Chapter 15

Accurate Estimates for the Exponential Decay of Semigroups with Non-Self-Adjoint Generators

15.1. Introduction

We review here a few examples of semigroups (or dynamical systems) of contractions in a Hilbert space with non-self-adjoint generators.

A question that occurs in many models is about the exponential decay with respect to time $t \geq 0$, which means finding the best $\lambda \in \mathbb{R}$ and $C > 0$ for

$$\|e^{-tA}\| \leq Ce^{-\lambda t}$$

or $$\|e^{-tA} - \sum_{j=1}^{N} e^{-\lambda_j t}\Pi_j p_j(t)\Pi_j\| \leq Ce^{-\lambda t}, \quad \lambda > \operatorname{Re}\lambda_j$$

when the Π_js are some spectral projectors associated with A and the eigenvalues λ_j and $p_j(t)$ is a matrix-valued non-constant polynomial in t when there is a Jordan block associated with λ_j.

Owing to

$$(A - z)^{-1} = \int_0^{\infty} e^{-t(A-z)}\, dt, \quad \operatorname{Re} z < 0$$

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and

$$e^{-tA}\psi = \frac{1}{2i\pi} \lim_{\varepsilon \to 0^+} \lim_{k \to +\infty} \int_{-\varepsilon+i\infty}^{-\varepsilon-i\infty} \frac{e^{-tz}}{1+\frac{z}{k}} (z-A)^{-1}\psi, \quad \forall \psi \in D(A)\,,$$

We see that the exponential decay of e^{-tA} is intimately related to resolvent estimates, i.e. estimates of $\|(z-A)^{-1}\|$ with respect to $z \in \mathbb{C}$.

A first standard result in this direction is the following.

GEARHART-PRÜSS-HWANG-GREINER THEOREM.– (See, for instance, [ENG 00, PAZ 83]):

1) If $\|(z-A)^{-1}\|$ is uniformly bounded in $\{\,\mathrm{Re} z \le \tau\}$, then there exists $C_\tau > 0$ such that $\|e^{-tA}\| \le C_\tau e^{-\tau t}$.

2) If $\|e^{-tA}\| \le C_\tau e^{-\tau t}$, then for every $\alpha < \tau$ the resolvent $\|(z-A)^{-1}\|$ is uniformly bounded in $\{\,\mathrm{Re} z \le \alpha\}$.

In many cases (e.g when A is sectorial), this allows us to prove

$$\lim_{t\to\infty} \frac{-\log \|e^{-tA}\|}{t} = \Sigma,$$

$$\text{with} \qquad \Sigma \stackrel{\text{def}}{=} \inf_{z \in \text{Spec}\,(A)} \mathrm{Re}\, z,$$

where all information about the constant C_τ disappears in the limit $t \to \infty$.

When A is a self-adjoint or normal operator, the functional calculus states

$$\|e^{-tA}\| \le \mathbf{1} \times e^{-t\Sigma}.$$

Of course, this is no more true when A is neither self-adjoint nor normal. Then, the question arises about controlling the constant C_λ in $\|e^{-tA}\| \le C_\lambda e^{-\lambda t}$ for $\lambda \le \Sigma$. If we think in terms of the resolvent, it is well known that there are differences between the localization of the spectrum and controlling the size of $\|(z-A)^{-1}\|$ when A is not self-adjoint. A typical example is the following perturbation of an $N \times N$ Jordan block

$$A = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 0 & 1 \\ \varepsilon & 0 & \dots & \dots & 0 \end{pmatrix},$$

with $\varepsilon > 0$ small. For $u = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ we have $\|Au\| = \mathcal{O}(\varepsilon)$ and $\|A^{-1}\| \geq \mathcal{O}(\varepsilon^{-1})$, while $\text{Spec}\,(A) = \left\{\varepsilon^{1/N} e^{\frac{2ik\pi}{N}}, k \in \{0, \ldots, N-1\}\right\}$ and $\text{dist}(0, \text{Spec}\,(A)) = \varepsilon^{1/N} \gg \varepsilon$.

Considering areas of the complex plane outside which the norm of the resolvent is "small" (a scale has to be introduced) is known as the *pseudospectrum*. Many works around resolvent estimates have been developed in the last 15 years, motivated by numerical analysis (see, for instance, [DAV 07, TRE 05]), the general analysis of linear partial differential equation (PDEs) (see, for instance, [DAV 05, DEN 04]) and the exponential decay for semigroups (see, for instance, [ECK 03, GAL 09, HÉR 04, HEL 10, HÉR 08a, HÉR 08b, HÉR 11]). Again, this makes sense when some scale (or small or large parameter) is introduced to the problem. The usual definition of pseudospectrum $\Psi\text{-Spec}_{\varepsilon}(A)$ of an operator A is parametrized by $\varepsilon > 0$ according to

$$\Psi\text{-Spec}_{\varepsilon}(A) = \left\{z \in \mathbb{C}, \|(A - z)^{-1}\| \geq \varepsilon^{-1}\right\} .$$

In semiclassical analysis for an operator $P(x, \varepsilon D_x)$ studied asymptotically as $\varepsilon \to 0$, it can be defined according to [DEN 04] as

$$\Psi\text{-Spec}\,(P(x, \varepsilon D_x)) = \left\{z \in \mathbb{C}, \lim_{\varepsilon \to 0} \varepsilon \log \|(z - P(x, \varepsilon D_x))^{-1}\| = +\infty\right\} .$$

Here, we rather consider the asymptotic behavior as $z \to \infty$. For a possibly parameter-dependent contraction semigroup A_{ε}, an accurate analysis of the exponential decay can be made when $\limsup_{\lambda \to \infty} |\lambda|^{\nu} \|(A_{\varepsilon} - i\lambda)^{-1}\| < +\infty$ for some $\nu > 0$. After setting $\lambda = \varepsilon^{-1}s$, $s \in \mathbb{R}$, the link with the notion of pseudospectrum is more obvious in the sense that the norm of the resolvent $\|\varepsilon A_{\varepsilon} - is)^{-1}\|$ is required not to be too large, namely bounded by $C\varepsilon^{\nu - 1}$ as $\varepsilon \to 0^{+}$ for any given $s \in \mathbb{R}^{*}$.

