Adiabatic theorems for particles coupled to massless fields

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Quantum Spectra and Transport,
Conference in Honor of Yosi Avron's 65th Birthday.

1. Introduction

In 1999 Yosi Avron and Alexander Elgart proved an adiabtic theorem without gap condition:

> *Traditionally, the adiabatic theorem is stated for Hamiltonians that have an eigenvalue which is separated by a gap from the rest of the spectrum. Folk wisdom is that some form of a gap condition is sine qua non for an adiabatic theorem to hold.*
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They went on to show that wise folks are not always right.

1. Introduction: recap on adiabatic theorems

Notation and setup

Let $H : \mathbb{R} \to \mathcal{L}(\mathcal{H})$, $t \mapsto H(t)$, be a time-dependent family of self-adjoint Hamiltonians and $U^\varepsilon(t, t_0)$ the solution of

$$\mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} U^\varepsilon(t, t_0) = H(t) U^\varepsilon(t, t_0) \qquad U^\varepsilon(t_0, t_0) = \mathrm{Id}\,.$$

Then the asymptotic limit $\varepsilon \to 0$ is the adiabatic limit.
Let $\sigma_*(t) \subset \sigma(H(t))$ be a subset of the spectrum and $P(t)$ the corresponding spectral projection.

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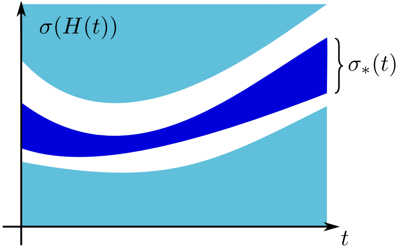
Adiabatic Theorem *Kato (1950)*

The gap condition and $H \in C^2$ imply for any $t_0, T \in \mathbb{R}$ that

$$\sup_{t \in [t_0, T]} \left\| P^\perp(t)\, U^\varepsilon(t, t_0)\, P(t_0) \right\| = \mathcal{O}(\varepsilon)$$



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Higher order adiabatic invariants: Lenard (1959), Garrido (1964)

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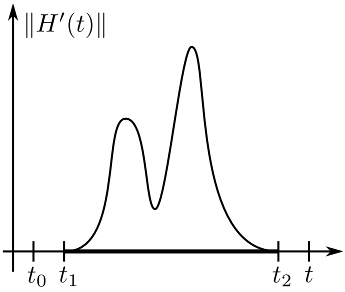
Improved Adiabatic Theorem 1

Version of Avron, Seiler, Yaffe (1987)

Assume in addition to the gap condition and $H \in C^{2+N}$ that $\mathrm{supp}\|H'\| \subset [t_1, t_2]$, then

$$\left\| P^{\perp}(t)\, U^{\varepsilon}(t, t_0)\, P(t_0) \right\| = \mathcal{O}(\varepsilon^{N+1})$$

for any $t_0 \leq t_1 < t_2 \leq t$.



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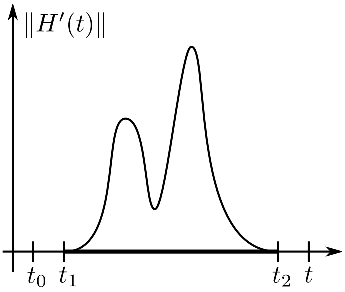

Non-adiabatic transitions $\mathcal{O}(\varepsilon^{N+1})$	$\ll$	Error of the adiabatic approximation $\mathcal{O}(\varepsilon)$

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Improved Adiabatic Theorem 2

Version of Nenciu (1981,1993), Berry (1990)

Assume the gap condition and $H \in C^{N+2}$, then there exist **super-adiabatic subspaces** $\mathrm{Ran}\, P_N^\varepsilon(t)$ with

$$\| P_N^\varepsilon(t) - P(t) \| = \mathcal{O}(\varepsilon) \quad \text{for all } t$$

and

$$P_N^\varepsilon(t) = P(t) \quad \text{if} \quad \tfrac{\mathrm{d}^j}{\mathrm{d}t^j} H(t) = 0 \quad \text{for} \quad j = 1, \ldots, N\,.$$

such that for $t_0, T \in \mathbb{R}$

$$\sup_{t \in [t_0, T]} \left\| P_N^{\varepsilon\perp}(t)\, U^\varepsilon(t, t_0)\, P_N^\varepsilon(t_0) \right\| = \mathcal{O}(\varepsilon^{N+1})\,.$$

