Estimates on the molecular dynamics for the predissociation process

Philippe BRIET & André MARTINEZ

Introduction

Quantum mechanics: Evolution described by the operator

$$\varphi \mapsto e^{-itP}\varphi$$

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In particular, if $P\varphi = E\varphi$, then $A(t,\varphi) = e^{-itE}$ and $S(t,\varphi) = 1$ (boundstate)

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But difficult to justify rigorously in general (resonant state $\notin L^2$).

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$$\langle e^{-itH_\kappa} g(H_\kappa)\varphi_0, \varphi_0\rangle = e^{-it\lambda_\kappa} a(\kappa) + \mathcal{O}(\kappa^2(1+t)^{-\nu})$$

($a(\kappa) = \|\varphi_0\|^2 + \mathcal{O}(k^2)$ and $\nu \geq 0$ depends on the regularity of g).

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[Also: Semiclassical result by Nakamura-Stefanov-Zworski (2003): Evolution operator (scalar case), with remainder $\mathcal{O}(h^\infty)$.]

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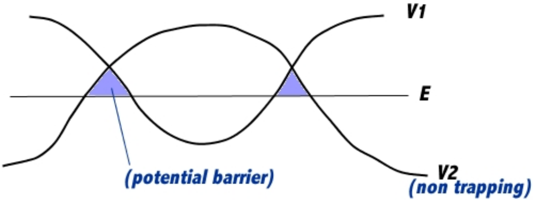
$$\mathcal{W}(x, hD_x) = \begin{pmatrix} 0 & W \\ W^* & 0 \end{pmatrix}$$

$W = w(x, hD_x)$ first-order semiclassical pseudodifferential operators.

Molecular predissociation

The two potentials:



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We fix $E = 0$.

General assumptions

Assumption 1. *The potentials V_1 and V_2 are smooth and bounded on $\mathbb{R}^n$, and satisfy,*

$$\text{The set } U := \{V_1 \leq 0\} \text{ is bounded ;} \tag{2}$$

$$\liminf_{|x|\to\infty} V_1 > 0; \tag{3}$$

$$V_2 \text{ has a strictly negative limit } -\Gamma \text{ as } |x| \to \infty; \tag{4}$$

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Assumption 2. *The potentials V_1 and V_2 extend to bounded holomorphic functions near a complex sector of the form,*
$\mathcal{S}_{R_0,\delta} := \{x \in \mathbb{C}^n\, ;\, |\mathrm{Re}\, x| \geq R_0\, ,\, |\mathrm{Im}\, x| \leq \delta |\mathrm{Re}\, x|\}$, *with* $R_0, \delta > 0$.
Moreover V_2 tends to its limit at ∞ in this sector and $\mathrm{Re}\, V_1$ stays away from $E = 0$ in this sector.

General assumptions

Assumption 3. *The symbol* $w(x,\xi)$ *of* W *extends to a holomorphic functions in* (x,ξ) *near,*

$$\widetilde{\mathcal{S}}_{R_0,\delta} := \mathcal{S}_{R_0,\delta} \times \{\xi \in \mathbb{C}^n\,;\, |\mathrm{Im}\,\xi| \leq \delta\langle \mathrm{Re}\, x\rangle\},$$

and, for real x, w *is a smooth function of* x *with values in the set of holomorphic functions of* ξ *near* $\{|\mathrm{Im}\,\xi| \leq \delta\}$. *Moreover, we assume that, for any* $\alpha \in \mathbb{N}^{2n}$, *it satisfies*

$$\partial^\alpha w(x,\xi) = \mathcal{O}(\langle \mathrm{Re}\,\xi\rangle) \text{ uniformly on } \widetilde{\mathcal{S}}_{R_0,\delta} \cup (\mathbb{R}^n \times \{|\mathrm{Im}\,\xi| \leq \delta\})\,. \quad (6)$$

General assumptions

Assumption [V] (Virial condition)

$$2V_2(x) + x\nabla V_2(x) < 0 \text{ on } \{V_2 \leq 0\},$$

or, more generally,

Assumption [NT]

$$E = 0 \text{ is a non-trapping energy for } V_2.$$

Resonances

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Resonances of H = eigenvalues of the complex distorted operator:

$$H_\theta := U_\theta H U_\theta^{-1} \qquad (\theta > 0)$$

$U_\theta \phi(x) := \det(I + i\theta dF(x))^{\frac{1}{2}} \phi(x + i\theta F(x))$, $F(x) \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$, $F(x) = 0$ for $|x| \leq R_0$, $F(x) = x$ for $|x| >> 1$.