This chapter aims to show that estimating the pair (C_{τ}, τ), and not only Σ, is crucial with effective practical consequences for parameter-dependent non-self-adjoint generators and that such an analysis is related to pseudospectral (resolvent) estimates that roughly look like $\|(A_{\varepsilon} - i\lambda)^{-1}\| = \mathcal{O}(|\lambda|^{-\nu})$. The various presented examples illustrate this and show that such accurate estimates require a refined analysis for every case, exploiting the specific structures and properties.

15.2. Relevant quantities for sectorial operators

A simple case for which accurate estimates can be given in a general setting is the case of sectorial operators, i.e. maximal accretive operators $(A, D(A))$ such that

$$\text{Num}(A) = \overline{\{\langle\psi, A\psi\rangle\,, \psi \in D(A)\,, \|\psi\| = 1\}}^{\mathbb{C}}$$

is contained in $\left\{|\arg z| \leq \frac{\pi}{2} - 2\alpha\right\}$ with $\alpha > 0$. More general examples will be discussed in section 15.3.2.

We work in a separable Hilbert space endowed with a scalar product $\langle\psi\,,\,\varphi\rangle$ right-$\mathbb{C}$-linear and left anti-linear. The associated norm is denoted by $\|\psi\|$ and the operator norm by $\|B\| = \sup_{\psi\neq 0} \frac{\|B\psi\|}{\|\psi\|}$ for $B \in \mathcal{L}(\mathcal{H})$.

Consider the quantities

$$\Sigma := \inf_{z\in \text{Spec}\,(A)} \text{Re}\, z, \qquad [15.1]$$

$$\Xi := \inf_{z\in \text{Num(A)}} \text{Re}\, z \quad (= \min_{z\in \text{Num(A)}} \text{Re}\, z \text{ here}), \qquad [15.2]$$

$$\Psi := \left(\sup_{\lambda\in\mathbb{R}} \|(A - i\lambda)^{-1}\|\right)^{-1}, \qquad [15.3]$$

where the letter Σ refers to spectrum and the letter Ψ to pseudospectrum.

Differentiating $\|e^{-tA}\psi\|^2$ for $\psi \in D(A)$ leads to

$$\|e^{-tA}\| \leq e^{-\Xi t} = \mathbf{1} \times e^{-\Xi t} \quad \text{with} \quad C_\Xi = 1,$$

while using the first resolvent formula

$$(A - z_2)^{-1} = \left[\text{Id} + (z_1 - z_2)(A - z_1)^{-1}\right]^{-1}(A - z_2)^{-1}$$

leads to

$$0 \leq \Xi \leq \Psi \leq \Sigma\,.$$

In [GAL 09], we proved the following.

LEMMA 15.1.– Let $(A, D(A))$ be a maximal accretive operator in a Hilbert space $\mathcal{H}$, with numerical range contained in the sector $\{z \in \mathbb{C}\,;\, |\arg z| \leq \frac{\pi}{2} - 2\alpha\}$ for some $\alpha \in (0, \frac{\pi}{4}]$. Assume that A is invertible and let

$$\Sigma = \inf \mathrm{Re}\,(\mathrm{Spec}\,(A)) > 0\,, \quad \text{and} \quad \Psi = \left(\sup_{\lambda\in\mathbb{R}} \|(A - i\lambda)^{-1}\|\right)^{-1}.$$

Then, the following statements hold:

1) If there exist $C \geq 1$ and $\mu > 0$ such that $\|e^{-tA}\| \leq C\, e^{-\mu t}$ for all $t \geq 0$, then

$$\Sigma \geq \mu \quad \text{and} \quad \Psi \geq \frac{\mu}{1 + \log(C)}\,.$$

2) For any $\mu \in (0, \Sigma)$, we have $\|e^{-tA}\| \leq C(A, \mu)\, e^{-\mu t}$ for all $t \geq 0$, where

$$C(A, \mu) = \frac{1}{\pi \tan\alpha}\Big(\mu N(A, \mu) + 2\pi\Big) \quad \text{and} \quad N(A, \mu) = \sup_{\lambda\in\mathbb{R}} \|(A - \mu - i\lambda)^{-1}\|\,.$$

3) If, moreover, $\mu \in (0, \Psi)$, the quantity $N(A, \mu)$ is not larger than $(\Psi - \mu)^{-1}$.

First note that the assumption that A is invertible is easily obtained in a general case possibly by replacing A with $c_0 + A$, with $c_0 > 0$ arbitrarily small.

Here, are some consequences:

– When $\mu = \frac{\Psi}{2}$ or, more generally, when μ is in the same scale as Ψ (extend it for $\mu = (1 - \delta)\Psi$), then statements 2) and 3) lead to

$$\|e^{-tA}\| \leq \frac{1 + 2\pi}{\pi \tan\alpha} e^{-\frac{\Psi t}{2}}\,. \qquad [15.4]$$

– While comparing with the uniform estimate $\|e^{-tA}\| \leq 1$ given by $\Xi \geq 0$, the estimate $\|e^{-tA}\| \leq C(A, \mu)e^{-\mu t}$ makes sense (i.e. it is better than the former one) only for $t \geq \frac{\log C(A,\mu)}{\mu}$.

