Adiabatic transitions of a two-level system coupled to a reservoir

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Outline

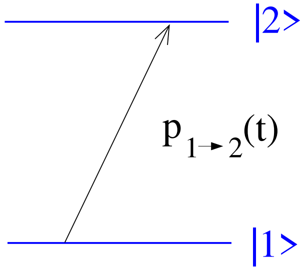
- Adiabatic and Landau-Zener transitions in closed systems
- Model: two level atom coupled to a free boson reservoir & Main results
- Sketch of the proof
- Conclusions & Perspectives

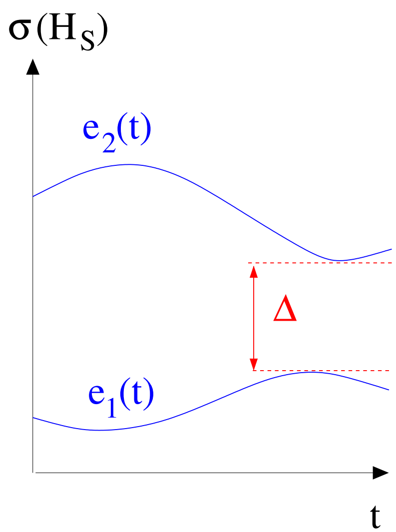
JOINT WORK WITH: Alain Joye & Marco Merkli

Adiabatic transitions in closed systems (1)

- Two-level atom with Hamiltonian $H_S(\varepsilon t)$ varying slowly in time
  $\tau = \varepsilon t$ rescaled time, $\varepsilon \ll 1$ adiabatic parameter.

- $e_i(\tau)$ eigenvalues of $H_S(\tau)$
  $P_i(\tau) = |\psi_i(\tau)\rangle\langle\psi_i(\tau)|$
  $= \text{eigenprojectors}$





- Assume (A.1) $e_i(\tau)$ and $P_i(\tau)$ depend smoothly on rescaled time
  (A.2) $P_i(\tau) = P_i(0)$ for $\tau \leqslant 0$
  (A.3) **Gap hypothesis:** $\Delta = \inf_{\tau \geqslant 0} |e_2(\tau) - e_1(\tau)| > 0.$

Adiabatic transition in closed systems (2)

- **ADIABATIC THEOREM:** **The probability of transition from one eigenstate of H_S into another vanishes in the adiabatic limit $\varepsilon \to 0$** and is given at the fixed recaled time t by

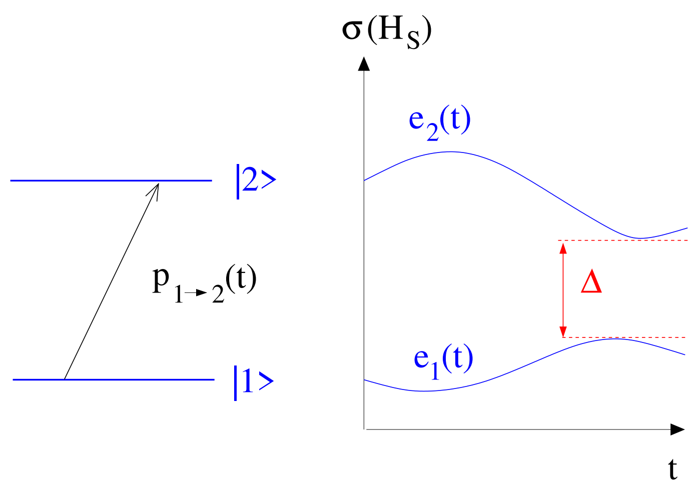
$$p^{(0)}(t;0) = \varepsilon^2 \frac{|\langle \psi_2(0)| W_K(t)^* \partial_t W_K(t) |\psi_1(0)\rangle|^2}{(e_2(t) - e_1(t))^2} + O(\varepsilon^3)$$

$W_K(t) =$ Kato operator defined by

$$\partial_t W_K(t) = \sum_{j=1}^{2} \partial_t P_j(t) P_j(t) \, W_K(t)$$

and $W_K(0) = \mathbb{1}$.

