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Small eigenvalues of semiclassical Boltzmann operators

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Analysis, modeling and numerical method for kinetic and related models

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Introduction

We are interested in Boltzmann equations of the form

$$\begin{cases} \partial_t u + X_0(u) + Q(u) = 0 \\ u_{|t=0} = u_0 \in L^1(\mathbb{R}^{2d}) \end{cases} \tag{1}$$

We aim at studying the return to equilibrium of the solutions of (1).

Here, Q is linear $\rightsquigarrow$ spectral analysis of the operator associated to (1) with

$$X_0 = v \cdot \partial_x - \partial_x W \cdot \partial_v$$

- Non-linear case without potential : Shizuta-Asano, Ukai, Desvillettes-Villani (1974-2005)
- Spatially homogeneous case : Barranger, Mouhot (2005-2006)
- Hypocoercivity : Hérau, Villani ($\sim$2006); Dolbeault-Mouhot-Schmeiser (2010); or recently Carrapatoso, Mischler, Robbe, Bernou, Tristani...

Denoting $h > 0$ a parameter proportional to the temperature of the system, (1) becomes

$$\begin{cases} h\partial_t f + v \cdot h\partial_x f - \partial_x W \cdot h\partial_v f + Q_h(f) = 0 \\ f_{|t=0} = f_0 \in L^2(\mathbb{R}^{2d}) \end{cases} \tag{2}$$

$\rightsquigarrow$ **semiclassical** study, i.e in the limit $h \to 0$ ("*low temperature*" regime) of the spectrum of the operator

$$\begin{aligned} P_h &= v \cdot h\partial_x - \partial_x W \cdot h\partial_v + Q_h \\ &= X_0^h + Q_h \end{aligned}$$

associated to equation (2).

Notations and assumptions

- $W \in \mathcal{C}^\infty(\mathbb{R}^d_x, \mathbb{R})$ is a **Morse** coercive function, at most quadratic at infinity with $n_0 \in \mathbb{N}_{\geq 2}$ local minima.
- $H_0 = -h^2\Delta_v + v^2 - hd = (h\partial_v + v)^* \circ (h\partial_v + v)$ is **the harmonic oscillator** in velocity,
- Π_h is the **orthogonal projector** on $\mathrm{Ker}\, H_0 = \mathrm{e}^{-\frac{v^2}{2h}} L^2(\mathbb{R}^d_x)$,

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We consider the collision operators

$$\begin{aligned} Q_h &= \frac{H_0}{1 + H_0} \qquad \text{“mild relaxation”} \\ &= (h\partial_v + v)^* \circ \mathrm{Op}_h(M_h) \circ (h\partial_v + v) \end{aligned}$$

and

$$\begin{aligned} \widetilde{Q}_h &= h(\mathrm{Id} - \Pi_h) \qquad \text{“linear relaxation”} \\ &= (h\partial_v + v)^* \circ \mathrm{Op}_h\left(\widetilde{M}_h\right) \circ (h\partial_v + v). \end{aligned}$$

Small eigenvalues of semiclassical operators

Quantum side :

- Simon, Robert, Martinez, Helffer-Sjöstrand (1980's); Dimassi (1990's) $\rightsquigarrow$ *Schrödinger*
- Helffer-Sjöstrand (1980's), Helffer-Morame; Fournais-Helffer (2000's), Bonnaillie-Noël-Hérau-Raymond (2016-2022) $\rightsquigarrow$ *Magnetic Laplacian*

Probabilistic side :

