\Lambda(t)$ has a gapped part $\sigma_*^\Lambda(t) \subset \sigma(H^\Lambda(t))$ of its spectrum in the following sense:

There exist continuous functions $f_\pm^\Lambda : \mathbb{R} \rightarrow \mathbb{R}$ and constants $g > \tilde{g} > 0$ such that

$$f_\pm^\Lambda(t) \in \rho(H^\Lambda(t)),$$

$$f_+^\Lambda(t) - f_-^\Lambda(t) \leq \tilde{g},$$

$$[f_-^\Lambda(t), f_+^\Lambda(t)] \cap \sigma(H^\Lambda(t)) = \sigma_*^\Lambda(t),$$

$$\text{dist} \left(\sigma_*^\Lambda(t), \sigma(H^\Lambda(t)) \setminus \sigma_*^\Lambda(t) \right) \geq g$$

for all $t \in \mathbb{R}$ and $L \geq L_0$.

We denote again by $P^\Lambda(t)$ the spectral projection of $H^\Lambda(t)$ corresponding to the spectrum $\sigma_*^\Lambda(t)$.

5. Adiabatic theorems for extended interacting systems

Super-adiabatic theorem for extended systems (Monaco, T. '17)

There exist smooth operator-valued functions $V^{\varepsilon, \Lambda}, K^{\varepsilon, \Lambda} \in C^1(\mathbb{R}, \mathcal{L}(\mathcal{F}^\Lambda))$ such that $V^{\varepsilon, \Lambda}(t)$ is **unitary** and $K^{\varepsilon, \Lambda}(t)$ is **self-adjoint** for all $t \in \mathbb{R}$. Let

$$H_a^{\varepsilon, \Lambda}(t) := H^\Lambda(t) + \varepsilon K^{\varepsilon, \Lambda}(t) \quad \text{and} \quad P^{\varepsilon, \Lambda}(t) := V^{\varepsilon, \Lambda}(t) P^\Lambda(t) V^{\varepsilon, \Lambda}(t)^*.$$

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The solution to

$$i\varepsilon \frac{d}{dt} U_a^{\varepsilon, \Lambda}(t, s) = H_a^{\varepsilon, \Lambda}(t) U_a^{\varepsilon, \Lambda}(t, s), \quad U_a^{\varepsilon, \Lambda}(s) = \mathbf{1}_{\mathcal{H}}$$

satisfies

$$U_a^{\varepsilon, \Lambda}(t, s)^* P^\Lambda(t) U_a^{\varepsilon, \Lambda}(t, s) = P^\Lambda(s)$$

and we define again the **super-adiabatic evolution** by

$$U_{sa}^{\varepsilon, \Lambda}(t, s) := V^{\varepsilon, \Lambda}(t) U_a^{\varepsilon, \Lambda}(t, s) V^{\varepsilon, \Lambda}(s)^*.$$

5. Adiabatic theorems for extended interacting systems

Super-Adiabatic Theorem for extended systems (continued)

Then for any $\zeta \in \mathcal{S}$ there exists a constant $C_\zeta < \infty$, such that for any initial state $\rho_0^{\varepsilon, \Lambda}$ with $P^{\varepsilon, \Lambda}(0) \rho_0^{\varepsilon, \Lambda} P^{\varepsilon, \Lambda}(0) = \rho_0^{\varepsilon, \Lambda}$ and any $B \in \mathcal{L}_{\zeta, 2}$ it holds that

$$\sup_{\Lambda} \frac{1}{|\Lambda|} \left| \text{tr} \left(\left(\rho^{\varepsilon, \Lambda}(t) - U_{\text{sa}}^{\varepsilon, \Lambda}(t) \rho_0^{\varepsilon, \Lambda} U_{\text{sa}}^{\varepsilon, \Lambda}(t)^* \right) B^\Lambda \right) \right| \leq C_\zeta |t| (1 + |t|)^d \varepsilon^N \|\Phi_B\|_{\zeta, 2},$$

where $\rho^{\varepsilon, \Lambda}(t)$ is the solution of

$$i\varepsilon \frac{d}{dt} \rho^{\varepsilon, \Lambda}(t) = [H^\Lambda(t), \rho^{\varepsilon, \Lambda}(t)], \quad \rho^{\varepsilon, \Lambda}(0) = \rho_0^{\varepsilon, \Lambda}.$$