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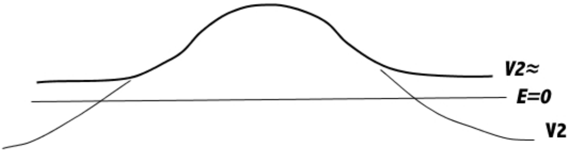
Anti-resonances = eigenvalues of $H_{-\theta}$ = conjugated of resonances

Resonances

In our situation, [M. Klein, 1987] $\Rightarrow$ near 0, the resonances are exponentially close to the eigenvalues of

$$\widetilde{H} := \begin{pmatrix} P_1 & 0 \\ 0 & \widetilde{P}_2 \end{pmatrix} + h\mathcal{W}(x, hD_x)$$

$$\widetilde{P}_2 := -h^2\Delta + \widetilde{V}_2$$



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Let $I(h) \subset [-\varepsilon_0, \varepsilon_0]$, and assume there exists $a(h) > 0$ s.t.

$$h^2/a(h) \to 0 \qquad (h \to 0);$$
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- $g^{(k)} = \mathcal{O}(a^{-k})$ uniformly $(k = 0, \dots, \nu)$.

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Theorem

For $t \geq 0$ and $\varphi = \sum_j \alpha_j \phi_j$, one has

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- $b_j(\varphi; h)$ = *residue at* ρ_j *of* $z \mapsto \langle (z-H)^{-1}\varphi, \varphi\rangle$

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- $b_j(\varphi; h)$ = *residue at* ρ_j *of* $z \mapsto \langle (z-H)^{-1}\varphi, \varphi\rangle$
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  $M(z) = m \times m$ *matrix* $= \mathrm{diag}(\lambda_1, \ldots, \lambda_m) + \mathcal{O}(h^2)$;

Results

Theorem

For $t \geq 0$ and $\varphi = \sum_j \alpha_j \phi_j$, one has

$$\langle e^{-itH} g(H)\varphi, \varphi\rangle = \sum_{j=1}^{m} e^{-it\rho_j} b_j(\varphi, h) + r(t, \varphi, h)$$

with

- $r(t,\varphi,h) = r_0(t,\varphi,h) + \mathcal{O}\left(h^4 a^{-2} \min_{0\leq k\leq \nu} a^{-k}(1+t)^{-k}\|\varphi\|^2\right)$,
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Corollary (Survival amplitude)

$$\langle e^{-itH}\varphi, \varphi \rangle = \sum_{j=1}^{m} e^{-it\rho_j} b_j(\varphi, h) + \mathcal{O}\left(\frac{h^2}{a}\right)\|\varphi\|^2.$$

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Theorem with $t = 0$

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Take $0 \leq g \leq 1$ and write,

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$$\langle e^{-itH}g(H)\varphi,\varphi\rangle = \lim_{\varepsilon\to 0_+}\frac{1}{2i\pi}\int_{\mathbb{R}} e^{-it\lambda}g(\lambda)\langle (R(\lambda+i\varepsilon)-R(\lambda-i\varepsilon))\varphi,\varphi\rangle d\lambda,$$

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Using the distortion and the location of resonances, this can be re-written,

$$\begin{aligned}\langle e^{-itH} g(H)\varphi, \varphi\rangle =& \frac{1}{2i\pi}\int_{\gamma} e^{-itz}\langle (R_\theta(z)\varphi_\theta, \varphi_{-\theta}\rangle dz \\ &+ \frac{1}{2i\pi}\int_{\gamma_-} e^{-itz} g(\mathrm{Re}\ z) T_\theta(z) dz,\end{aligned}$$

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- $T_\theta(z) := \langle(R_\theta(z)\varphi_\theta,\varphi_{-\theta}\rangle - \langle(R(z)\varphi,\varphi\rangle$.

Sketch of proof

Thus, by Cauchy formula,

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with $K = \mathcal{O}(h^2/a)$.

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Also using $e^{-izt} = (1+t)^{-k}\left(1 + i\frac{d}{dz}\right)^k e^{-izt}$, the estimate follows,

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$$\mathcal{G}_0(z) := \begin{pmatrix} H_0^\theta - z & L_- \\ L_+ & 0 \end{pmatrix} \quad ; \quad \mathcal{G}(z) := \begin{pmatrix} H_\theta - z & L_- \\ L_+ & 0 \end{pmatrix}$$

$$L_-(\mu_1, \dots, \mu_m) := \sum_{j=1}^m \mu_j \phi_j^\theta \quad ; \quad L_+ u := L_-^* u = (\langle u, \phi_1^{-\theta} \rangle, \dots, \langle u, \phi_m^{-\theta} \rangle).$$

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$$\mathcal{G}_0(z)^{-1} = \begin{pmatrix} \widehat{R}_0^\theta(z) & L_- \\ L_+ & z - \Lambda \end{pmatrix},$$

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Sketch of proof

We compute,

$$\mathcal{G}(z)\mathcal{G}_0(z)^{-1} =: \begin{pmatrix} A_{11} & A_{12} \\ 0 & I_{\mathbb{C}^m} \end{pmatrix}.$$

$$A_{11} = I_2 + h\mathcal{W}_\theta \widehat{R}_0^\theta(z) = \begin{pmatrix} 1 & \mathcal{O}(h) \\ \mathcal{O}(h/a) & 1 \end{pmatrix} = \mathcal{O}(h/a);$$

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$\Rightarrow$ Result.

THANK YOU !