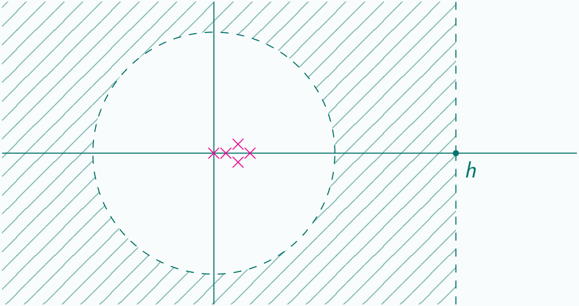
- Helffer-Sjöstrand (1980's); Helffer-Klein-Nier, Bovier-Gayrard-Klein (2000's) $\rightsquigarrow$ *Witten Laplacian*
- Hérau-Hitrik-Sjöstrand (2008) $\rightsquigarrow$ *Kramers-Fokker-Planck*
- Robbe (2016) $\rightsquigarrow$ *Boltzmann equation*
- Le Peutrec-Michel, Bony-Le Peutrec-Michel (2020's) $\rightsquigarrow$ *KFP without supersymmetry*

$\rightarrow$ We adapt the methods from the latter to some **non local** frameworks.

Preliminary result

Theorem 1 [Robbe 2015, N. 2022]

- P_h admits **0** as a **simple eigenvalue**
- $\mathrm{Spec}(P_h) \cap \{\mathrm{Re}\, z \leq h\}$ consists of exactly $\mathbf{n_0}$ **eigenvalues** that are $O(\mathrm{e}^{-c/h})$
- The resolvent estimate $\boldsymbol{(P_h - z)^{-1} = O(1/h)}$ holds uniformly on $\{\mathrm{Re}\, z \leq h\} \backslash B(0, \frac{h}{2})$



Ideas of proof

1st difficulty : P_h is not self-adjoint (in particular no min-max principle) $\rightsquigarrow$ use the **spectral projector**

$$\Pi_0 = \frac{1}{2i\pi} \int_{|z|=\frac{h}{2}} (z - P_h)^{-1} \mathrm{d}z$$

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2nd difficulty : P_h is not elliptic $\rightsquigarrow$ **hypocoercive** techniques

- We find a subspace $F \subset L^2$ of **dimension** n_0 and an **auxiliary** bounded operator L such that

$$\mathrm{Re} \left\langle (1 + L) P_h u , u \right\rangle \gtrsim h\|u\|^2 \qquad \forall u \in F^\perp$$

  $\rightsquigarrow$ We deduce the **resolvent estimate** $(z - P_h)^{-1} = O(1/h)$
- We show that $\Pi_0 L^2 = \Pi_0 F$ and has dimension n_0 $\square$

Plan of the talk

Goal : Provide a sharp description of the n_0 "small eigenvalues" of the operator P_h.

Plan :

1. Strategy heuristic : construction of **gaussian quasimodes** for the **mild relaxation** operator $X_0^h + Q_h$.
2. Study of the **linear relaxation** operator $X_0^h + \widetilde{Q}_h$.
3. **Return to equilibrium** et **metastability**.

Boltzmann operator with *mild relaxation* : $P_h = X_0^h + Q_h$

Theorem

Let $\mathbf{m}$ *a local minimum of* W. *There exist*

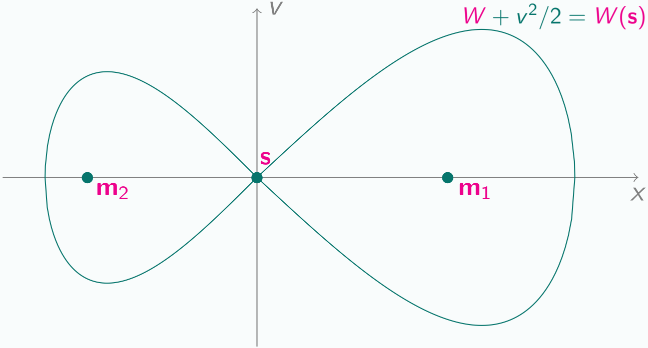
$S(\mathbf{m}) > 0$ *and* $a_h(\mathbf{m}) \sim \sum_{k\geq 0} h^k a_k(\mathbf{m})$

that we can compute and such that

$$\lambda(\mathbf{m}, h) = h\, a_h(\mathbf{m}) \mathrm{e}^{-\frac{2S(\mathbf{m})}{h}}.$$

Strategy Heuristic

To simplify, let us suppose that we have the following picture in $\mathbb{R}^{2d}$:



In particular, $n_0 = 2$ and $W(\mathbf{m}_1) < W(\mathbf{m}_2)$.