– When $\mu \in (\Psi, \Sigma)$, then the statement 1) implies that the constant $C(A, \mu)$ is greater than $e^{\frac{\mu}{\Psi} - 1}$. In particular, when $\Sigma \gg \Psi$, an exponential time decay with rate $\mu = \frac{\Sigma}{2}$ (extend it $\mu = (1 - \delta)\Sigma$) occurs with a constant $C(A, \mu)$ that is exponentially large, more precisely larger than $\frac{1}{3}e^{\frac{\Sigma}{2\Psi}}$. The exponential decay $\|e^{-tA}\| \leq C(A, \Sigma/2)e^{-\Sigma t/2}$ makes sense for $t \geq \frac{1}{2\Psi}$.

It really becomes better than [15.4] when $t \gg \frac{1}{\Psi}$.

A similar analysis with less explicit resolvent bounds can be carried out for non-sectorial operators, by making use of subelliptic estimates (see the example given in section 15.3.2).

We conclude this general discussion with a remark given by Helffer and Sjöstrand in [HEL 10] about a more general (no sectoriality is assumed) but less explicit control of the constant $C(A,\mu)$ in $\|e^{-tA}\| \leq C(A,\mu)e^{-\mu t}$: by setting $r(\tau) = \frac{1}{N(A,\tau)}$ and by assuming that the continuous function m fulfills $m(t) \geq \|e^{-tA}\|$, the estimate

$$\|e^{-tA}\| \leq \frac{e^{-\tau t}}{r(\tau)\|m^{-1}\|_{e^{\tau \cdot} L^2([0,a])}\|m^{-1}\|_{e^{\tau \cdot} L^2([0,\tilde{a}])}}$$

holds for all pairs $(a,\tilde{a}) \in (0,t)^2$ such that $a + \tilde{a} = t$. In particular, with $m(t) = \hat{m}(t)e^{-\tau t}$, the estimate can be improved succesively or asymptotically as $k \to \infty$ by considering the sequence

$$\frac{\hat{m}_{k+1}(t)}{r(\tau)} = \min\left\{\frac{1}{\int_0^{t/2}\left(\frac{r(\tau)}{\hat{m}_k(s)}\right)^2 ds}, \frac{\hat{m}_k(t)}{r(\tau)}\right\}.$$

15.3. Natural examples

Among natural examples, we distinguish the examples coming from the linearization of some nonlinear problem, while studying the stability of equilibria or traveling waves for the linear problems. The first example is a simplified version of the linearization of the incompressible 2D-Navier Stokes equation in the vortex formulation around Oseen vortices (see [GAL 02, GAL 05, GAL 09, VIL 09, DEN 13]). The second example is provided by the Feller semigroup associated with the Langevin dynamics, which solves the Kramers–Fokker–Planck equation, which produces naturally non-self-adjoint generators (see, for instance [RIS 89, NEL 02]). More general non-self-adjoint generators are given by what the probabilists call the non-reversible stochastic processes.

15.3.1. *An example related to linearized equations of fluid mechanics*

After his work with Wayne [GAL 02, GAL 05], Gallay proposed to consider the following simplified one-dimensional model

$$H_\varepsilon = -\partial_x^2 + x^2 + i\frac{f(x)}{\varepsilon}, \text{ on } \mathbb{R}$$

with the assumption

$$\forall\alpha \in \mathbb{N}, \exists C_\alpha > 0, \forall x \in \mathbb{R}, \quad |\partial_x^\alpha f(x)| \leq C_\alpha \langle x\rangle^{-k-|\alpha|}$$

where we used the notation $\langle x\rangle = \sqrt{1+x^2}$ and k is assumed positive. While conducting numerical experiments, computing Spec (H_ε) and solving the equation $\partial_t u = -H_\varepsilon u$, Gallay realized that the observed numerical decay of $\|e^{-tH_\varepsilon}u_0\|$ had nothing to do with the computed spectrum. This simple one-dimensional problem actually provides a very nice illustration of the general discussion presented in section 15.2.

In [GAL 09–theorem 1.8], we proved that the constant $\Psi(\varepsilon)$ defined like Ψ in [15.3] for $A = H_\varepsilon$ satisfies

$$C^{-1}\varepsilon^{-\frac{2}{k+4}} \leq \Psi(\varepsilon) \leq C\varepsilon^{-\frac{2}{k+4}}.$$

The constant C_ε in $\|e^{-tH_\varepsilon}\| \leq C_\varepsilon e^{-\frac{\Psi(\varepsilon)t}{2}}$ satisfies $C_\varepsilon = \mathcal{O}(\varepsilon^{-1})$. When the function f is chosen as

$$f(x) = \frac{1}{(1+x^2)^{k/2}} \quad \text{with } k > 0\,,$$

we proved in [GAL 09, proposition 1.9]

$$\Sigma(\varepsilon) \geq C^{-1}\varepsilon^{-\min\left\{\frac{1}{2},\frac{2}{k+2}\right\}},$$

where $\Sigma(\varepsilon)$ is defined like [15.1]. Consider $k > 2$ for the sake of simplicity. The constant C_ε in $\|e^{-tH_\varepsilon}\| \leq C_\varepsilon e^{-\frac{\Sigma(\varepsilon)t}{2}}$ satisfies $C_\varepsilon \geq \frac{1}{3}\exp[c\varepsilon^{-\frac{4}{(k+4)(k+2)}}]$. This example thus provides a typical situation where $\Sigma(\varepsilon) \gg \Psi(\varepsilon)$, also with $\Psi(\varepsilon) \gg \Xi(\varepsilon) = 1$. The numerical observation made by Gallay, which was checked and completed in [GAL 09], can be summarized with the following picture, representing upper bounds for $\|e^{-tH_\varepsilon}\|$ with respect to time.

While conducting his numerical experiments, Gallay was stopped the computation when $\|e^{-tH_\varepsilon}u_0\|$ was small compared to $\|u_0\|$ ...but before reaching the regime $t \geq \varepsilon^{\frac{2}{k+2}}\log[C(\varepsilon)]$ where the exponential decay estimate is really governed by the spectrum.

