Geometric Kramers-Fokker-Planck operators with boundary conditions

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Outline

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

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 $g = g_{ij}(q)dq^i dq^j$, $g^{-1} = (g^{ij})$

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

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

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

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

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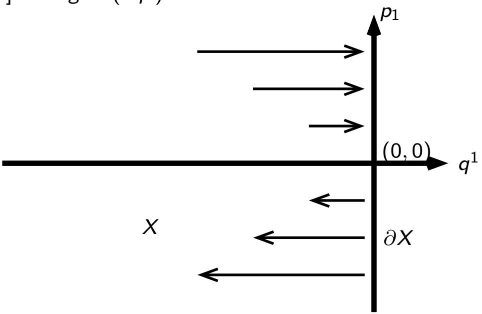
A simple case

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 $p_1 < 0$.

It can be written $\gamma_{odd}\, u = \mathrm{sign}(p_1)\gamma_{ev}\, u$ with $\gamma_{ev}\, u = \frac{u(0,p_1) + u(0,-p_1)}{2}$.

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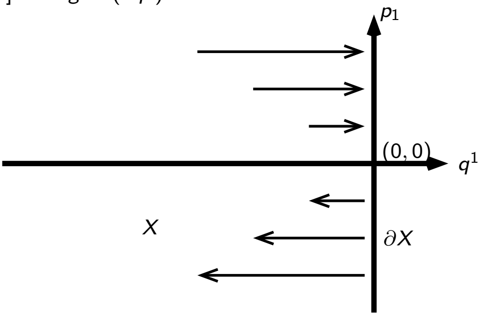

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General BC

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 $\partial X = \left\{q^1 = 0\right\}$:

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

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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.
- $A\Pi_{ev} = \Pi_{ev} A$
- either $\mathrm{Re}\, A(q, r) \geq c_A > 0$ unif. or $A(q, r) \equiv 0$.

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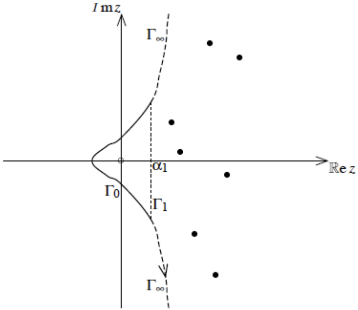
Questions

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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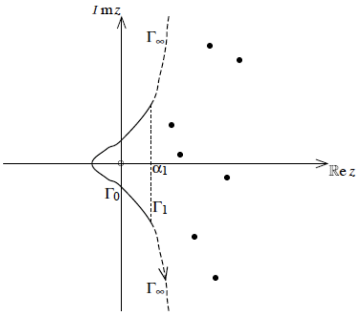

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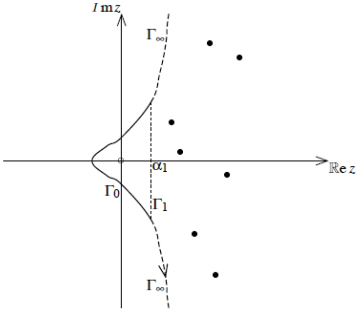

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SDE's: B. Lapeyre (1990) 1D specular reflection, Bossy–Jabir (2011) specular reflection. Bertoin (2007) non-elastic 1D boundary conditions. Very few results for the PDE interpretation

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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

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

The adjoint of $K_{\pm,A,g}$ is $K_{\mp,A^*,g}$.

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 $\pi_{\mathcal{H}^{s'}} : \mathcal{H}^{s'} \to Q$.

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Notations and first result

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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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Corollaries

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

When $\overline{Q}$ is compact, $K^{-1}_{\pm,A,g}$ is compact $\to$ discrete spectrum.

The integration by parts imply $\|u\|^2_{L^2(Q,\mathcal{H}^1)} \leq \|(K_{\pm,A,g} - i\lambda)u\|\|u\|$ and a potential term $\mp\partial_q V(q)\partial_p$ with V Lipschitz is a nice perturbation $\to$ All the results are still valid with such a potential term.

PT-symmetry if $UAU^* = A^*$, $UK_{\pm,A,g}U^* = K_{\mp,A^*,g} = K^*_{\pm,A,g}$ 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 $\pi_F : F \to Q$ with a metric g^F and a connection ∇^F . The pull-back bundle $F_X = \pi^* F$ with $\pi : \overline{X} = \overline{T^*Q} \to \overline{Q}$ is then endowed with the metric $g^{F_X} = \pi^* g^F$ and the connection

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Covariant derivative $\tilde{\nabla}^{F_X}_T(s^k(x)f_k) = Ts^k(x)f_k + s^k(x)\nabla^{F_X}_T f_k$. $\quad x = (q,p)$.

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:

- For specular reflection the jump changes the velocity (p_1, p') with $p_1 > 0$ into $(-p_1, p')$;
- For the absorption, the particle is sent to an external stationary point $\mathfrak{e}$ when the particle hits the boundary.

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

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Hypoelliptic Laplacian: partial differential operator acting on differential forms= sections of $\bigwedge T^*X$, of which the main part is a scalar geometric KFP operator. (REF Bismut and Lebeau).

With the basis $(e^I \hat{e}_J = e^{i_1} \wedge \ldots \wedge e^{i_{|I|}} \wedge \hat{e}_{j_1} \wedge \ldots \wedge \hat{e}_{j_{|J|}})$ of $\bigwedge T^*_x X$, $x \in \partial X$, $e^i = dq^i$, $\hat{e}_j = dp_j - \Gamma^\ell_{ij} p_\ell dq^i$, the involution $\mathbf{j}_k$ is defined pointwise by

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

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Hypoelliptic Laplacian, a p-form version

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It is a very classical one for boundary value problems (see for example Hörmander-Chap 20 or Boutet de Montvel (1970))

- 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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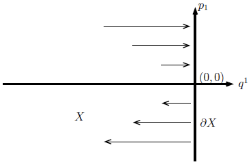

Fig.1: The boundary $\partial X = \{q^1 = 0\}$ and the vector field $p_1\partial_{q^1}$ are represented. For the absorbing case, the boundary condition says $\gamma u(p_1) = 0$ for $p_1 < 0$ and corresponds to the case ($j = 1$ and $A = 1$).

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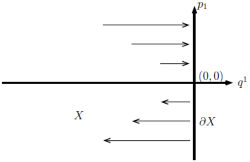

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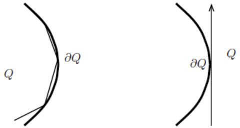

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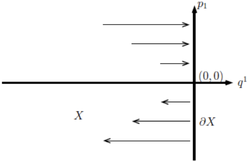

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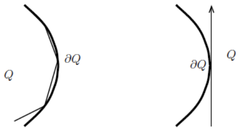

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Pb 1 solved by introducing adapted Fourier series and a quantization of the function $\mathrm{sign}(p_1)$.

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 $(h = 2^{-j})$.

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...