Geometric Kramers-Fokker-Planck operators with boundary conditions

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Microlocal analysis and spectral theory
in honor of J. Sjöstrand
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Outline

- Presentation of the problem
- Main results
- Applications
- Elements of proofs

I do not have much more time left, so let me close by trying to give you a little bit of the flavor of how Witten's assertion comes about at least in this simplest case. He did not *prove* it by mathematical standards in his wonderful paper [8]. For that we had to wait for the quite difficult papers of Helder and Sjöstrand [5], where of course Smale's transversality condition enters. (In fact, it is nowadays possible to write long *Comptes*

Raoul Bott: Morse theory indomitable (IHES 1988)

Geometric Kramers-Fokker-Planck operators

In the euclidean space, the operator

$$P_{\pm} = \pm p.\partial_q - \partial_q V(q).\partial_p + \frac{-\Delta_p + |p|^2}{2} \quad , \quad x = (q,p) \in \Omega \times \mathbb{R}^d$$

is associated with the Langevin process

$$dq = pdt \quad , \quad dp = -\partial_q V(q)dt - pdt + dW$$

$\overline{Q} = Q \sqcup \partial Q$ riem. mfld with bdy , $X = T^*Q$, $\partial X = T^*_{\partial Q}Q$.
Metric $g = g_{ij}(q)dq^i dq^j$, $g^{-1} = (g^{ij})$

$$P_{\pm,Q,g} = \pm \mathcal{Y}_{\mathcal{E}} + \frac{-\Delta_p + |p|_q^2}{2} \,, \quad \Delta_p = g_{ij}(q)\partial_{p_i}\partial_{p_j}$$

$$\mathcal{E}(q,p) = \frac{|p|_q^2}{2} = \frac{g^{ij}(q)p_i p_j}{2} \,,$$

$$\mathcal{Y}_{\mathcal{E}} = g^{ij}(q)p_i\partial_{q^j} - \frac{1}{2}\partial_{q^k} g^{ij}(q)p_i p_j \partial_{p_k} = g^{ij}(q)p_i e_j \,, \quad e_j = \partial_{q^j} + \Gamma_{ij}^{\ell} p_\ell \partial_{p_j} \,.$$

acting on $\mathcal{C}^\infty(\overline{X};\mathfrak{f})$. $P_{\pm,Q,g}$ = scalar part of Bismut's hypoelliptic Laplacian.

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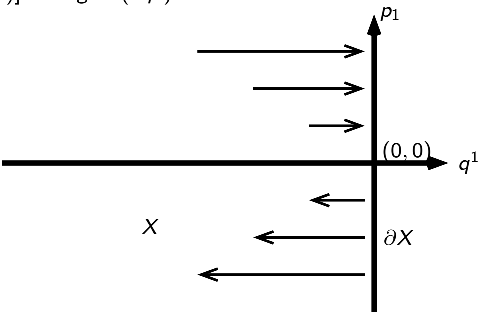
A simple case

Take $\overline{Q} = (-\infty, 0)]$ with $g = (dq^1)^2$.



Specular reflection: $u(0, -p_1) = u(0, p_1)$ for $p_1 > 0$.
It can be written $\gamma_{odd}\, u = 0$ with $\gamma_{odd}\, u = \frac{u(0,p_1) - u(0,-p_1)}{2}$.
Absorption: $u(0, p_1) = 0$ for $p_1 < 0$.
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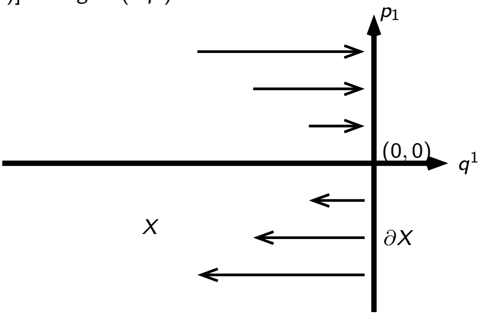

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General BC

Metric locally on ∂Q: $(dq^1)^2 \oplus^\perp m(q^1, q')$. Consider $\mathfrak{f}$-valued functions, $\mathfrak{f}$ Hilbert space.