The estimate of $\Psi(\varepsilon)$ actually results from the competition of various (micro)-local models, some of which are localized at a distance of order ε^{-m} with $m > 0$ as $\varepsilon \to 0$.

A more accurate discussion is presented in [GAL 09]. When $f(x) = (1 + x^2)^{-k/2}$ or when f has some holomorphic properties, the accurate computation of the low-lying spectrum, that is an asymptotic expansion for $\Sigma(\varepsilon)$ in powers of ε, is possible but has not yet been done.

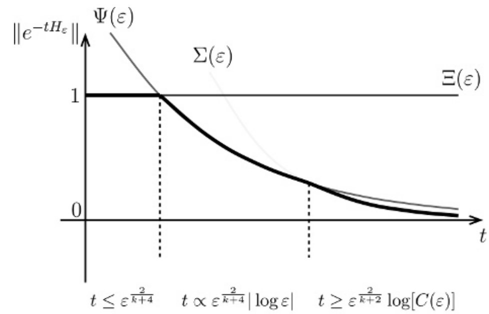

Figure 15.1. $\varepsilon^{\frac{2}{k+4}} \leq\leq \varepsilon^{\frac{2}{k+2}}$ *but* $C(\varepsilon)$ *is exponentially large*

15.3.2. *Kramers–Fokker–Planck operators*

When considering the Langevin process in $\mathbb{R}^{2d}_{x,v}$,

$$dx = vdt$$
$$dv = -\tfrac{1}{m}(\partial_x V)(x)dt - \gamma_0 v dt - \sqrt{\tfrac{2\gamma_0}{m\beta}} dW_t,$$

where $m > 0$ is the mass of particles, γ_0 the friction coefficient and $\beta = \frac{1}{k_B T}$ is the inverse temperature, we are led to consider the operator

$$K = \left[v.\partial_x - \frac{1}{m}(\partial_x V)(x).\partial_v \right] + \frac{\gamma_0}{m\beta} \left[-\Delta_v + \frac{m^2\beta^2 v^2}{4} - \frac{m\beta}{2} \right]$$

in $L^2(\mathbb{R}^{2d}, dxdv)$. For any $V \in \mathcal{C}^\infty(\mathbb{R}^d_x)$, K is essentially maximal accretive on $\mathcal{C}^\infty_0(\mathbb{R}^{2d}_{x,v})$ and the semigroup $(e^{-tK})_{t \geq 0}$ is well defined. Note that K is not self-adjoint and

$$K^* = -\left[v.\partial_x - \frac{1}{m}(\partial_x V)(x).\partial_v \right] + \frac{\gamma_0}{m\beta} \left[-\Delta_v + \frac{m^2\beta^2 v^2}{4} - \frac{m\beta}{2} \right]$$

Assume $C^{-1}\langle x \rangle^\mu - C \leq V(x) \leq C\langle x \rangle^\mu + C$ for some $\mu > 1$. Then, the Maxwellian distribution function $M(x, v) = e^{-\frac{\beta}{2}(\frac{mv^2}{2} + V(x))}$ is an equilibrium: $M \in \ker K$. In [HÉR 04], we proved

$$\|e^{-tK}u - c_u M\|_{L^2} \leq Q(m, \beta, \gamma_0, \omega, t)e^{-\omega t}, \quad c_u = \int M(x, v)u(x, v)\, dxdv,$$

where ω is the spectral gap of some Witten Laplacian (self-adjoint Schrödinger-type operator) associated with the reversible stochastic process

$$dx = -(\partial_x V)(x)dt - \sqrt{\frac{2}{\beta}}dW_t,$$

and where the prefactor $Q(m, \beta, \gamma_0, \omega, t)$ can be written as

$$Q(t_1, \ldots, t_5) = C_Q \prod_{j=1}^{5} (t_j + t_j^{-1})^{R_Q}.$$

The important thing is that the prefactor of $e^{-\omega t}$ was checked to be algebraically controlled, so that the range of times within which the exponential decay estimate is valid is really comparable to $\frac{1}{\omega}$.

Two properties are important in the (pseudo-)spectral analysis of K: global subellipticity and PT-symmetry.

15.3.2.1. *Global subellipticity for K*

Even in the simple case when $d = 1$ and $V(x) = x^2$, the operator K is not sectorial, although the spectrum is contained in a sector (see [RIS 89, HEL 05 – section 5.5, HIT 09]). Hence, controlling the norm $\|(K - \mu - i\lambda)\|$ with respect to $\lambda \in \mathbb{R}$ for a given μ (even $\mu = 0$) does not come at once from simple *a priori* estimates. If we think that sectoriality is often associated with ellipticity and that subellipticity is a kind of degenerate ellipticity, we may expect to have some control of $\|(K - \mu - i\lambda)^{-1}\|$ in the limit $\lambda \to \pm\infty$ for a given μ.

The following result can be extracted from [HÉR 04], [ECK 03] and [HEL 05], in particular section 6.1].

PROPOSITION 15.1.– Let $(K, D(K))$ be a maximal accretive operator in $\mathcal{H}$. Assume that there exists a non-negative (self-adjoint) operator $(\Lambda, D(\Lambda))$, $\Lambda \geq 1$, with $D(\Lambda^2) \overset{\text{dense}}{\subset} D(K)$, $\nu > 0$ and $C > 0$ such that

$$\forall u \in D(\Lambda^2)\,, \quad \|Ku\| \leq C\|\Lambda^2 u\|$$
$$\forall u \in D(\Lambda^2)\,, \forall \lambda \in \mathbb{R}, \quad \|\Lambda^\nu u\| \leq C\left(\|(K - i\lambda)u\| + \|u\|\right)\,.$$

Then, the spectrum of K lies in

$$S_K = \left\{ z \in \mathbb{C}, |z+1| \leq C'|\operatorname{Re} z + 1|^{\frac{2}{\nu}}\,, \operatorname{Re} z \geq -\frac{1}{2} \right\}.$$

Moreover, when $z \notin S_K$ with $\operatorname{Re} z \geq -\frac{1}{2}$, the resolvent is estimated by

$$\|(z-K)^{-1}\| \leq C'|z+1|^{-\nu/2}.$$

By assuming, for example, $|\partial_x^\alpha V(x)| \leq C_\alpha \langle x\rangle^{2n-|\alpha|}$, $V(x) \geq C^{-1}\langle x\rangle^{2n} - C$ and $|\partial_x V(x)| \geq C^{-1}\langle x\rangle^{2n-1}$ with $n > 1/2$, the above conditions were verified with

$$\Lambda^2 = 1 - \Delta_x + x^2 - \Delta_v + v^2,$$

and $\nu = \min\left\{\frac{1}{4}, \frac{1}{4n-2}\right\}$, an exponent that is not optimal and can be improved under more specific assumptions.