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$$i\varepsilon \frac{d}{dt} \rho^{\varepsilon, \Lambda}(t) = [H^\Lambda(t), \rho^{\varepsilon, \Lambda}(t)], \quad \rho^{\varepsilon, \Lambda}(0) = \rho_0^{\varepsilon, \Lambda}.$$

If $\frac{d^n}{dt^n} H(t') = 0$ for some $t' \in \mathbb{R}$ and all $n = 1, \dots, N$, then

$$V^{\varepsilon, \Lambda}(t') = \text{id} \quad \text{and} \quad K^{\varepsilon, \Lambda}(t') = 0.$$

5. Adiabatic theorems for extended interacting systems

We only highlight some new aspects of the proof:

Recall from section 3 that

$$\begin{aligned}\frac{d}{dt} \left(U(t)^* U_{\text{sa}}(t) \right) &= \\ &= \frac{i}{\varepsilon} U(t)^* V(t) \left(V(t)^* H(t) V(t) - H_a(t) + i\varepsilon \dot{V}(t)^* V(t) \right) V(t)^* U_{\text{sa}}(t) \\ &=: \frac{i}{\varepsilon} U(t)^* R(t) U_{\text{sa}}(t).\end{aligned}$$

For the norm-estimates at fixed Λ , it was sufficient to show that

$$\|R^{\varepsilon, \Lambda}(t)\| = \mathcal{O}(|\Lambda| \varepsilon^{N+1}).$$

Now one needs to show that $R^{\varepsilon, \Lambda}$ is a local Hamiltonian with

$$\|\Phi_{R^{\varepsilon}}(t)\| = \mathcal{O}(\varepsilon^{N+1}).$$

Then a clever use of **Lieb-Robinson propagation bounds** allows to prove the theorem.

5. Adiabatic theorems for extended interacting systems

Recall that

$$V^{\varepsilon, \Lambda}(t) = e^{i\varepsilon \sum_{n=1}^N \varepsilon^{n-1} A_n^\Lambda(t)}$$

and

$$K^{\varepsilon, \Lambda}(t) = \sum_{n=1}^N \varepsilon^n K_n^\Lambda(t)$$

appearing in the construction of $R^{\varepsilon, \Lambda}(t)$ were constructed inductively starting from $K_1 = [\dot{P}, P]$ and H by taking commutators and inverting the map $\text{ad}_H(\cdot) = [H, \cdot]$ restricted to off-diagonal operators.

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Now there are two problems:

- ▶ The spectral projection P and thus also Kato's generator of parallel transport $K_1 = [\dot{P}, P]$ are **not** local Hamiltonians.
- ▶ While ad_H maps local Hamiltonians to local Hamiltonians, its inverse restricted to off-diagonal operators does not.

5. The local inverse of ad_H

The following construction is based on the one used by *Hastings, Wen '05* and *Bachmann, Michalakis, Nachtergaele, Sims '12* in the context of the so called **quasi-adiabatic flow** and by *Bachmann, de Roeck, Frass '17* in their version of the adiabatic theorem for extended systems.

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First note that for $g > \tilde{g} > 0$ one can find a real-valued, odd function $\mathcal{W}_{g,\tilde{g}} \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ satisfying

$$\sup_{s \in \mathbb{R}} |s|^n |\mathcal{W}_{g,\tilde{g}}(s)| < \infty \quad \text{for all } n \in \mathbb{N},$$

and with a Fourier transform satisfying

$$\widehat{\mathcal{W}}_{g,\tilde{g}}(\omega) = \frac{-i}{\sqrt{2\pi\omega}} \quad \text{for } |\omega| \geq g \quad \text{and} \quad \widehat{\mathcal{W}}_{g,\tilde{g}}(\omega) = 0 \quad \text{for } |\omega| \leq \tilde{g}.$$

5. The local inverse of ad_H

Lemma: The local inverse of ad_H

The map

$$\mathcal{I}_H^\wedge : \mathcal{A}_\wedge \rightarrow \mathcal{A}_\wedge, \quad A \mapsto \mathcal{I}_H^\wedge(A) := \int_{\mathbb{R}} \mathcal{W}_{g, \tilde{g}}(s) e^{iH^\wedge s} A e^{-iH^\wedge s} ds$$

satisfies

$$\mathcal{I}_H^\wedge|_{\mathcal{A}_\wedge^{\text{od}}} = i \text{ad}_H|_{\mathcal{A}_\wedge^{\text{od}}}^{-1}$$

and

$$P^\wedge \mathcal{I}_H^\wedge(A) P^\wedge = 0 \quad \text{for all } A \in \mathcal{A}_\wedge.$$