We take

$$f_{ker}(x,v) = \exp\left(-\frac{W(x)+v^2/2}{h}\right) \in \mathrm{Ker}\, P_h.$$

We aim at choosing f the closest possible to the **generalized eigenspace** of P_h :

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$\rightarrow$ denoting

$$\Pi_0 = \frac{1}{2i\pi}\int_{|z|=\frac{h}{2}} (z - P_h)^{-1}\mathrm{d}z,$$

we have

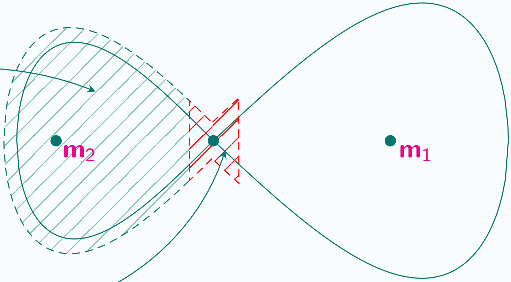
$$\begin{aligned}(1-\Pi_0)f &= \frac{1}{2i\pi}\int_{|z|=\frac{h}{2}} \left(z^{-1} - (z-P_h)^{-1}\right) f \,\mathrm{d}z \\ &= \frac{-1}{2i\pi}\int_{|z|=\frac{h}{2}} z^{-1}(z-P_h)^{-1} P_h f \,\mathrm{d}z.\end{aligned}$$

$\rightsquigarrow$ We want $P_h f$ to be **the smallest possible**.

We define the **gaussian quasimode**

$$f_\ell(x,v) = \theta_\ell(x,v)\exp\left(-\frac{W(x)+v^2/2}{h}\right)$$

$\theta_\ell = 1$



$$\theta_\ell(x,v) = \tfrac{1}{2} + \int_0^{\ell(x,v)} \zeta(y)\,\mathrm{e}^{-y^2/2h}\mathrm{d}y$$

$$\theta_\ell(x,v) = \frac{1}{2} + \int_0^{\ell(x,v)} \mathrm{e}^{-y^2/2h}\mathrm{d}y$$

We easily compute

$$\nabla\theta_\ell = \mathrm{e}^{-\ell^2/h}\nabla\ell.$$

$$\Longrightarrow\ X_0^h f_\ell = \omega_\ell^{tran}(x,v)\exp\left(-\frac{W + \frac{v^2}{2} + \ell^2}{h}\right)$$

with $\omega_\ell^{tran} = O_{L^\infty}(1)$.

$\rightsquigarrow$ "X_0^h sends the ℓ-**gaussian quasimode** on the ℓ-**elliptized** phase."

⚠ here Q_h is **non local** $\rightsquigarrow$ computation of $Q_h f_\ell$?

Lemma

There exists a matrix $M_h(v, \eta) \in S^{\mathbf{0}}$ of symbols ***analytic*** *in η such that*

$$Q_h = (h\partial_v + v)^* \circ \mathrm{Op}_h(M_h) \circ (h\partial_v + v).$$

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$$\Rightarrow Q_h f_\ell = (h\partial_v + v)^* \circ \mathrm{Op}_h(M_h) \left[\exp\left(-\frac{W + \frac{v^2}{2} + \ell^2}{h} \right) \partial_v \ell \right]$$

$$= \omega_\ell^{col}(x,v) \exp\left(-\frac{W + \frac{v^2}{2} + \ell^2}{h} \right) + \text{ negligible terms.}$$

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$$= \omega_\ell^{col}(x,v) \exp\left(- \frac{W + \frac{v^2}{2} + \ell^2}{h} \right) + \text{ negligible terms.}$$

$$\Longrightarrow \quad P_h f_\ell(x,v) = \omega_\ell(x,v) \exp\left(- \frac{W + \frac{v^2}{2} + \ell^2}{h} \right)$$

with $\omega_\ell = O_{L^\infty}(1)$.