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Exponential bounds

Joye, Pfister (1991), Nenciu (1993), Sjöstrand (1993), Jung (2000)

For $t \mapsto H(t)$ analytic there are $P^\varepsilon(t)$ such that one replace $\mathcal{O}(\varepsilon^{N+1})$ by $\mathcal{O}(\mathrm{e}^{-\frac{\gamma}{\varepsilon}})$ in the previous result.

More than bounds: transition probabilities

Zener (1932); . . . ; Joye, Kunz, Pfister (1991), Joye (1993)

Let $t \mapsto H(t)$ be analytic and matrix-valued, let $\sigma_*(t) = \{E(t)\}$ be a simple eigenvalue and let $\lim_{t\to\pm\infty} \|H'(t)\| = 0$. Then

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

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More than bounds: adiabatic transition histories

Berry (1990); Hagedorn, Joye (2004); Betz, T. (2005)

Let $t \mapsto H(t)$ be analytic and 2×2-real-matrix-valued, let $\sigma_*(t) = \{E(t)\}$ be a simple eigenvalue and let $\lim_{t\to\pm\infty} \|H'(t)\| = 0$. Then

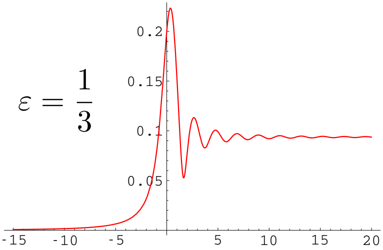
$$\lim_{t_0\to-\infty} \left\| P^{\varepsilon\perp}(t)\, U^{\varepsilon}(t,t_0)P^{\varepsilon}(t_0) \right\|^2 = 4\sin^2\left(\tfrac{\pi\gamma}{2}\right) \mathrm{e}^{-\frac{2\tau_c}{\varepsilon}} \left(\mathrm{erf}\left(\tfrac{t}{\sqrt{2\varepsilon\tau_c}}\right) - 1\right)^2$$

where $P^{\varepsilon}(t)$ are the optimal super-adiabatic projections.

1. Introduction: recap on adiabatic theorems

Plots of $t \mapsto \|P^{\perp}(t)U^{\varepsilon}(t,t_0)P(t_0)\|$ for $t_0 \ll 0$

$$\varepsilon = \frac{1}{3}$$



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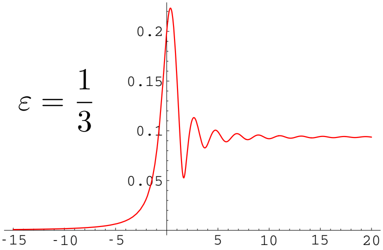
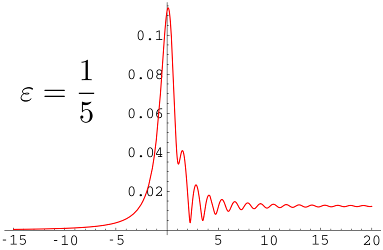


$\varepsilon = \dfrac{1}{5}$



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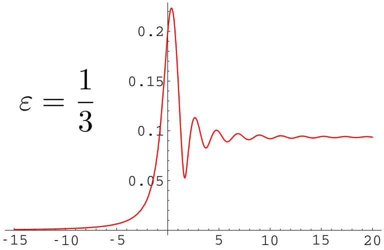

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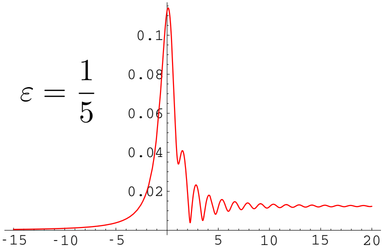
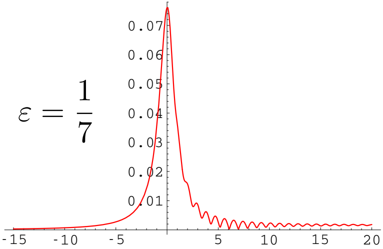