Let j be a unitary involution in $\mathfrak{f}$ and define along $\partial X = \{q^1 = 0\}$:

$$\gamma_{odd} = \Pi_{odd}\gamma = \frac{\gamma(q', p_1, p') - j\gamma(q', -p_1, p')}{2},$$

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Let the boundary condition on the trace $\gamma u = u\big|_{\partial X}$ be

$$\gamma_{odd}\, u = \pm \mathrm{sign}(p_1) A \gamma_{ev}\, u \quad , \quad \Pi_{ev} A = A \Pi_{ev}.$$

Formal integration by part

$$\mathrm{Re}\,\langle u\,,\, P_{\pm,Q,g} u\rangle = \frac{\|\nabla_p u\|^2_{L^2(X,dqdp;\mathfrak{f})} + \||p|_q u\|^2_{L^2(X,dqdp;\mathfrak{f})}}{2} \pm \frac{1}{2}\int_{\partial X} |\gamma u|(q',p)^2\; p_1\, dq' dp$$

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Assumptions:

- $A = A(q, |p|_q)$ is local in q and $|p|_q$ (local elastic collision at the boundary);
- $A(q, |p|_q) \in \mathcal{L}(L^2(S^*_{\partial Q} Q, |\omega_1| dq' d\omega; \mathfrak{f}))$ with $\|A(q,r)\| \leq C$ unif.
- either $\mathrm{Re}\, A(q,r) \geq c_A > 0$ unif. or $A(q,r) \equiv 0$.

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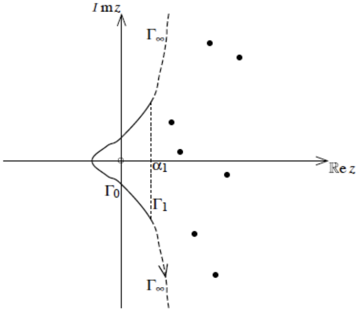
Questions

Do such boundary conditions with (A, j) define a maximal accretive realization $K_{\pm,A,g}$ of $P_{\pm,Q,g}$?

Can we specify the domain of $K_{\pm,A,g}$ and the regularity (and decay in p) estimates for the resolvent ? Global subelliptic estimates ?

$K_{\pm,A,g}$ "cuspidal" ?



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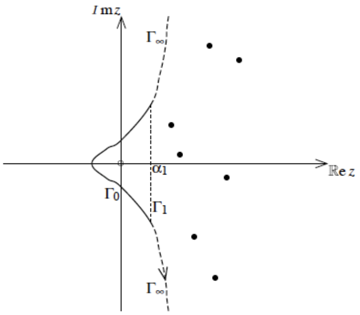

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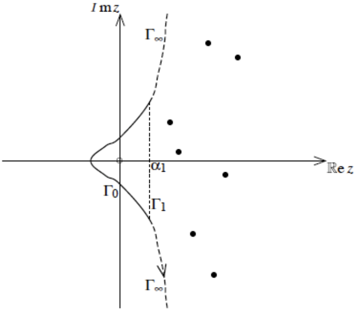

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Some related works and motivations

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SDE's: B. Lapeyre (1990) 1D specular reflection, Bossy–Jabir (2011) specular reflection. Bertoin (2007) non-elastic 1D boundary conditions. Very few results for the PDE interpretation

Quasi Stationary Distribution ($\to$ molecular dynamics algorithms): Le Bris–Lelièvre–Luskin–Perez (2012) and Lelièvre–N. (2013) Elliptic case, Witten Laplacian. But Langevin is a more natural model !

Exponentially small eigenvalues of Witten Laplacians on p-forms in the low temperature limit: Le Peutrec–Viterbo–N. (2013) Artificial boundary value problems are introduced.

Series of works by Bismut and Lebeau (2004$\to$2011) about the hypoelliptic Laplacian. Phase-space hypoelliptic and non self-adjoint version of Witten's deformation of Hodge theory.

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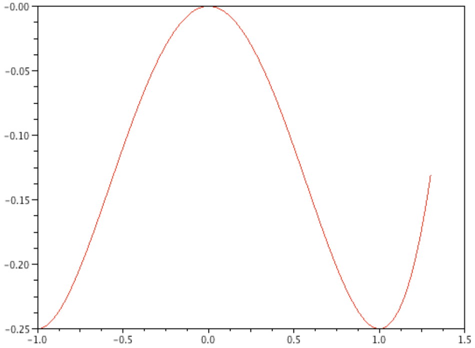
QSD Simulations by T. Lelièvre

Comparison of QSD simulations: Witten with Dirichlet BC (blue line), Langevin with absorbing BC (histogram).
Friction $b = 10$, $dt = 0.01$, 2000 time-step, 10000 independent particles.