$\rightsquigarrow$ "P_h sends the ℓ-**gaussian quasimode** on the ℓ-**elliptized** phase."

Conditions on ℓ : We want to choose ℓ such that

- 0 is a local **minimum** of $W + \frac{v^2}{2} + \ell^2$
- ω_ℓ vanishes **at order 2** at 0.

$$\rightsquigarrow \quad \Phi \begin{pmatrix} \ell_x \\ \ell_v \end{pmatrix} = -M_h(0,0)\, \ell_v \cdot \ell_v \begin{pmatrix} \ell_x \\ \ell_v \end{pmatrix}$$

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Denoting $\tilde{\lambda}_h := \langle P_h f_\ell, f_\ell \rangle$, we then get

Lemma

- $\tilde{\lambda}_h = h\, \tilde{a}_h\, \mathrm{e}^{-\frac{2S(\mathbf{m}_2)}{h}}$ *with* $\tilde{a}_h \sim \sum_{k\geq 0} h^k a_k$ *that we can compute*
- $\|P_h f_\ell\| = O(h\tilde{\lambda}_h^{1/2})$.

Proof :

- $\langle P_h f_\ell, f_\ell \rangle = \Big\langle \mathrm{Op}_h(M_h)\,(h\partial_v + v)\,f_\ell\,,\ (h\partial_v + v)\,f_\ell \Big\rangle$
- $P_h f_\ell = \omega_\ell \exp\Big(- \frac{W + \frac{v^2}{2} + \ell^2}{h} \Big)$

$+$ Laplace method $\square$

Proof :

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- $P_h f_\ell = \omega_\ell \exp\Big(-\frac{W+\frac{v^2}{2}+\ell^2}{h}\Big)$

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Conclusion :

We go from quasimodes to actual **eigenfunctions** :

$$(f_{ker}, f_\ell) \xrightarrow{\Pi_0} (f_{ker}, \Pi_0 f_\ell) \xrightarrow[\text{Schmidt}]{\text{Gram}} (f_{ker}, \boldsymbol{\varphi_2})$$

Interaction matrix : $\mathcal{M} = \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\lambda_h} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \underbrace{\langle \boldsymbol{P_h \varphi_2, \varphi_2} \rangle}_{=\tilde{\lambda}_h(1+O(\sqrt{h}))} \end{pmatrix}$

$\square$

Boltzmann operator with *linear relaxation* : $P_h = X_0^h + \widetilde{Q}_h$

Theorem

Let $\mathbf{m}$ *a local minimum of* W*.*
There exist $S(\mathbf{m}) > 0$ *and* $a_0(\mathbf{m})$ *that we can compute and such that*

$$\lambda(\mathbf{m}, h) \sim h\, a_0(\mathbf{m}) \mathrm{e}^{-\frac{2S(\mathbf{m})}{h}}.$$

Proposition

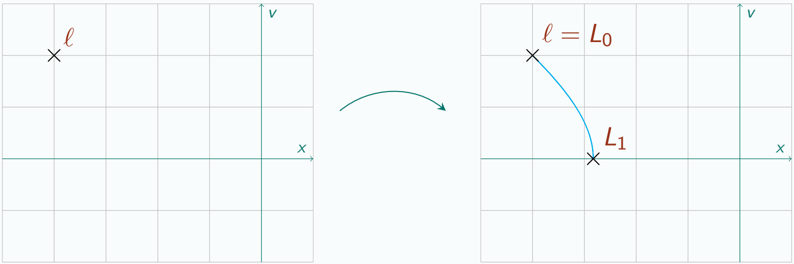
We have

$$\widetilde{Q}_h f_\ell(x,v) = \int_0^1 \partial_y(L_y)\, \mathrm{e}^{-\frac{W(x)+v^2/2+L_y\cdot(x,v)^2}{h}}\, \mathrm{d}y \ \cdot (x,v)$$

with

$$L_y = \Big(4y\ell_v^2 + (y+1)^2\Big)^{-1/2}\Big((1+y)\ell_x, (1-y)\ell_v\Big).$$