$\varepsilon = \frac{1}{7}$



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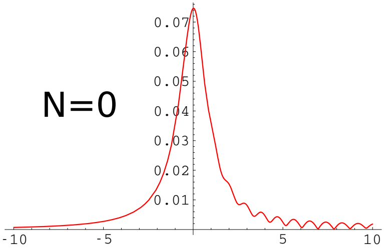
Plots of $t \mapsto \| P_N^{\varepsilon\perp}(t) U^{\varepsilon}(t, t_0) P_N^{\varepsilon}(t_0) \|$ for $t_0 \ll 0$ and $\varepsilon = \frac{1}{7}$.

N=0



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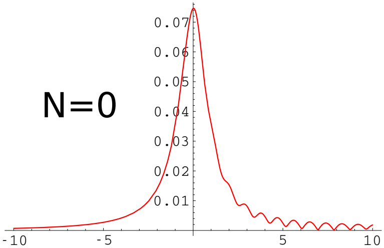

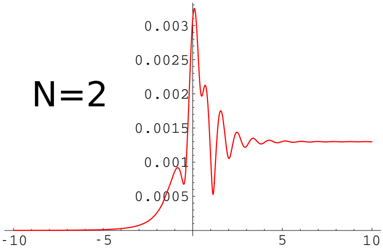

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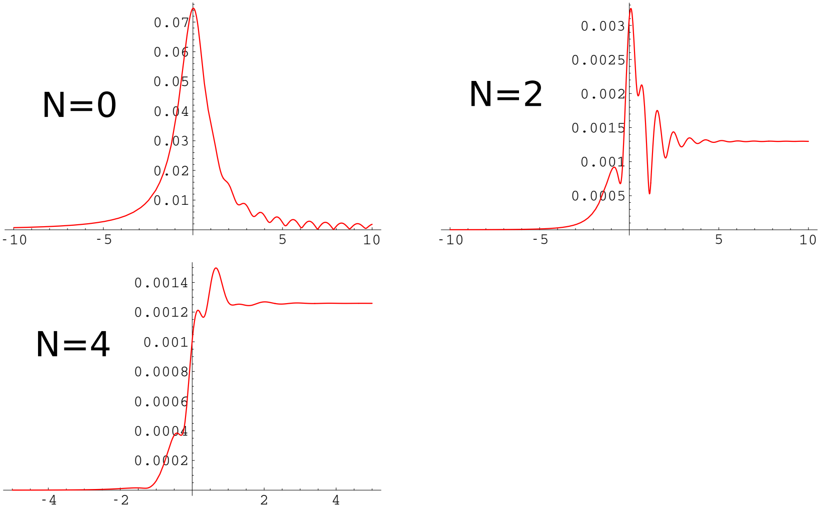

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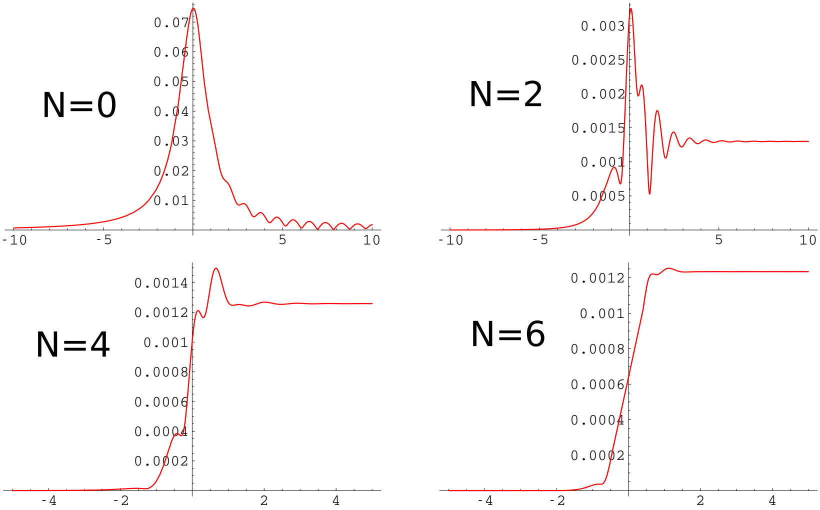