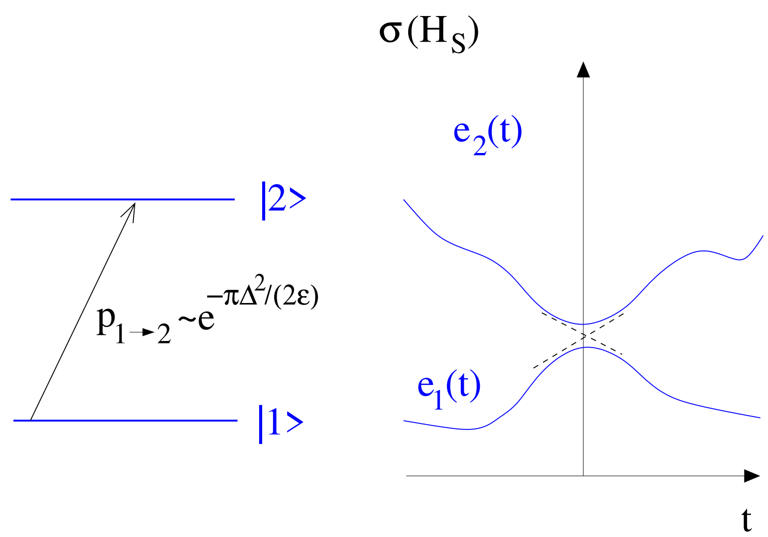
[Kato, J. Phys. Soc. Japan '50,...]



Landau-Zener formula

- Assume that $H_S(\varepsilon t)$ has an **avoided crossing** at $t = 0$, in the visicinity of which it *varies linearly with time*,

$$H_S(\varepsilon t) = \frac{1}{2}\begin{pmatrix} \varepsilon t & \Delta \\ \Delta & -\varepsilon t \end{pmatrix}$$



- **LANDAU-ZENER FORMULA:** (under appropriate smoothness assumptions) the probability of transition is exponentially small,

$$p^{(0)}(\infty; -\infty) = \exp\Big(-\frac{\pi\Delta^2}{2\varepsilon}\Big)$$

[Landau '32, Zener '32, Majorana '32, ...]

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- Model: 2-level atom coupled to a free boson reservoir
  & Main result

2-level atom coupled to a free boson reservoir

The 2-level atom is weakly coupled to a free boson bath by a **time-dependent interaction Hamiltonian**

$$H_{\rm int}(\varepsilon t) = \lambda B(\varepsilon t) \otimes (a(g) + a^*(g))/\sqrt{2}\ , \quad \lambda = \text{coupling const.}$$

◇ **linear coupling** in the bosonic anihilation and creation op. $a(g)$ and $a^*(g) = \int \mathrm{d}^3 k\, g(k) a_k^*$, with $g \in L^2(\mathbb{R}^3)$= form factor

◇ the s.a. operator $B(\varepsilon t)$ (acts on the atom Hilbert space $\mathbb{C}^2$) **varies slowly with time** with the same adiabatic parameter ε as for the atom Hamiltonian $H_S(\varepsilon t)$.

From now on: $t \to \varepsilon t$ = rescaled time

◇ $B(t)$ **commutes with** $H_S(t)$ at all times
$\hookrightarrow$ **no dissipation of energy** (pure dephasing dynamics).

$$H_S(t) = \sum_j e_j(t) P_j(t)\ ,\ B(t) = \sum_j b_j(t) P_j(t)$$

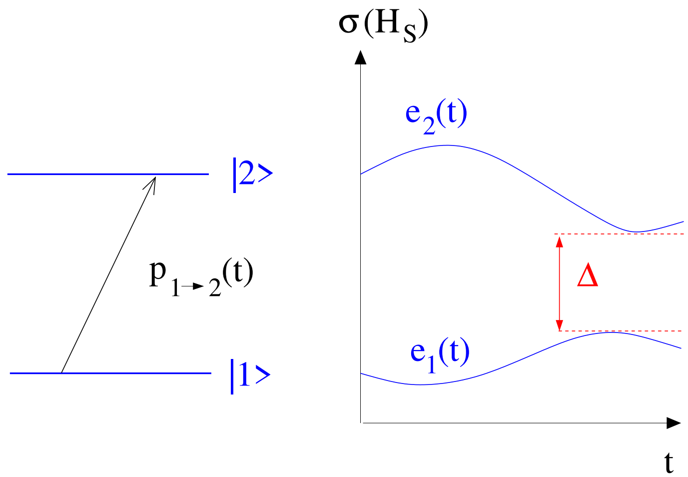
Adiabatic transition probability

- At $t = 0$, atom and bosons are decoupled and in their GS $\rho(0) = |\psi_1(0)\rangle\langle\psi_1(0)| \otimes |0\rangle\langle 0|$ (bath at zero temperature).