Potential $V(q) = \frac{q^4}{4} - \frac{q^2}{2}$ **,** $-1 \leq q \leq 1.3$

QSD Simulations by T. Lelièvre

Comparison of QSD simulations: Witten with Dirichlet BC (blue line), Langevin with absorbing BC (histogram).
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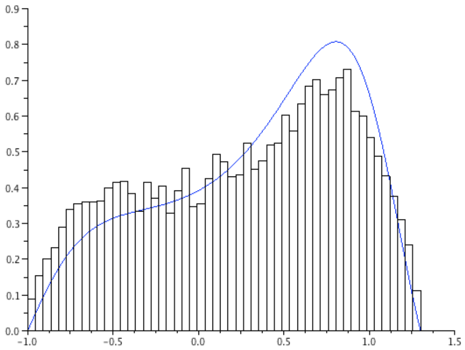

Quasi-stationnary particle density w.r.t q

Notations and first result

Call $\mathcal{O}_{Q,g} = \frac{-\Delta_p + |p|_q^2}{2}$ and set $\mathcal{H}^{s'}(q) = (d/2 + \mathcal{O}_{Q,g})^{-s'/2} L^2(T_q^*Q, dp; \mathfrak{f})$ and globally $\mathcal{H}^{s'} = (d/2 + \mathcal{O}_{Q,g})^{-s'/2} L^2(X, dqdp; \mathfrak{f})$. $H^s(Q; \mathcal{H}^{s'})$ is the Sobolev space of H^s-sections of the hermitian fiber bundle $\pi_{\mathcal{H}^{s'}} : \mathcal{H}^{s'} \to Q$.

Remember the BC's $\gamma_{odd} u = \pm \mathrm{sign}(p_1) A \gamma_{ev} u$

- $A\Pi_{ev} = \Pi_{ev} A$;
- $A = A(q, |p|_q)$ is local in q and $|p|_q$ (local elastic collision at the boundary);
- $A(q, |p|_q) \in \mathcal{L}(L^2(S^*_{\partial Q} Q, |\omega_1| dq' d\omega; \mathfrak{f}))$ with $\|A(q,r)\| \leq C$ unif.
- either $\mathrm{Re}\, A(q,r) \geq c_A > 0$ unif. or $A(q,r) \equiv 0$.

Theorem 1: With the domain $D(K_{\pm,A,g})$ characterized by

$$u \in L^2(Q; \mathcal{H}^1) \quad , \quad P_{\pm,Q,g} u \in L^2(X, dqdp; \mathfrak{f}) ,$$
$$\gamma u \in L^2_{loc}(\partial X, |p_1| dq' dp; \mathfrak{f}) \quad , \quad \gamma_{odd} u = \pm \mathrm{sign}(p_1) A \gamma_{ev} u ,$$

the operator $K_{\pm,A,g} - \frac{d}{2}$ is maximal accretive and

$$\mathrm{Re}\, \langle u \,,\, (K_{\pm,A,g} + \frac{d}{2}) u \rangle = \|u\|^2_{L^2(Q, dq; \mathcal{H}^1)} + \mathrm{Re}\, \langle \gamma_{ev} u \,,\, A \gamma_{ev} u \rangle_{L^2(\partial X, |p_1| dq' dp; \mathfrak{f})} .$$

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Subelliptic estimates when $A = 0$

Theorem 2: When A=0 there exists $C > 0$ and for all $\Phi \in \mathcal{C}_b^\infty([0,+\infty))$ satisfying $\Phi(0) = 0$ a constant C_Φ such that

$$\langle\lambda\rangle^{\frac{1}{4}}\|u\| + \langle\lambda\rangle^{\frac{1}{8}}\|u\|_{L^2(Q;\mathcal{H}^1)} + \|u\|_{H^{1/3}(Q;\mathcal{H}^0)} + \langle\lambda\rangle^{\frac{1}{4}}\|(1+|p|_q)^{-1}\gamma u\|_{L^2(\partial X,|p_1|dq'dp;\mathfrak{f})} \leq C\|(K_{\pm,0,g} - i\lambda)u\|\,,$$

and

$$\|\Phi(d_g(q,\partial Q))\mathcal{O}_{Q,g}u\| \leq C\|\Phi\|_{L^\infty}\|(K_{\pm,0,g} - i\lambda)u\| + C_\Phi\|u\|\,,$$

hold for all $u \in D(K_{\pm,0,g})$ and all $\lambda \in \mathbb{R}$.