Moreover, if $A \in \mathcal{L}_{S, \infty}$, then

$$\{\mathcal{I}_H^\wedge(A^\wedge)\} \in \mathcal{L}_{S, \infty}.$$

5. The local inverse of ad_H (proof)

Inserting the spectral decomposition of $H = \sum_n E_n P_n$ into the definition of \mathcal{I} , we find that

$$\begin{aligned}\mathcal{I}_H(A) &= \sum_{n,m} \int_{\mathbb{R}} \mathcal{W}_{g,\tilde{g}}(s) e^{iE_n s} P_n A P_m e^{-iE_m s} ds \\ &= \sqrt{2\pi} \sum_{n,m} \widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) P_n A P_m.\end{aligned}$$

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Inserting the spectral decomposition of $H = \sum_n E_n P_n$ into the definition of \mathcal{I} , we find that

$$\begin{aligned}\mathcal{I}_H(A) &= \sum_{n,m} \int_{\mathbb{R}} \mathcal{W}_{g,\tilde{g}}(s) e^{iE_n s} P_n A P_m e^{-iE_m s} ds \\ &= \sqrt{2\pi} \sum_{n,m} \widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) P_n A P_m.\end{aligned}$$

For $E_n \in \sigma_*$ and $E_m \in \sigma(H) \setminus \sigma_*$ it holds that $|E_m - E_n| \geq g$, i.e. $\widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) = \frac{-i}{\sqrt{2\pi}(E_m - E_n)}$. Hence, for $A = A_{\text{od}}$ it holds that

$$\begin{aligned}-i[H, \mathcal{I}_H(A)] &= i\sqrt{2\pi} \sum_{n,m} \widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) P_n A P_m (E_m - E_n) \\ &= \sum_{n \in \sigma_*, m \notin \sigma_*} P_n A P_m + \sum_{n \notin \sigma_*, m \in \sigma_*} P_n A P_m \\ &= PAP^\perp + P^\perp AP = A_{\text{od}} = A.\end{aligned}$$

5. The local inverse of ad_H (proof)

Inserting the spectral decomposition of $H = \sum_n E_n P_n$ into the definition of \mathcal{I} , we find that

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On the other hand, since for $E_n, E_m \in \sigma_*$ it holds that $|E_m - E_n| \leq \tilde{g}$, i.e. $\widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) = 0$, we have that

$$P \mathcal{I}_H(A) P = \sqrt{2\pi} \sum_{n \in \sigma_*, m \in \sigma_*} \widehat{\mathcal{W}}_{g,\tilde{g}}(E_m - E_n) P_n A P_m = 0.$$

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The claim that $\mathcal{I}_H(\mathcal{L}_{S,\infty}) \subset \mathcal{L}_{S,\infty}$ is highly non-trivial and uses again Lieb-Robinson bounds.

5. Adiabatic theorems for extended interacting systems

Now there are two problems:

- ▶ The spectral projection P and thus also Kato's generator of parallel transport $K_1 = [\dot{P}, P]$ are **not** local Hamiltonians.
- ▶ While ad_H maps local Hamiltonians to local Hamiltonians, its inverse restricted to off-diagonal operators does not.

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The first problem is solved by replacing K_1 by $\mathcal{I}_H(\dot{H})$, since

$$\begin{aligned} [\mathcal{I}_H(\dot{H}), P] &= \mathcal{I}_H([\dot{H}, P]) = \mathcal{I}_H \left(\left[\sum_n (\dot{E}_n P_n + E_n \dot{P}_n, P) \right] \right) \\ &= \sum_n E_n \mathcal{I}_H([\dot{P}_n, P]) = - \sum_n E_n \mathcal{I}_H([P_n, \dot{P}]) \\ &= - \left[\sum_n E_n P_n, \mathcal{I}_H(\dot{P}) \right] = [H, \mathcal{I}_H(\dot{P})] \\ &= i\dot{P} = i[[\dot{P}, P], P] = [K_1, P] \end{aligned}$$

and therefore $\mathcal{I}_H(\dot{H})_{\text{od}} = K_1$ and $P\mathcal{I}_H(\dot{H})P = 0$.