"$\widetilde{Q}_h$ sends the ℓ-GQ on a **superposition** of the L_y-elliptized phases":



Lemma

The matrices of symbols

$$\widetilde{M}_h(v,\eta) = \int_0^1 (y+1)^{d-2} \mathrm{e}^{-\frac{y}{h}(v^2+\eta^2)} \mathrm{d}y \, \mathrm{Id} \quad \in S^{\mathbf{1/2}}$$

$$\widetilde{g}_h(v,\eta) = \int_0^1 (y+1)^{d-1} \mathrm{e}^{-\frac{y}{h}\left(v^2+\eta^2\right)} \mathrm{d}y \, (-i\eta + v) \quad \in S^{\mathbf{1/2}}$$

are such that

$$\begin{aligned} \widetilde{Q}_h &= (h\partial_v + v)^* \circ \mathrm{Op}_h\left(\widetilde{M}_h\right) \circ (h\partial_v + v) \\ &= \mathrm{Op}_h\left(\widetilde{g}_h\right) \circ (h\partial_v + v). \end{aligned}$$

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$$= \mathrm{Op}_h\left(\widetilde{g}_h\right) \circ (h\partial_v + v).$$

Proof of Proposition :

- $f_\ell(x,v) = \theta_\ell(x,v) \exp\left(-\frac{W(x)+v^2/2}{h}\right)$
- $(h\partial_v + v) f_\ell(x,v) = h\,\mathrm{e}^{-\frac{1}{h}\left(W+\frac{v^2}{2}+\ell^2\right)} \ell_v$

Finally, $\mathrm{Op}_h\left(\widetilde{g}_h\right)\left[\mathrm{e}^{-\frac{1}{h}\left(W+\frac{v^2}{2}+\ell^2\right)}\ell_v\right](x,v)$ equals

$$(2\pi h)^{-d}\int_{v'}\mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v'^2}{2}+\ell^2(x,v')\right)}$$

$$\times\left(\int_\eta \mathrm{e}^{\frac{i}{h}(v-v')\cdot\eta}\,\widetilde{g}_h\Big(\frac{v+v'}{2},\eta\Big)\mathrm{d}\eta\right)\,\mathrm{d}v'\ell_v$$

$$=\boxed{\int_0^1\partial_y(L_y)\,\mathrm{e}^{-\frac{W(x)+v^2/2+L_y\cdot(x,v)^2}{h}}\,\mathrm{d}y\,\cdot(x,v)}\qquad\square$$

Problem :

$$X_0^h f_\ell \approx \mathrm{e}^{-\frac{1}{h}\left(W+\frac{v^2}{2}+\ell^2\right)} \qquad \not\approx \qquad \widetilde{Q}_h f_\ell \approx \int_0^1 \mathrm{e}^{-\frac{1}{h}\left(W+\frac{v^2}{2}+L_y^2\right)} \mathrm{d}y$$

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Idea :

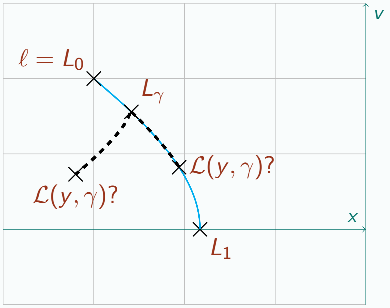
$$f_\ell \quad \rightsquigarrow \quad F_\ell := \int_0^1 k(\gamma) f_{L_\gamma} \mathrm{d}\gamma$$

$$\begin{aligned} \Longrightarrow \; X_0^h F_\ell(x,v) &= \int_0^1 k(\gamma)\, X_0^h f_{L_\gamma}(x,v) \mathrm{d}\gamma \\ &= \int_0^1 \omega_1(\gamma,x,v)\, \mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_\gamma\cdot(x,v)^2\right)} \mathrm{d}\gamma \end{aligned}$$