Theorem 3: Assume $\mathrm{Re}\, A(q, |p|_q) \geq c_A > 0$ uniformly. There exists $C > 0$, for all $t \in [0, \frac{1}{18})$ a constant $C_t > 0$ and for all $\Phi \in \mathcal{C}_b^\infty([0, +\infty))$ satisfying $\Phi(0) = 0$ a constant C_Φ such that

$$\langle\lambda\rangle^{\frac{1}{4}}\|u\| + \langle\lambda\rangle^{\frac{1}{8}}\|u\|_{L^2(Q;\mathcal{H}^1)} + C_t^{-1}\|u\|_{H^t(Q;\mathcal{H}^0)} + \langle\lambda\rangle^{\frac{1}{8}}\|\gamma u\|_{L^2(\partial X, |p_1|\,dq'\,dp;\mathfrak{f})} \leq C\|(K_{\pm,A,g} - i\lambda)u\|\,,$$

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The operator $K_{\pm,A,g}$ is cuspidal.

When $\overline{Q}$ is compact, $K_{\pm,A,g}^{-1}$ is compact $\rightarrow$ discrete spectrum.

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PT-symmetry if $jAj = A^*$, $UK_{\pm,A,g}U^* = K_{\mp,A^*,g} = K^*_{\pm,A,g}$ when $Uu(q,p) = u(q,-p)$.

The results hold (with additional conditions for the PT-symmetry) when $Q \times \mathfrak{f}$ is replaced by a hermitian bundle $\pi_F : F \rightarrow Q$ with a metric g^F and a connection ∇^F . The pull-back bundle $F_X = \pi^* F$ with $\pi : \overline{X} = \overline{T^*Q} \rightarrow \overline{Q}$ is then endowed with the metric $g^{F_X} = \pi^* g^F$ and the connection

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DEF: General geometric Kramers-Fokker-Planck operator (including hypoelliptic Laplacian)

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Scalar case: $\mathfrak{f} = \mathbb{C}$

Specular reflection: $j = 1\,,\; A = 0\,.$

Absorption: $j = 1\,,\; A = \mathrm{Id}\,.$

The two above cases can be interpreted in terms of stochastic processes by completing the Langevin process with a jump process when $X(t)$ hits the boundary:

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More general jump processes: Set $\partial X_{\pm} = \{(0, q', p_1, p')\,, \pm p_1 > 0\}$. More general Markov kernel from ∂X_+ to $\partial X_- \sqcup \{\mathfrak{e}\}$ can be considered. $\mathrm{Re}\, A \geq c_A$ means that a positive fraction is sent to $\mathfrak{e}$

Doubling the manifold: In the position variable the Neumann and Dirichlet boundary value problems for $-\Delta_q$ can be introduced by considering even and odd solutions after the extension by reflection $(q^1, q') \to (-q^1, q')$.
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Doubling the manifold: In the position variable the Neumann and Dirichlet boundary value problems for $-\Delta_q$ can be introduced by considering even and odd solutions after the extension by reflection $(q^1, q') \to (-q^1, q')$.
Here the extension by reflection is $(q^1, q', p_1, p') \to (-q^1, q', -p_1, p')$.

- Even case=specular reflection: $j = 1$ and $A = 0$.
- Odd case: $j = -1$ and $A = 0 \to$ does not preserve the positivity.

Hypoelliptic Laplacian

Set $\eta(U,V)=\langle \pi_* U\,,\,\pi_* V\rangle_g-\omega(U,V)$ for $U,V\in TX=T(T^*Q)$ where $\omega=dp\wedge dq$ is the symplectic form on X. The non degenerate form η^* is defined by duality and then extended to $\bigwedge T_x^*X$, $x=(q,p)$.
Call d^X the differential on X and $\overline{d}_\eta^X$ the "codifferential" defined by

$$\int_X \langle (d^X s)(x)\,,\,s'(x)\rangle_\eta~dqdp=\int_X \langle s(x)\,,\,(\overline{d}_\eta^X s')(x)\rangle_\eta~dqdp\,.$$

Deformation à la Witten: For $\mathcal{H}(q,p)=\frac{|p|_q^2}{2}+V(q)$, the deformed differential and codifferential are defined by

$$d_{\mathcal{H}}^X=e^{-\mathcal{H}}d^X e^{\mathcal{H}}\quad,\quad \overline{d}_{\eta,\mathcal{H}}^X=e^{\mathcal{H}}\overline{d}_{\mathcal{H}}^X e^{-\mathcal{H}}\,.$$