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- ▶ The spectral projection P and thus also Kato's generator of parallel transport $K_1 = [\dot{P}, P]$ are **not** local Hamiltonians.
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The second problem is solved by now taking

$$A_\mu = \mathcal{I}_H(L_\mu - Q_\mu) \quad \text{and} \quad K_\mu = (Q_\mu - L_\mu) + i \text{ad}_H(A_\mu)$$

instead of

$$A_\mu = i \text{ad}_H^{-1}(L_\mu - Q_\mu)_{\text{od}} \quad \text{and} \quad K_\mu = (Q_\mu - L_\mu)_{\text{dia}}.$$

Due to the fact that $P\mathcal{I}_H(B)P = 0$ for any $B \in \mathcal{A}$, the $P \cdots P$ -blocks of A_μ and K_μ remain unchanged. Hence, the actions of the adiabatic evolution U_a and of the superadiabatic transformation V remain unchanged when acting on states in $\text{ran}P$.

5. Adiabatic theorems for extended interacting systems

Remarks:

- ▶ In *Monaco, T. '17* we prove a more general statement: If the driving \dot{H} is supported near a subspace of dimension d_1 and the observable B is supported near a subspace of dimension d_2 and the intersection of these subspaces has dimension d_{12} , then the normalization $|\Lambda|^{-1} = L^{-d}$ in the trace per unit volume can be replaced by $L^{-d_{12}}$.

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- ▶ We also provide an explicit asymptotic expansion of

$$U_{\text{sa}}^{\varepsilon, \Lambda}(t) \rho_0^{\varepsilon, \Lambda} U_{\text{sa}}^{\varepsilon, \Lambda}(t)^* .$$

If $\sigma_* = \{E\}$ is a single non-degenerate eigenvalue, then

$$U_{\text{sa}}^{\varepsilon, \Lambda}(t) \rho_0^{\varepsilon, \Lambda} U_{\text{sa}}^{\varepsilon, \Lambda}(t)^* = P(t) + i\varepsilon \left[(H(t) - E(t))^{-1} P^\perp(t), \dot{P}(t) \right] + \mathcal{O}(\varepsilon^2) .$$

6. Derivation of the Kubo formula for the Hall conductance

The adiabatic theorem with error bounds uniform in the system size now allows to redo the derivation of the **Kubo formula for the Hall conductance** given independently by *Avron, Seiler '85* and *Niu, Thouless '84* with error estimates uniform in the system size Λ .

6. Derivation of the Kubo formula for the Hall conductance

Let H be a uniformly finite-range gapped Hamiltonian and define

$$\mathfrak{N}_j := \sum_{x \in \Lambda_j} a_x^* a_x \in \mathcal{A}_\Lambda^{\mathfrak{N}},$$

that is, the number operator counting particles in the right, resp. upper, half $\Lambda_j := \{x \in \Lambda \mid x_j \geq 0\}$, $j = 1, 2$, of the square Λ .

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that is, the number operator counting particles in the right, resp. upper, half $\Lambda_j := \{x \in \Lambda \mid x_j \geq 0\}$, $j = 1, 2$, of the square Λ . Then the interaction of the Hamiltonian $H(\beta_1, \beta_2)$ is defined in two steps as

$$\Phi_{H(\beta_1, 0)}^\Lambda(X) := \begin{cases} e^{-i\beta_1 \mathfrak{N}_1} \Phi_H^\Lambda(X) e^{i\beta_1 \mathfrak{N}_1} & \text{if } X \cap \Lambda_1 \neq \emptyset, X \cap \Lambda \setminus \Lambda_1 \neq \emptyset, \\ & \text{and } \text{dist}(X, \{x_1 = 0\}) \leq r \\ \Phi_H^\Lambda(X) & \text{otherwise,} \end{cases}$$

and then

$$\Phi_{H(\beta_1, \beta_2)}^\Lambda(X) := \begin{cases} e^{-i\beta_2 \mathfrak{N}_2} \Phi_{H(\beta_1, 0)}^\Lambda(X) e^{i\beta_2 \mathfrak{N}_2} & \text{if } X \cap \Lambda_2 \neq \emptyset, \\ & X \cap \Lambda \setminus \Lambda_2 \neq \emptyset, \\ & \text{and } \text{dist}(X, \{x_2 = 0\}) \leq r \\ \Phi_{H(\beta_1, 0)}^\Lambda(X) & \text{otherwise.} \end{cases}$$