- $U_{\lambda,\varepsilon}(t)$ atom-bath evolution operator, given by the time-rescaled Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t U_{\lambda,\varepsilon}(t) = \big(H_S(t)\otimes \mathbb{1} + H_{\rm int}(t) + \mathbb{1}\otimes H_R\big) U_{\lambda,\varepsilon}(t)$$

- **Goal:** determine the transition probability from one eigenstate of the atom into another at the fixed rescaled time $t > 0$ in the limits $\varepsilon \ll 1$, $\lambda \ll 1$.



$$p^{(\lambda,\varepsilon)}(t) = \mathrm{tr}\left(P_2(t)\otimes \mathbb{1}\, U_{\lambda,\varepsilon}(t) P_1(0)\otimes |0\rangle\langle 0|\, U_{\lambda,\varepsilon}(t)^*\right)$$

Bath time-autocorrelation function

Bath autocorrelation function for free bosons with Hamiltonian $H_R = \int \mathrm{d}^3k\, \omega(k) a_k^* a_k$ and linear dispersion $\omega(k) = |k|$:

$$\gamma(t) = \left\langle \mathrm{e}^{\mathrm{i}t\omega} g, g \right\rangle = \int \mathrm{d}^3k\, |g(k)|^2 \mathrm{e}^{-\mathrm{i}t|k|}$$

Fourier transform $\widehat{\gamma}(\omega) \geqslant 0$ (= power spectrum function).

- E.g. rotation-invariant form factor g

$$g(k) = g_0 |k|^{\frac{m}{2}-1} \exp\left(-\tfrac{|k|}{2}\right) \quad \text{with } m > 0$$

$$\Rightarrow \ \gamma(t) = 4\pi g_0 \tfrac{\Gamma(m+1)}{(1+\mathrm{i}t)^{m+1}} \ , \ \ \widehat{\gamma}(\omega) = 8\pi^2 g_0^2\, \omega^m \mathrm{e}^{-\omega}\, \mathbf{1}_{\{\omega \geqslant 0\}}$$

- Time-independent case: decoherence induced by the atom-bath coupling essentially depends on low frequency behavior of $\widehat{\gamma}(\omega)$:
  - $m \leqslant 1$ (*Ohmic or sub-Ohmic regime*): $\rho_{12}(t) \to 0$ as $t \to \infty$
  - $m > 1$ (*super-Ohmic regime*): decoherence factor

$$\exp(-\lambda^2 b_{12}^2 \textstyle\int_0^t \mathrm{d}s \int_0^s \mathrm{d}\tau \,\mathrm{Re}\, \gamma(\tau)) \to \mathrm{e}^{-d_\infty} > 0 \text{ as } t \to \infty$$

Main result

- Assume (A1) $e_i(t)$, $b_i(t)$ and $P_i(t)$ depend smoothly on t

  (A2) $P_i(t) = P_i(0)$ for $t \leqslant 0$

  (A3) **Gap hypothesis:** $\Delta = \inf_{t\geqslant 0} |e_2(t) - e_1(t)| > 0$.

  (A4) The **bath autocorrelation function** satifies

  $|\gamma(t)| \leqslant c\, t^{-m-1}$ for any $t > t_0$ with $m > 0 \ \Rightarrow \gamma \in L^1$

  $\widehat{\gamma}(\omega) \sim \gamma_0\, \omega^m$ as $\omega \to 0+$ with $m > 0$.

- **THEOREM:** *(Joye-Merkli-DS '19)* If $\lambda \ll \varepsilon^{\frac{1}{m_<+2}} \ll 1$ with $m_< = \min\{m, 1\} > 0$, the transition probability is given by

$$p^{(\lambda,\varepsilon)}(t) = p^{(0)}(t) + \frac{\lambda^2}{2\varepsilon} \int_0^t \mathrm{d}s\, p^{(0)}(s) b_{12}^2(s) \widehat{\gamma}\big(e_{12}(s)\big) + O(\varepsilon^r)$$

$p^{(0)}(t)$ = transition proba in the absence of bath, $\quad r > 2$

$e_{12}(s) = e_1(s) - e_2(s)$, $b_{12}(s) = b_1(s) - b_2(s)$ Bohr frequencies

Comments on the theorem

$$p^{(\lambda,\varepsilon)}(t) = p^{(0)}(t) + \frac{\lambda^2}{2\varepsilon}\int_0^t \mathrm{d}s\, \underbrace{p^{(0)}(s) b_{12}^2(s)\widehat{\gamma}\big(e_{12}(s)\big)}_{\geqslant 0, \quad =0 \text{ when } e_{12}(s)<0} + O(\varepsilon^r)$$

★ 1. If λ scales like $\sqrt{\varepsilon}$, the transition proba increases due to the coupling with the bath by an amount $\approx p^{(0)}(t)$ if tunneling from excited to ground state, and is left unchanged if tunneling from ground to excited state.