15.3.2.2. *PT-symmetry of K*

To get an accurate estimate of ω in the low-temperature regime $\beta \to \infty$, which can be translated into some semiclassical limit, in their recent work [HÉR 11], Hérau, Hitrik and Sjöstrand used the following "PT-symmetry" of K:

If U denotes the unitary transform $Uf(x,v) = f(x,-v)$, then

$$UKU^* = K^*. \qquad [15.5]$$

This is not exactly the PT-symmetry in the sense of [BEN 05], which rather refers to parity $Pf(x) = f(-x)$ and time $Tf(x) = \overline{f(x)}$ symmetries, with the condition

$$PTH = HPT$$

But the former condition can be written as

$$PHP = THT,$$

where the right-hand side simply equals H^* when $H = H(q,p)$ with $p = \frac{1}{i}\nabla$ with the additional symmetry $H(q,-p) = H(q,p)$ (e.g. $H(q,p) = p^2 + V(q)$ is a Schrödinger-type operator). This is exactly the condition [15.5] with $U = U^* = P$.

If we forget the microlocal geometric constructions of [HÉR 11], the strategy of this article for analyzing the low-lying spectrum of the Kramers–Fokker–Planck operator in the limit $\beta \to \infty$ can be summarized by the next proposition, applied with $A = K$, of which we give a complete proof.

PROPOSITION 15.2.– Let $(A, D(A))$ be a closed densely defined operator in a separable Hilbert space $\mathcal{H}$, such that $(1+A)^{-1}$ is compact, so that Spec (A) is discrete, and $D(A) = D(A^*)$. Assume that there exists a unitary operator, $U^* = U^{-1}$, such that $U^*AU = A^*$. Then, the spectrum Spec (A) is invariant by complex conjugation.

If additionally there exists $\gamma > 0$ and a bounded contour Γ around $z = 0$, symmetric with respect to $z \to \overline{z}$ such that:

– the real part $\operatorname{Re} A = A + A^*$ is non-negative with $\min \operatorname{Spec}(\operatorname{Re} A) \setminus \{0\} = \gamma > 0$, and $U\Pi_0 = \Pi_0 U = \Pi_0$ by setting $\Pi_0 = 1_{\{0\}}(\operatorname{Re} A)$;

– with $\Pi_\Gamma = \frac{1}{2\pi i}\int_\Gamma (z-A)^{-1}\, dz$ and $A\Pi_\Gamma = \Pi_\Gamma A = \Pi_\Gamma A \Pi_\Gamma$,

$$\operatorname{Tr}\left[\frac{1}{2\pi i}\int_\Gamma A(z-A)^{-1}\, dz\right] = \operatorname{Tr}\left[A\Pi_\Gamma\right] \in [0, \frac{\gamma}{2}) ; \quad [15.6]$$

then the following properties hold:

– $\langle u, v\rangle_U = \langle u, U^* v\rangle$ is a Hermitian positive definite form on $E_\Gamma = \operatorname{Ran}\Pi_\Gamma$;

– $A\big|E_\Gamma$ is self-adjoint and non-negative for the scalar product $\langle\ ,\ \rangle_U$;

– E_Γ admits a basis of eigenvectors of A, $(e_1, \ldots, e_N)$, orthonormal for the scalar product $\langle\ ,\ \rangle_U$;

– there exists a constant $C_{\Gamma,\gamma} > 0$ such that for all $z \in \mathbb{C}$ being inside the contour Γ, the inequality

$$\|(z-A)^{-1}\big|_{E_\Gamma}\| \leq \frac{C_{\Gamma,\gamma}}{\operatorname{dist}(z, \langle\lambda_1, \ldots, \lambda_N\rangle)} .$$

holds with the initial norm on $\mathcal{L}(\mathcal{E}_-)$.

REMARK 15.1.– This does not prove resolvent estimates for A and z inside Γ, because Π_Γ is not *a priori* an orthogonal projection. Actually, in practice, resolvent estimates have to be proved first in order to control $\|\Pi_\Gamma\|$ and also to verify condition [15.6]. But once it is done in a rough sense, the self-adjointness property with respect to $\langle\ ,\ \rangle_U$ can be used to have finer spectral results. This summarizes part of the analysis of [HÉR 11].