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This suggests to define

Non-adiabatic transitions	$:=$	Transitions with respect to the optimal super-adiabatic subspaces

Adiabatic theorem without gap condition

Avron, Elgart (1999), Bornemann (1998)

Let $\sigma_*(t) = \{E(t)\}$ be an eigenvalue and let $t \mapsto P(t)$ be finite rank and C^2. Then for $t_0, T \in \mathbb{R}$

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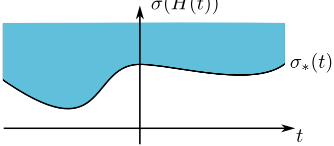

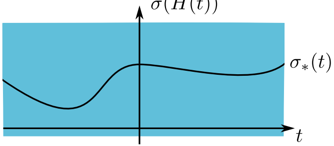

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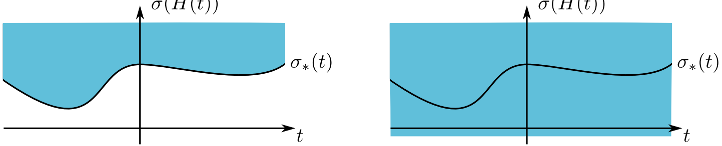

Applications:

- Dicke model (Avron, Elgart 1998)
- Nelson model (T. 2001)
- Isothermal processes (Abou-Salem, Fröhlich 2005)

Adiabatic theorems for resonances
Abou-Salem, Fröhlich (2007); Faraj, Mantile, Nier (2011); T., Wachsmuth (2012)

Adiabatic theorems can still hold if the eigenvalue $E(t)$ is replaced by a resonance.

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Adiabatic theorems for non-self-adjoint generators
Nenciu, Rasche (1992); Abou-Salem (2005); Joye (2007); Avron, Fraas, Graf, Grech (2012), Schmid (2012)

Adiabatic theorems can still hold e.g. for generators of contraction semigroups.

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- The super-adiabatic subspaces have a clear physical meaning.

2. Massless scalar bosons (jointly with J. von Keler (2012))

Consider a field of massless scalar bosons with point sources at the positions $x_j(t)$, $j = 1, \ldots, N$, and an UV-cutoff in the coupling,

$$H(t) = \mathrm{d}\Gamma(|k|) + \sum_{j=1}^{N} e_j \, \Phi\left(\frac{\hat{\varphi}(k)}{\sqrt{|k|}} \, \mathrm{e}^{\mathrm{i}k \cdot x_j(t)} \right) .$$

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If $\sum_{j=1}^{N} e_j = 0$, then $H(t)$ has a ground state eigenvalue $E_{\mathrm{inf}}(t)$ with spectral projection $P(t)$.

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It is not difficult to prove an adiabatic theorem with

$$\left\| \, P^{\perp}(t) \, U^{\varepsilon}(t, t_0) \, P(t_0) \, \right\| = \mathcal{O}(\varepsilon \ln(\varepsilon^{-1})) \, .$$

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$$\left\| \, P^{\perp}(t) \, U^{\varepsilon}(t, t_0) \, P(t_0) \, \right\| = \mathcal{O}(\varepsilon \ln(\varepsilon^{-1})) \, .$$

However, even in the absence of a spectral gap one can use the machinery of adiabatic perturbation theory to construct super-adiabatic projections $P^{\varepsilon}(t)$ that satisfy

$$\left\| \, P^{\varepsilon\perp}(t) \, U^{\varepsilon}(t, t_0) \, P^{\varepsilon}(t_0) \, \right\| = \mathcal{O}(\varepsilon) \, .$$

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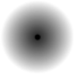
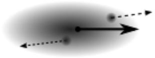
	$t \leq t_1$	$t_1 < t < t_2$	$t \geq t_2$
$\psi(t)$			