Hypoelliptic Laplacian $\quad \mathcal{U}_{\mathcal{H}}^2=(d_{\mathcal{H}}^X+\overline{d}_{\eta,\mathcal{H}}^X)^2\,.$
With the basis $(e^I\hat{e}_J=e^{i_1}\wedge\ldots\wedge e^{i_{|I|}}\wedge\hat{e}_{j_1}\wedge\ldots\wedge\hat{e}_{j_{|J|}})$ with $e^i=dq^i$, $\hat{e}_j=dp_j-\Gamma_{ij}^{\ell}p_\ell dq^i$, consider the weight operator

$$\langle p\rangle^{\pm\widehat{\deg}}(\omega_I^J e^I\hat{e}_J)=\langle p\rangle^{\pm|J|}\omega_I^J e^I\hat{e}_J\,.$$

Then $\langle p\rangle^{-\widehat{\deg}}\circ\mathcal{U}_{\mathcal{H}}^2\circ\langle p\rangle^{+\widehat{\deg}}$ is a geometric Kramers-Fokker-Planck operator.
(Note $e^i=\pi^*(dq^i)$, $\hat{e}_j=\pi^*(dp_j)=\pi^*(\partial_{q^j})$.)

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A proposal for "Dirichlet" and "Neumann" realization of the hypoelliptic Laplacian.

Remember $g^X = g \oplus g^{-1}$ with $g(e^i, e^j) = g^{ij}$, $g(\hat{e}_i, \hat{e}_j) = g_{ij}$ and $g(e^i, \hat{e}_j) = 0$ and the natural extension to $\bigwedge T_x^* X$.

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defines a unitary involution on $F^X = \pi^* F$ for $k = 0$ and $k = 1$.

"Neumann" realization: Take $k = 0$, $j = \mathbf{j}_0$ and $A = 0$.

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- Have a good understanding of the simplest $1D$-problem.
- Use some separation of variables for straight half-spaces.
- Look at the general local problem by sending it to the straight half-space problem with a change of variables and try to absorb the corresponding perturbative terms.

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Problems

Pb 1 The simplest $1D$ problem is actually a $2D$-problem with p-dependent coefficients. Moreover it looks like a corner problem.

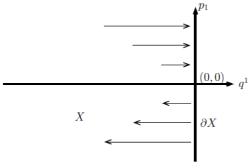

Fig.1: The boundary $\partial X = \{q^1 = 0\}$ and the vector field $p_1 \partial_{q^1}$ are represented. For the absorbing case, the boundary condition says $\gamma u(p_1) = 0$ for $p_1 < 0$ and corresponds to the case ($j = 1$ and $A = 1$).

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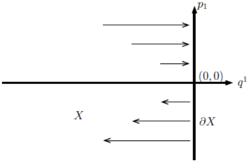

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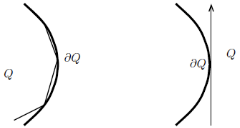

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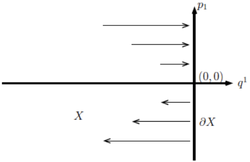

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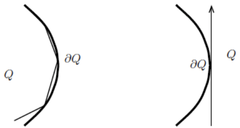

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Pb 1 solved by introducing adapted Fourier series and a quantization of the function $\mathrm{sign}(p_1)$.

Pb 2 solved by introducing a dyadic partition of unity in the p-variable and by using the 2nd resolvent formula for the corresponding semiclassical problems ($h = 2^{-j}$) .

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Take $\mathfrak{f} = \mathbb{C}$, $j = 1$ for simplicity. One wants to prove that

$$\begin{cases} p\partial_q u + (\frac{1}{2} + \mathcal{O})u = [p\partial_q + \frac{-\partial_p^2 + p^2 + 1}{2}]u = f\,, \\ \gamma_{odd} u = \mathrm{sign}(p) A \gamma_{ev} u\,, \end{cases}$$

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$A_0 = \sum_{\nu \in \pm(2\mathbb{N}^*)^{-\frac{1}{2}}} \nu |e_\nu\rangle\langle e_\nu|$ in $\mathcal{H}^1$ with $e_\nu = i^{\frac{\mathrm{sign}(\nu)}{2\nu^2}} \nu \varphi_{[\frac{1}{2\nu^2} - 1]}(p - \frac{1}{\nu})$ and φ_n, n^{th} normalized Hermite function.