PROOF.– The PT-symmetry implies

$$(z-A^*)^{-1} = (z-U^*AU)^{-1} = U^*(z-A)^{-1}U$$

when the resolvent in z is defined, so that

$$\overline{\operatorname{Spec}(A)} = \operatorname{Spec}(A^*) = \operatorname{Spec}(A)$$

and the spectrum $\mathrm{Spec}\,(A)$ is symmetric with respect to the real axis. The maximal accretivity of A gives $\mathrm{Spec}\,(A) \subset \{z \in \mathbb{C},\ \mathrm{Re}\, z \geq 0\}$. Another consequence is that if the integration contour Γ is symmetric with respect to the real axis and the holomorphic function $z \to f(z)$ satisfies $\overline{f(\overline{z})} = f(z)$ then

$$f_\Gamma(A)^* = \frac{-1}{2i\pi} \int_\Gamma \frac{f(\bar{z})}{(\bar{z} - A^*)}\, d\bar{z} = U^* \left[\frac{1}{2i\pi} \int \frac{f(z)}{(z - A)}\, dz \right] U = U^* f_\Gamma(A) U\,,$$

and, in particular

$$\mathrm{Tr}\, [f_\Gamma(A)] = \frac{1}{2} \left(\mathrm{Tr}\, [f_\Gamma(A)] + \mathrm{Tr}\, [U^* f_\Gamma(A) U] \right) = \mathrm{Re}\, \mathrm{Tr}\, [f_\Gamma(A)] \quad \in \mathbb{R}\,.$$

Therefore, the condition [15.6] makes sense (take $f(z) = z$) when there are eigenvalues of A with small real parts and multiplications that are not too big. On the space $E_\Gamma = \mathrm{Ran}\, \Pi_\Gamma$, $(u, v) \mapsto \langle u\,,\, v\rangle_U = \langle u\,,\, U^* v\rangle$ is a Hermitian form and it is a scalar product when $\langle u\,,\, u\rangle_U > 0$ for any non-zero $u \in E_\Gamma$. When $u \in E_\Gamma$ with $\|u\| = 1$, it can be completed in an orthonormal basis $(e_1 = u, e_2, \ldots, e_N)$ of E_Γ for the scalar product $\langle\ ,\ \rangle$. We have

$$\begin{aligned}
\frac{\gamma}{2} > \mathrm{Tr}\, (A \Pi_\Gamma) &= \mathrm{Re} \left(\sum_{j=1}^{N} \langle e_j\,,\, A e_j \rangle \right) \\
&= \sum_{j=1}^{N} \langle e_j\,,\ \mathrm{Re}\, A e_j \rangle \geq \langle u\,,\ \mathrm{Re}\, A u \rangle \geq \gamma \|(1 - \Pi_0) u\|^2\,,
\end{aligned}$$

and

$$\|(1 - \Pi_0) u\|^2 < \frac{1}{2}\,.$$

Now compute

$$\begin{aligned}
\langle u\,,\, U^* u \rangle &= \langle u\,, \Pi_0 U^* u \rangle + \langle u\,,\, (1 - \Pi_0) U^* u \rangle \\
&= \|\Pi_0 u\|^2 + \langle (1 - \Pi_0) u\,,\, U (1 - \Pi_0) u \rangle \\
&\geq \|\Pi_0 u\|^2 - \|(1 - \Pi_0) u\|^2 = 1 - 2 \|(1 - \Pi_0) u\|^2 > 0\,.
\end{aligned}$$

Let A_Γ be the restriction of A to E_Γ, which is a finite dimensional Hilbert space with the scalar product $\langle\ \ \rangle_U$ (and $\langle\ ,\ \rangle$). For $u, v \in E_\Gamma$, the series of equalities

$$\begin{aligned}\langle u\,,\,A_\Gamma v\rangle_U = \langle u\,,\,U^*(A\Pi_\Gamma)v\rangle &= \langle u\,,(A\Pi_\Gamma)^*U^*v\rangle = \langle (A\Pi_\Gamma)u\,,\,U^*v\rangle \\ &= \langle A_\Gamma u\,,\,v\rangle_U\end{aligned}$$

says that A_Γ is self-adjoint on $(E_\Gamma, \langle\ ,\ \rangle_U)$. The two statements follow for the scalar product $\langle\ ,\ \rangle_U$ and the norm $\|\ \|_U$. Since on the finite dimensional space E_Γ, the norms $\|\ \|_U$ and $\|\ \|$ are equivalent, the last statement also holds in the initial norm.

15.4. Artificial examples

We now consider artificial non-self-adjoint deformations of initially self-adjoint operators, in order to have a good mathematical definition of spectral objects (e.g. the definition of quantum resonances), or in order to have some additional flexibility in an optimization process (see the second example).

15.4.1. *Adiabatic evolution of quantum resonances in the one-dimensional case*

Consider a one-dimensional Schrödinger operator

$$H^h = -h^2\Delta + V(x)$$

with $\operatorname{supp} V \subset [a,b]$, $-\infty < a < b < +\infty$.

Quantum resonances can be defined by introducing an exterior deformation (see e.g. [CYC 87]) according to

$$U_\theta\psi(x) = \begin{cases} e^{\theta/2}\psi(e^\theta(x-b)+b) & \text{for} \quad x > b \\ \psi(x) & \text{when} \quad a < x < b \\ e^{\theta/2}\psi(e^\theta(x-a)+a) & \text{for} \quad x < a\,, \end{cases}$$

and

$$\begin{aligned} H^h(\theta) &= U_\theta H^h U_{-\theta} \\ &= -h^2 e^{-2\theta\times 1_{\mathbb{R}\setminus[a,b](x)}}\Delta + V(x) \\ D(H^h(\theta)) &= \left\{ u \in H^2(\mathbb{R}\setminus\{a,b\})\,,\ \begin{array}{l} e^{-\frac{\theta}{2}}u(b^+) = u(b^-)\,, \\ e^{-\frac{3\theta}{2}}u'(b^+) = u'(b^-)\,, \\ e^{-\frac{\theta}{2}}u(a^-) = u(a^+)\,, \\ e^{-\frac{3\theta}{2}}u'(a^-) = u'(a^+)\,, \end{array} \right\}. \end{aligned}$$

When θ is real, $U(\theta)$ is unitary and the spectrum of $H^h(\theta)$ does not change. When $\theta = i\tau$ with $\tau > 0$, the essential spectrum of $H^h(i\tau)$ lies in $e^{-2i\tau}\mathbb{R}_+$ and this rotation of the essential spectrum unveils resonances (see [BAL 71, SIM 79, CYC 87]) as complex eigenvalues of $H^h(i\tau)$ with negative imaginary parts and which do not depend any more on τ. For shape resonances, when V models well in a semiclassical island, the imaginary parts of (interesting) resonances have exponentially small imaginary parts, $\Gamma_j^h = -\operatorname{Im}(E_j^h) = \mathcal{O}(e^{-\frac{C_j}{h}})$. The inverse $\frac{1}{\Gamma_j^h}$ is interpreted as a lifetime of a quantum meta-stable state well described by the associated eigenvector $\psi_j^h(i\tau)$ of $H^h(i\tau)$.