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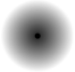
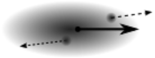
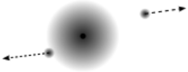
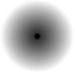
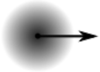
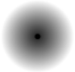
$\psi(t)$			
$\psi_{\mathrm{ad}}(t)$			
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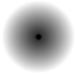
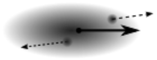
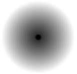
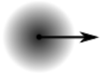
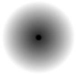
$\psi(t)$			
$\psi_{\mathrm{ad}}(t)$			
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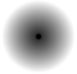
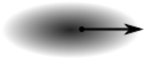
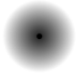
$\psi_{\mathrm{su}}(t)$			
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2. Massless scalar bosons (jointly with J. von Keler (2012))

Physics check: Radiated energy

Let the initial state $\psi(t_0) \in \mathrm{Ran} P^\varepsilon(t_0)$ be the dressed vaccuum. Then the energy of the bosons created relative to the dressed vaccuum, i.e. of $\psi_{\mathrm{rad}}(t) := P^{\varepsilon\perp}(t)\psi(t)$, is

$$E_{\mathrm{rad}}(t) = \frac{\varepsilon^3}{12\pi} \int_{t_0}^{t} |\ddot{d}(s)|^2 \, \mathrm{d}s \; + \; o(\varepsilon^3) \, .$$

Here $\ddot{d}(t)$ is the second derivative of the dipole moment $d(t) := \sum_{j=1}^{N} e_j \, \ddot{x}_j(t)$.

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Note that defining $\psi_{\mathrm{rad}}(t) := P^{\perp}(t)\psi(t)$ would give a radiated energy of order ε^2 depending on the instantaneous velocities.

3. Heavy particles coupled to massless scalar bosons

If we replace the time-dependent Hamiltonian for the field

$$H(t) = \mathrm{d}\Gamma(|k|) + \sum_{j=1}^{N} e_j \, \Phi\left(\frac{\hat{\varphi}(k)}{\sqrt{|k|}} \, \mathrm{e}^{\mathrm{i}k\cdot x_j(t)}\right)$$

by a time-independent Hamitlonian for heavy particles interacting with the field

$$H^\varepsilon = -\sum_{j=1}^{N} \frac{\varepsilon^2}{2m_j}\Delta_{x_j} + \mathrm{d}\Gamma(|k|) + \sum_{j=1}^{N} e_j \, \Phi\left(\frac{\hat{\varphi}(k)}{\sqrt{|k|}} \, \mathrm{e}^{\mathrm{i}k\cdot x_j}\right) ,$$

one can still apply adiabatic methods to understand the asymptotics of the unitary group

$$U^\varepsilon(t) := \mathrm{e}^{-\mathrm{i}H^\varepsilon \frac{t}{\varepsilon}}$$

for $\varepsilon \to 0$.

3. Heavy particles coupled to massless scalar bosons

(jointly with L. Tenuta, CMP 2008)

Theorem: almost invariant subspaces

For any $E \in \mathbb{R}$ there are orthogonal projections P^ε projecting on the subspace of dressed electrons such that

$$\left\| P^{\varepsilon\perp} U^\varepsilon(t) P^\varepsilon \chi(H^\varepsilon \le E) \right\| = \mathcal{O}(\varepsilon |t|) .$$

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Theorem: effective dynamics

The evolution of the reduced density matrix for states starting in the range of P^ε is unitarily equivalent to the evolution generated by

$$H^\varepsilon_{\mathrm{eff}} = -\sum_{j=1}^{N} \tfrac{\varepsilon^2}{2m_j^\varepsilon}\Delta_{x_j} + E_{\mathrm{inf}}(x) + \varepsilon^2 H_{\mathrm{Darwin}}$$

up to $\mathcal{O}(\varepsilon^2)$ when tested against semiclassical observables.