6. Derivation of the Kubo formula for the Hall conductance

Then

$$\partial_{\beta_j} H(\beta_1, \beta_2) \stackrel{=} i [H(\beta_1, \beta_2), \mathcal{N}_j] = -\dot{\mathcal{N}}_j,$$

where, however, only the particle flow through the line $x_j = 0$ is counted. Hence, $\partial_{\beta_j} H(\beta_1, \beta_2)$ is interpreted as the “current through the line $x_j = 0$ operator”.

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Now consider the time-dependent Hamiltonian

$$H(t) := H(0, t\delta V)$$

modelling a voltage drop δV at the line $x_2 = 0$.

One is interested in the induced current through the line $x_1 = 0$, i.e. in the expectation value of

$$I(t) := \partial_{\beta_1} H(\beta_1, t\delta V)|_{\beta_1=0}.$$

6. Derivation of the Kubo formula for the Hall conductance

Assume that $H(0, t\delta V)$ has a gapped nondegenerate ground state $\varphi_0(t)$ for all $t \in [0, 2\pi/\delta V)$, i.e. $P(t) = |\varphi_0(t)\rangle\langle\varphi_0(t)|$.

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Using the super-adiabatic theorem including first order corrections to the adiabatic evolution one finds that

$$\begin{aligned}\mathrm{tr}\left(\rho^{\delta V}(t)I(t)\right) &= \mathrm{tr}\left((P(t) + \delta V P_1(t)) \partial_1 H(t)\right) \\ &= \delta V \mathrm{tr}\left(\left[(H(t) - E(t))^{-1} P^\perp(t), \partial_2 P(t)\right] \partial_1 H(t)\right) \\ &= \delta V \mathrm{tr}\left(P(t) [\partial_1 P(t), \partial_2 P(t)]\right) \\ &= \delta V \cdot 2 \mathrm{Im} \langle \partial_1 \varphi_0(0, t \delta V), \partial_2 \varphi_0(0, t \delta V) \rangle + \mathcal{O}(\delta V^2),\end{aligned}$$

where the error term is **uniform in the system size**.

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where the error term is **uniform in the system size**.

We thus proved that the Hall conductance for the finite system at finite voltage δV is given by

$$\sigma_{12}^{\delta V, \Lambda}(t) = 2 \mathrm{Im} \left\langle \partial_1 \varphi_0^\Lambda(0, \delta V t), \partial_2 \varphi_0^\Lambda(0, \delta V t) \right\rangle + \mathcal{O}(\delta V).$$

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Klein and Seiler '90 showed that this formula holds with the error estimate replaced by $\mathcal{O}(|\delta V|^\infty)$, however, not uniformly in the system size. But their argument can presumably be transferred to the present setting (*de Roeck '17*, private communication).

6. Quantization of the Hall conductance

Hastings and Michalakis '14 proved that

$$2 \operatorname{Im} \left\langle \partial_1 \varphi_0^\Lambda(0, 0), \partial_2 \varphi_0^\Lambda(0, 0) \right\rangle \in \frac{1}{2\pi} \mathbb{Z} + \mathcal{O}(|\Lambda|^{-\infty}).$$

(see also *Bachmann, Bols, de Roeck, Fraas '17*). Note that they take the Kubo formula we just derived as the definition of Hall conductance.

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Avron, Seiler '85 and *Niu, Thouless '84* originally observed that the conductance averaged over the “flux torus” is quantized,

$$\begin{aligned} & \frac{1}{(2\pi)^2} \int_{\mathbb{T}^2} 2 \operatorname{Im} \left\langle \partial_1 \varphi_0^\Lambda(\beta), \partial_2 \varphi_0^\Lambda(\beta) \right\rangle d\beta \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{T}^2} \operatorname{tr} \left(P^\Lambda(\beta) \left[\partial_1 P^\Lambda(\beta), \partial_2 P^\Lambda(\beta) \right] \right) d\beta \in \frac{1}{2\pi} \mathbb{Z} \end{aligned}$$

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