$\rightarrow$ What about $\widetilde{Q}_h F_\ell$?

$$\widetilde{Q}_h F_\ell(x,v) = \int_0^1 k(\gamma)\, \widetilde{Q}_h f_{L_\gamma}(x,v)\mathrm{d}\gamma$$

$$= \int_0^1 k(\gamma) \int_0^1 \partial_y \mathcal{L}(y,\gamma)\, \mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+\mathcal{L}(y,\gamma)\cdot(x,v)^2\right)} \mathrm{d}y\, \mathrm{d}\gamma \cdot (x,v)$$



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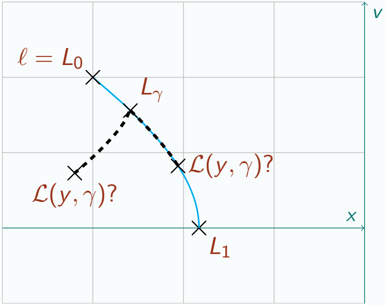

Lemma

There exists $\Gamma_\gamma : [0,1] \to [0,1]$ such that

$$\mathcal{L}(y,\gamma) = L_{\Gamma_\gamma(y)}.$$

Therefore,

$$\widetilde{Q}_h F_\ell(x,v) = \int_0^1 k(\gamma) \int_0^1 \partial_y L_{\Gamma_\gamma(y)} \,\mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_{\Gamma_\gamma(y)}\cdot(x,v)^2\right)} \mathrm{d}y\,\mathrm{d}\gamma \cdot (x,v)$$

$$\overset{z=\Gamma_\gamma(y)}{=} \int_0^1 \int_0^z k(\gamma)\mathrm{d}\gamma\, \partial_z L_z \cdot (x,v) \mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_z\cdot(x,v)^2\right)} \mathrm{d}z$$

$$= \int_0^1 \omega_2(z,x,v)\,\mathrm{e}^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_z\cdot(x,v)^2\right)} \mathrm{d}z$$

Goal :

$$\omega_1(z,x,v) + \omega_2(z,x,v) = 0 \qquad \forall z \in [0,1]$$

Therefore,

$$\widetilde{Q}_h F_\ell(x,v) = \int_0^1 k(\gamma) \int_0^1 \partial_y L_{\Gamma_\gamma(y)}\, e^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_{\Gamma_\gamma(y)}\cdot(x,v)^2\right)} \mathrm{d}y\, \mathrm{d}\gamma \cdot (x,v)$$

$$\overset{z=\Gamma_\gamma(y)}{=} \int_0^1 \int_0^z k(\gamma)\mathrm{d}\gamma\, \partial_z L_z \cdot (x,v) e^{-\frac{1}{h}\left(W(x)+\frac{v^2}{2}+L_z\cdot(x,v)^2\right)} \mathrm{d}z$$

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Goal :

$$\underbrace{\omega_1(z,x,v)}_{\approx k(z)} + \underbrace{\omega_2(z,x,v)}_{\approx \frac{1}{R(z)}\int_0^z k(\gamma)\mathrm{d}\gamma} = 0 \qquad \forall z \in [0,1]$$

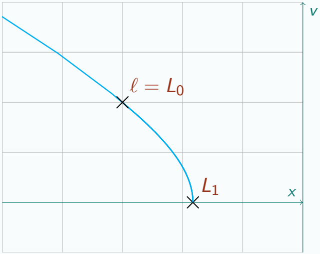
$\rightsquigarrow$ ODE on k :

$$\begin{cases} K'(z) = \dfrac{1}{R(z)} K(z) \\ K(0) = 0 \end{cases}$$

only solution $\equiv 0$... ☹

$\rightsquigarrow$ Use the **singularity** at $\gamma_1 < 0$ of $1/R$: replace $[0,1]$ by $]\gamma_1, 1]$...