2. If $\sqrt{\varepsilon} \ll \lambda \ll \varepsilon^{1/(m_<+2)}$, the bath strongly helps the atom to decay from excited state to ground state in a finite time ($p^{(\lambda,\varepsilon)}(t) \gg p^{(0)}(t)$ if $e_1 > e_2$)

★ The 2^{nd} term is proportional to $\lambda^2\varepsilon$ (since $p^{(0)}(t) = O(\varepsilon^2)$)
$\hookrightarrow$ similar result as for dephasing Lindbladian dynamics (Born Markov approx.) *[Avron-Fraas-Graf-Grech '10, Fraas-Hänggli '16]*

Error terms

★ If $\lambda \approx \varepsilon^q$, $q > (m_< + 2)^{-1}$, error terms are of order ε^r with $r = \min\{3, q + \frac{3+m_<}{2}, 2q + 1 + \frac{m}{2m - m_< + 2}, 4q + m_<, 6q\}$

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Expansion of the wave operator

1. Adiabatic evolution operator $V_{\lambda,\varepsilon}(t)$ given by

$$\mathrm{i}\varepsilon\partial_t V_{\lambda,\varepsilon}(t) = \big(H(t) + \mathrm{i}\varepsilon \sum_j \partial_t P_j(t) P_j(t) \otimes 1\big) V_{\lambda,\varepsilon}(t)$$

$\Rightarrow V_{\lambda,\varepsilon}(t) = W_{\mathrm{K}}(t) \otimes \mathbb{1}\ \Psi_{\lambda,\varepsilon}(t)$ with dynamical phase operator $\Psi_{\lambda,\varepsilon}(t)$ diagonal in the eigenbasis of $H_S(0)$

2. Dyson expansion of the "wave operator" $\Omega_{\lambda,\varepsilon}(t) = V^*_{\lambda,\varepsilon}(t) U_{\lambda,\varepsilon}(t)$

$$= \sum_{k\geqslant 0} (-1)^k \int_{0\leqslant s_k \leqslant \cdots \leqslant s_1 \leqslant t} \mathrm{d}^k s\, \Psi^*_{\lambda,\varepsilon}(s_1) \widetilde{K}(s_1) \Psi_{\lambda,\varepsilon}(s_1) \cdots \Psi^*_{\lambda,\varepsilon}(s_k) \widetilde{K}(s_k) \Psi_{\lambda,\varepsilon}(s_k)$$

with $\widetilde{K}(t) = W^*_k(t) \sum_j \partial_t P_j(t) P_j(t) W_k(t)$ independent of ε.

3. Transition probability:

$$p^{(\lambda,\varepsilon)}(t) = \big\| P_2(0) \Omega_{\lambda,\varepsilon}(t) |\psi_1(0)\rangle \otimes |0\rangle \big\|^2 = \big\| \sum_{k\geqslant 1} |\omega^{(k)}_{\lambda,\varepsilon}(t)\rangle \big\|^2$$

$\hookrightarrow$ **only the first term in the Dyson expansion contributes.**

Exact calculations & Integrations by Parts

4. The dynamical phase operator can be determined exactly in terms of the bosonic Weyl operators $W(f) = \mathrm{e}^{(a(f)+a^*(f))/\sqrt{2}}$:

$$\Psi_{\lambda,\varepsilon}(t) = \sum_j \mathrm{e}^{-\mathrm{i}(\varphi_j(t,0)-\zeta_j(t,0))} P_j(0) \otimes \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon}H_R} W(F_j(t,0))$$

with $\varphi_j(t,\tau) = \varepsilon^{-1}\int_\tau^t \mathrm{d}s\, e_j(s)$ **dynamical phase for H_S**

$\zeta_j(t,\tau)$, $F_j(t,\tau)$ **bath functions proportional to λ^2/ε^2**

5. Integrate twice by parts and use $\langle 0|W(F)|0\rangle = \mathrm{e}^{-\|F\|^2/4}$

$$\Rightarrow \quad \|\omega^{(1)}_{\lambda,\varepsilon}(t)\|^2 = p^{(0)}(t) - 2\varepsilon^2 \mathrm{Re}\left\{ \int_0^t \mathrm{d}s \int_0^s \mathrm{d}\tau\, \mathrm{e}^{-\mathrm{i}\varphi_{12}(s,\tau)} \times \partial_\tau \left(\frac{1}{e_{21}(\tau)} \partial_\tau \left(\mathrm{e}^{(\mathrm{i}\zeta_{12}-\eta_{12})(s,\tau)} e_{21}(\tau) q_{1\to 2}(s,\tau) \right)\right)\right\}$$

with $\zeta_{12}(s,\tau)$, $\eta_{12}(s,\tau) \propto \lambda^2/\varepsilon^2$

$e_{12}(\tau) = e_1(\tau) - e_2(\tau)$ and $q_{1\to 2}(s,\tau)$ independent of ε, λ.