4. Spontaneous emission of photons in dynamical molecules

(jointly with J. Wachsmuth, CMP 2012)

Units: Bohr raduis $= \frac{1}{2m\alpha}$ and Rydberg $= 2m\alpha^2$

$$
\begin{aligned}
H^{\varepsilon,\alpha} \;=\; & \varepsilon^2 \sum_{j=1}^{N_{\mathrm{n}}} \Big(p_{j,x} - 2\sqrt{\pi}\alpha^{\frac{3}{2}} Z_j\, A_\lambda(\alpha x_j) \Big)^2 && \text{nuclei} \\
& + \sum_{j=1}^{N_{\mathrm{e}}} \Big(p_{j,y} - 2\sqrt{\pi}\alpha^{\frac{3}{2}}\, A_\lambda(\alpha y_j) \Big)^2 && \text{electrons} \\
& + H_{\mathrm{f}} && \text{photons} \\
& + V_{\mathrm{e}}(y) + V_{\mathrm{en}}(x,y) + V_{\mathrm{n}}(x) && \text{electrostatic potentials}
\end{aligned}
$$

$\Rightarrow$ two small parameters, $\varepsilon := \sqrt{\frac{m}{M}}$ and $\alpha \approx \frac{1}{137}$.

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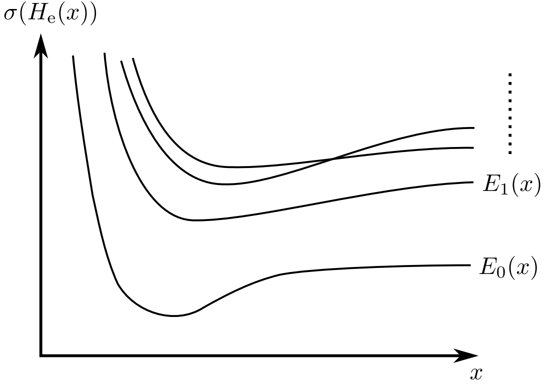

4. Spontaneous emission of photons in dynamical molecules

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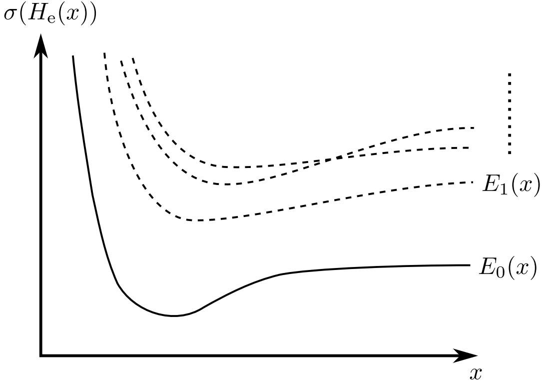
In contrast to the standard Born-Oppenheimer problem, the excited electronic levels turn into resonances:



4. Spontaneous emission of photons in dynamical molecules

(jointly with J. Wachsmuth, CMP 2012)

Theorem: spontaneous emission probability

Let $E_j > E_i$ and $\Psi = \psi \otimes \Omega \in (P_j^\varepsilon \otimes P_\Omega)\, \chi_E(H^{\varepsilon,\alpha})\mathcal{H}$. Then

$$\left\| P_i^\varepsilon \, \mathrm{e}^{-\mathrm{i}\frac{t}{\varepsilon} H^{\varepsilon,\alpha}} \, \Psi \right\|^2 \; = \; \frac{4\alpha^3}{3} \frac{1}{\varepsilon} \int_0^t \mathrm{d}s \, \left\langle \psi(s), \, |D_{ij}|^2 \Delta_E^3 \, \psi(s) \right\rangle_{\mathcal{H}_{\mathrm{nuc}}} \, + \, o(\alpha^3/\varepsilon)$$

uniformly on bounded intervals in time.

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Here $\psi(s) := \mathrm{e}^{-\mathrm{i}\frac{s}{\varepsilon} H_{j,\mathrm{BO}}} \, \psi$ is the nuclear wave function according to the standard BO-approximation,

$$D_{ij}(x) = \sum_{\ell=1}^{N_\mathrm{e}} \langle \varphi_i(x), y_\ell \varphi_j(x) \rangle_{\mathcal{H}_{\mathrm{el}}}$$

is the dipole matrix element and $\Delta_E(x) = E_j(x) - E_i(x)$ the energy gap.

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For the proof one has to use super-adiabatic projections $P_j^{\varepsilon,\alpha}$ corresponding to dressed electrons.

5. Conclusion

- Non-adiabatic transitions for gapless systems have physical significance. Computing them requires careful distinction between the error of the adiabatic approximation and true non-adiabatic transitions. A useful tool are super-adiabatic projections.

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Many Thanks and Happy Birthday!