Conclusion



$\Rightarrow$ The remainder terms depend (continuously) on $z \in]\gamma_1, 1]$ and blow up at γ_1...

$\rightsquigarrow$ We work on $[\gamma_1 + \varepsilon, 1]$

$\Rightarrow$ The $O\left(\sqrt{h}\right)$ become $O_\varepsilon\left(\sqrt{h}\right)$

In the end :

$$\boxed{\boldsymbol{\lambda_h} = \tilde{\lambda}_h\left(1 + O_\varepsilon\left(\sqrt{h}\right)\right)} \qquad \square$$

Return to equilibrium and metastability

Corollary [Helffer-Sjöstrand 2010, Bony et al. 2021, N. 2022]

There exist some projectors $\mathbb{P}_1, \ldots, \mathbb{P}_{n_0}$ *such that*

$$f_t = \mathbb{P}_1 f_0 + O\left(\mathrm{e}^{-t\lambda_2} \|f_0\|\right)$$

as well as some time intervals $[t_k^-, t_k^+]$ *during which*

$$f_t = \sum_{j=1}^{k} \mathbb{P}_j f_0 + O\left(h^\infty \|f_0\|\right) \qquad \forall t \in [t_k^-, t_k^+].$$

$$
\begin{aligned}
e^{-tP_h} &= e^{-tP_h}\Pi_0 + O\left(e^{-cht}\right) \qquad \text{(Gearhart-Prüss)} \\
&= \sum_{j=1}^{n_0} e^{-t\lambda_j}\mathbb{P}_j + O\left(e^{-cht}\right) \\
&= \mathbb{P}_1 + O\left(e^{-t\lambda_2}\right) \quad \rightsquigarrow \textbf{return to equilibrium}
\end{aligned}
$$

$$\begin{aligned}
e^{-tP_h} &= e^{-tP_h}\Pi_0 + O\left(e^{-cht}\right) \qquad \text{(Gearhart-Prüss)} \\
&= \sum_{j=1}^{n_0} e^{-t\lambda_j}\mathbb{P}_j + O\left(e^{-cht}\right) \\
&= \mathbb{P}_1 + O\left(e^{-t\lambda_2}\right) \quad \rightsquigarrow \textbf{return to equilibrium}
\end{aligned}$$

$$\begin{aligned}
e^{-tP_h} + O\left(e^{-cht}\right) &= \sum_{j=1}^{n_0} e^{-t\lambda_j}\mathbb{P}_j \\
&= \sum_{j=1}^{k}\mathbb{P}_j + \sum_{j=2}^{k}\left(e^{-t\lambda_j} - 1\right)\mathbb{P}_j + \sum_{j=k+1}^{n_0} e^{-t\lambda_j}\mathbb{P}_j \\
&\overset{t\geqslant t_k^-}{=} \sum_{j=1}^{k}\mathbb{P}_j + \sum_{j=2}^{k}\left(e^{-t\lambda_j} - 1\right)\mathbb{P}_j + O\left(h^\infty\right) \\
&\overset{t\leqslant t_k^+}{=} \sum_{j=1}^{k}\mathbb{P}_j + O\left(h^\infty\right) \quad \rightsquigarrow \textbf{metastability} \qquad \square
\end{aligned}$$

Perspectives

- Consider cases with multiple *collision invariants* [Post-doc with F. Hérau] :

$$\operatorname{Ker} Q_h = \operatorname{Vect}\left(\mathrm{e}^{-v^2/2h}, v_1\,\mathrm{e}^{-v^2/2h}, \dots, v_d\,\mathrm{e}^{-v^2/2h}, v^2\,\mathrm{e}^{-v^2/2h}\right).$$

- Consider the linearized Boltzmann and Landau operators [Carrapatoso et al.]

- Study on domains bounded in space [Nier, Lelièvre et al., Bernou et al.] : $\mathbb{R}^{2d} \rightsquigarrow \Omega \times \mathbb{R}^d_v$.

Thank you !