Contribution of the $1^{\rm st}$ term of the Dyson series

$$\|\omega^{(1)}_{\lambda,\varepsilon}(t)\|^2 = p^{(0)}(t) - 2\varepsilon^2 \mathrm{Re}\Big\{ \int_0^t \mathrm{d}s \int_0^s \mathrm{d}\tau\, \mathrm{e}^{-\mathrm{i}\varphi_{12}(s,\tau)} \times \partial_\tau\Big(\frac{1}{e_{21}(\tau)}\partial_\tau\big(\mathrm{e}^{(\mathrm{i}\zeta_{12}-\eta_{12})(s,\tau)} e_{21}(\tau) q_{1\to 2}(s,\tau)\big)\Big)\Big\}$$

6. The fastly oscillating bath phase ζ_{12} and damping exponent η_{12} and their derivatives up to $2^{\rm nd}$ order are given by integrals involving the bath autocorrelation function $\gamma(t)$, that are evaluated in the limit $\varepsilon, \lambda \ll 1$ by relying on

$$\gamma \in L^1(\mathbb{R})\ ,\ \gamma(-t) = \overline{\gamma(t)} \quad \text{and} \quad \int_0^\infty \mathrm{d}t\, \mathrm{Re}\,\gamma(t) = 0$$

$\hookrightarrow$ the main contribution comes from the term $\partial_\tau^2(\mathrm{i}\zeta_{12} - \eta_{12})$,

$$\Rightarrow\ \|\omega^{(1)}_{\lambda,\varepsilon}(t)\|^2 = p^{(0)}(t) + \frac{\lambda^2}{2\varepsilon}\int_0^t \mathrm{d}s\, p^{(0)}(s) b_{12}^2(s)\widehat{\gamma}\big(e_{12}(s)\big)$$

up to errors $O(\varepsilon^3) + O(\lambda^2 \varepsilon^{1+\frac{m}{2m-m_<+2}}) + O(\lambda^4\varepsilon^{m_<}) + O(\lambda^6)$

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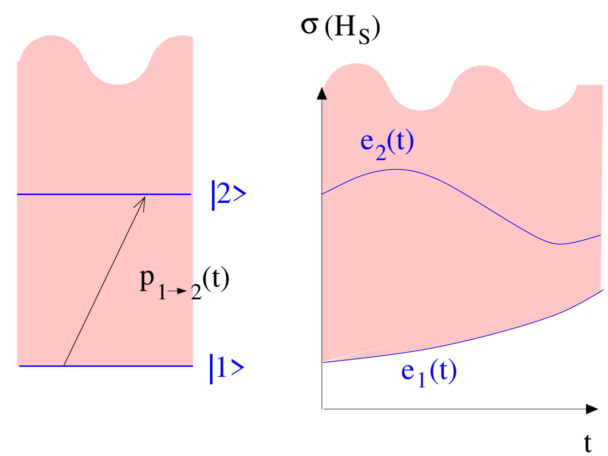
Conclusions & Perspectives

★ Rigorous proof that the coupling with the bath modifies the transition proba by a positive term $\propto \lambda^2 \varepsilon$ determined explicitely up to small errors when $\lambda \ll \varepsilon^{1/3}$ if $m \geqslant 1$ or $\lambda \ll \varepsilon^{1/(m+2)}$ if $m < 1$ (recall that $m > 0$ is s.t. $\widehat{\gamma}(\omega) \sim \gamma_0 \, \omega^m$ as $\omega \to 0+$).

★ The system + bath has a continuous spectrum $\sigma_{ac}(t) = [e_1(t), \infty)$ and **no gap**
$\hookrightarrow$ we got a more precise adiabatic theo than for general gapless time-depend. Hamiltonians with continuous spectra showing that $p_{1\to 2} \to 0$ as $\varepsilon \to 0$
[Avron-Elgart, Teufel, Elgart-Hagedorn '10]



★ **Open problem:** improve control over the error terms for Landau-Zener Hamiltonians with an avoided crossing: errors of order $O(\lambda^2 \varepsilon^{1+\frac{m}{2m-m_<+2}}) + O(\lambda^4 \varepsilon^{m_<}) + O(\lambda^6)$?

That's all!

THANK YOU FOR YOUR ATTENTION!