The time adiabatic evolution of quantum resonant states arises for slowly time-dependent Hamiltonians (here time-dependent potential): set $H^h(\theta, t) = U_{i\tau}[-h^2\Delta + V(x;t)]U_{i\tau}^{-1}$, take $\psi_j^h(i\tau;0)$ an eigenvector of $H_j^h(\tau;0)$ and consider the evolution equation

$$i\varepsilon\partial_t\psi = H^h(i\tau;t)\psi \quad , \quad \psi(t=0) = \psi_j^h(i\tau;0)\,.$$

The question is whether the solution $\psi(t)$ remains close to $\mathbb{C}\psi_j^h(i\tau;t)$ for $t \neq 0$ in the limit $\varepsilon \to 0$.

In the self-adjoint case, that is when $i\tau = 0$, and $E_j^h(t)$ is a simple real eigenvalue of $H^h(t)$ isolated from the rest of the spectrum, the result is true (see, e.g. [KAT 95, NEN 93]). It relies in a crucial way on the uniform estimate $\|U(t,s)\| \leq 1$ when $U(t,s)$ is the dynamical system solving $i\varepsilon\partial_t U(t,s) = H^h(t)U(t,s)$, $U(s,s) = \mathrm{Id}$. The adiabatic evolution of resonant states arises, for instance, in the modeling of some electronic devices and is clearly used as an assumption without justification in the works of Jona-Lasinio *et al.* and Presilla and Sjöstrand [JON 95, PRE 96].

For $\tau \neq 0$, the operator $H^h(i\tau, t)$ is not self-adjoint and the dynamical system $U_{i\tau}(t,s)$ solving $i\varepsilon\partial_t U_{i\tau}(t,s) = H^h(i\tau;t)U_{i\tau}(t,s)$, $U_{i\tau}(s,s) = \mathrm{Id}$ is not made of unitary operators. Even for a fixed t_0, $\left(e^{-i\frac{t}{\varepsilon}H^h(i\tau;t_0)}\right)_{t\geq 0}$ is not a semigroup of contractions for $iH^h(i\tau;t_0)$ is not accretive. Actually, the boundary term in

$$\begin{aligned} \operatorname{Re}\langle\psi\,, H^h(i\tau;t_0)\psi\rangle_{L^2(\mathbb{R})} &= h^2\sin(2\tau)\int_{\mathbb{R}\setminus[a,b]} |\psi'|^2\,dx \\ &\quad + \operatorname{Re}\left[ih^2(\bar{\psi}\psi'(b) - \bar{\psi}\psi'(a))(e^{-2i\tau} - e^{-i\tau})\right] \end{aligned}$$

has no sign. Meanwhile, the essential spectrum of $iH^h(i\tau;t_0)$ is $e^{i(\frac{\pi}{2}-2\tau)}\mathbb{R}_+$ and we conclude that $\Sigma = \inf \operatorname{Re}\operatorname{Spec} H^h(i\tau;t_0)$ is 0. So, uniform estimates for $U_{i\tau}(t,s)$ seem difficult to obtain, especially if we add the difficulty of a time-dependent Hamiltonian and the size of $\varepsilon = e^{-\frac{C}{h}}$, in which we are interested.

To solve this difficulty, we decided in [FAR 11] to introduce an additional artificial deformation of $H^h = -h^2\Delta + V(x)$ depending on a second parameter θ_0:

$$\begin{aligned} H^h_{\theta_0}(\theta) &= U_\theta H^h_{\theta_0} U_{-\theta} \\ &= -h^2 e^{-2\theta \times 1_{\mathbb{R}\setminus[a,b]}} \Delta_{\theta_0} + V \\ D(H^h_{\theta_0}(\theta)) &= \left\{ u \in H^2(\mathbb{R} \setminus \{a,b\}) \,, \begin{array}{l} e^{-\frac{\theta_0+\theta}{2}} u(b^+) = u(b^-) \,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(b^+) = u'(b^-) \,, \\ e^{-\frac{\theta_0+\theta}{2}} u(a^-) = u(a^+) \,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(a^-) = u'(a^+) \,, \end{array} \right\} . \end{aligned}$$

A simple integration by parts shows that when $\theta = \theta_0 = i\tau$, the operator $iH^h_{i\tau}(i\tau)$ is maximal accretive. With a time-dependent potential, this leads to a dynamical system of contractions $(U_{i\tau}(t,s))_{s\leq t}$ and the analysis of the adiabatic evolution of the modified resonant states can be carried out. Of course, we have to check that the modification parametrized by θ_0 is a small perturbation of the initial model. Under some additional assumptions on the potential $V(x;t)$, we checked that all the relevant stationary physical quantities (and up to some extent the dynamical behavior) are affected by a relatively-$\mathcal{O}(\theta_0)$ small error. This holds even for the exponentially small quantities $\Gamma^h_j = \mathcal{O}(e^{-\frac{C_j}{h}})$ that are changed by an $\mathcal{O}(\Gamma_j \theta_0^{1/4})$ term, where θ_0 can be chosen as $\theta_0 = i\tau$ with $\tau = e^{-\frac{c}{h}}$.

For the dynamics, the comparison of $H^h_{\theta_0}(0)$ and $H^h(0)$ meets the discussion of Kato in [KAT 95] about the definition of wave operators $\mathrm{s} - \lim_{t\to\pm\infty} e^{itA} e^{-it(A+B)}$ when B is a non-self-adjoint perturbation of the self-adjoint operator A with an absolutely continuous spectrum (see [FAR 11] and [MAN 13] for more details).