Defined $\mathcal{D}_s = \left\{ u = \sum_{\nu \in \pm(2\mathbb{N}^*)^{-\frac{1}{2}}} u_\nu e_\nu\,, \sum_{\nu \in \pm(2\mathbb{N}^*)^{-\frac{1}{2}}} |\nu|^{2s} |u_\nu|^2 < +\infty \right\}$.

Then $\mathcal{D}_0 = \mathcal{H}^1$, $\mathcal{D}_{-1} = \left\{ u \in \mathcal{D}'(\mathbb{R}^*)\,, pu \in \mathcal{H}^{-1} \right\}$ and

$$\mathcal{D}_{-\frac{1}{2}} = L^2(\mathbb{R}, |p|dp)$$

with a different scalar product. If $Se_\nu = \mathrm{sign}(\nu) e_\nu$ then

$$\langle u\,, Sv\rangle_{\mathcal{D}_{-\frac{1}{2}}} = \langle u\,, \mathrm{sign}(p) v\rangle_{L^2(\mathbb{R}, |p|dp)} = \int_{\mathbb{R}} \overline{u}(p) v(p)\; pdp\,.$$

Set $\mathcal{E}(\mathbb{R}_-)=\left\{u\in L^2(\mathbb{R}_-,dq;\mathcal{H}^1); p\partial_q\in L^2(\mathbb{R}_-,dq;\mathcal{H}^{-1})\right\}$. There is a continuous and onto trace operator $\gamma:\mathcal{E}(\mathbb{R}_-)\to\mathcal{D}_{-\frac{1}{2}}$.

After setting $\tilde{f}=(\frac{1}{2}+\mathcal{O})^{-1}f=\sum_{\nu\in\pm(2\mathbb{N}^*)^{-\frac{1}{2}}}f_\nu e_\nu$, the well posedness of

$$\left\{\begin{array}{l}(p\partial_q+(\frac{1}{2}+\mathcal{O}))u=f\\ T\gamma u=f_\partial\in\mathcal{T}\quad\text{with}\quad T\in\mathcal{L}(\mathcal{D}_{-\frac{1}{2}};\mathcal{T})\end{array}\right.$$

is equivalent to the well posedness in $\mathcal{D}_{-\frac{1}{2}}$ of

$$\left\{\begin{array}{l}(1+S)\gamma=0,\\ T\gamma=f'_\partial\in\mathcal{T}\quad T\in\mathcal{L}(\mathcal{D}_{-\frac{1}{2}};\mathcal{T})\end{array}\right.$$

The Calderon projector (kill the exponentially growing modes when solving $\nu\partial_q u_\nu+u_\nu=0$) is $1_{\mathbb{R}_-}(S)$ and $\mathrm{Ran}1_{\mathbb{R}_-}(S)=\ker 1_{\mathbb{R}_+}(S)=\ker\left(\frac{1+S}{2}\right)$.

With $M=S\circ\mathrm{sign}(p)$, solving $\gamma_{odd}-\mathrm{sign}(p)A\gamma_{ev}=f'_\partial$ and $(1+S)\gamma=0$ is equivalent to

$$(\mathrm{Id}+MA)\gamma_{ev}=-f'_\partial\quad,\quad\gamma_{odd}=-S\gamma_{ev}\,.$$

But $((A,D(A))$ max. acc. in $L^2(\mathbb{R},|p|dp))\Leftrightarrow\left((MA,D(A))\text{ max. acc. in }\mathcal{D}_{-\frac{1}{2}}\right)$.
Conclusion: $K_{\pm,A}$ is maximal accretive.

1D case

Set $\mathcal{E}(\mathbb{R}_-) = \left\{u \in L^2(\mathbb{R}_-, dq; \mathcal{H}^1); p\partial_q \in L^2(\mathbb{R}_-, dq; \mathcal{H}^{-1})\right\}$. There is a continuous and onto trace operator $\gamma : \mathcal{E}(\mathbb{R}_-) \to \mathcal{D}_{-\frac{1}{2}}$.

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Conclusion: $K_{\pm,A}$ is maximal accretive.

Conclusion

This solves only the basic functional analysis.
There are still a lot of things to be investigated:

- Non self-adjoint spectral problems.
- Boundary value problems.
- Parameter dependent asymptotics (large friction, small temperature=semiclassical).
- Multiple wells and tunnel effect...