15.4.2. *Optimizing the sampling of equilibrium distributions*

A basic question of stochastic modeling concerns the sampling of an equilibrium distribution function

$$\psi_\infty(x) = \frac{1}{Z} e^{-V(x)} \quad \text{with } Z = \int_{\mathbb{R}^N} e^{-\beta V(x)}\, dx$$

for an energy function V defined on $\mathbb{R}^N$ with N presumably large.

One way to do this is by considering the reversible stochastic process

$$dX_t = -\nabla V(X_t) dt + \sqrt{2} dW_t \,.$$

The efficiency of the sampling can be measured by considering the exponential return to the equilibrium

$$\|e^{t\mathcal{L}}\psi - (\int_{\mathbb{R}^N} u\psi_\infty \, dx)\|_{L^2(\psi_\infty dx)} \leq Ce^{-\lambda t}\|u\|_{L^2(\psi_\infty dx)}$$

with

$$\mathcal{L} = -\nabla V(x).\nabla_x + \Delta_x \,.$$

In the above reversible case ($\mathcal{L}$ is self-adjoint in $L^2(\mathbb{R}^N;\psi_\infty dx)$), the constant C equals 1 and, for instance, when V fulfills strong convexity conditions, λ is estimated by the minimal eigenvalue of Hess $V(x_0)$ with $V(x_0) = \min_{x\in\mathbb{R}^N} V(x)$.

An alternative approach consists of considering a non-reversible process by changing the drift term and keeping the same invariant measure:

$$dX_t = (-\nabla V(X_t) + b(X_t))dt + \sqrt{2}dW_t \quad \text{with } \operatorname{div}(be^{-V}) \equiv 0\,.$$

The invariant measure is still $\psi_\infty \, dx$ and the semigroup generator becomes

$$(-\nabla V(x) + b(X)).\nabla_x + \Delta_x \,.$$

The simplest case is the linear case when

$$V(x) = \frac{x^t Sx}{2} \quad , \quad \nabla V(x) = Sx \quad , \quad S^t = S \in \mathcal{M}_N(\mathbb{R})\,, S > 0\,,$$
$$b(x) = -JSx \quad , J^t = -J \in \mathcal{M}_N(\mathbb{R})\,,$$

with $\psi_\infty(x) = e^{-\frac{x^t Sx}{2}}$ and

$$\mathcal{L}_J = -((I+J)Sx).\nabla_x + \Delta_x$$

and the return to the equilibrium is given by

$$\|e^{t\mathcal{L}_J}u - (\int_{\mathbb{R}^N} u\psi_\infty \, dx)\|_{L^2(\psi_\infty dx)} \leq C_S(J)e^{-\lambda_S(J)t}\|u\|_{L^2(\psi_\infty dx)}\,.$$

The question is whether $\lambda_S(J)$ can be optimized (maximized) with respect to $J = -J^t \in \mathcal{M}_N(\mathbb{R})$, and then whether the constant $C_S(J_{opt})$ is well controlled with respect to S and N. In [LEL 13], we proved:

– The optimal value $\lambda_{S,opt} = \frac{\mathrm{Tr}\,[S]}{N}$ can be reached by constructing a pair $\tilde{J} = S^{1/2}JS^{1/2} = -\tilde{J}^t$ and $Q = Q^t > 0$ such that

$$\tilde{J}Q - Q\tilde{J} = -QS - SQ + \frac{2\mathrm{Tr}\ [S]}{N}Q\,. \qquad [15.7]$$

– For a well-chosen optimal J_{opt}, the constant $C_S(J_{opt})$ is bounded by $C_N\kappa(S)^{7/2}$ where $\kappa(S)$ is the condition number $\kappa(S) = \|S\|\|S^{-1}\|$ and $C_N = \mathcal{O}(N^3)$ (a better control with respect to N is possible).

Solving [15.7] can be done first by constructing an orthonormal basis of eigenvectors for Q via a Gram-Schmidt algorithm. Choosing the eigenvalues of Q provides a lot of flexibility in the construction of J_{opt}.

The estimate $C_S(J_{opt}) \leq C_N\kappa(S)^{7/2}$ relies on an inequality for Wick-ordered products, sometimes used in bosonic quantum field theory (the reader is referred, for instance, to [DER 00, AMM 08, AMM 13]), which says that the quartic operator

$$\sum_{1\leq i,j,k,\ell\leq N} A_{(i,j),(k,\ell)}a_i^*a_j^*a_ka_\ell$$

$$\text{with} \qquad a_i = \frac{1}{\sqrt{2}}(\partial_{x_i} + x_i) \quad , \quad a_i^* = \frac{1}{\sqrt{2}}(-\partial_{x_i} + x_i)$$

is non-negative whenever the matrix $A = A^* \in \mathcal{M}_{N^2}(\mathbb{C})$ is non-negative.

15.5. Conclusion

Our list of examples is by far not exhaustive since many works by many authors have been devoted in the last 10 years to these kind of questions. The discussion in section 15.2 and examples therein show that when the generator A is not self-adjoint (or normal), the exponential decay estimated by $\|e^{-tA}\| \leq Ce^{-\lambda t}$

– has to be considered in terms of the pair (C, λ), instead of the only rate λ;

– has a more robust translation in terms of resolvent estimates (pseudospectrum when a scale is introduced), rather than simply localizing the spectrum.

Finally, although some general tools were developed for some classes of problems, sectorial operators (see section 15.2), subelliptic operators (see section 15.3.2), semiclassical operators in [DEN 04] or differential operators with general complex valued quadratic symbols (see [HÖR 95, PRA 08, PRA 11, HIT 09]) this often requires some refined analysis and makes use of many specific structures of the problem.

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