Geometric Kramers-Fokker-Planck operators with boundary conditions

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Beijing, april 30th 2014

Outline

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

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

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

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

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

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

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

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

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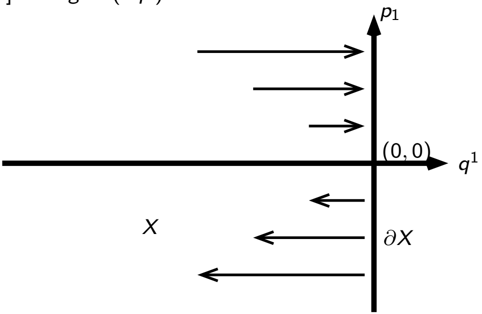
acting on $\mathcal{C}^\infty(\overline{X};\mathfrak{f})$. $P_{\pm,Q,g}=$ scalar part of Bismut's hypoelliptic Laplacian.

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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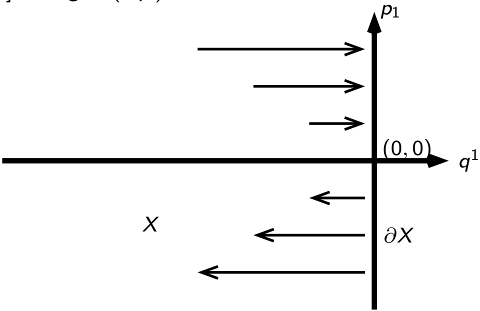

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General BC

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

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

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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

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

$$= \frac{\|\nabla_p u\|^2_{L^2(X,dqdp;\mathfrak{f})} + \||p|_q u\|^2_{L^2(X,dqdp;\mathfrak{f})}}{2} + \underbrace{\mathrm{Re}\,\langle \gamma_{ev} u\,,\, A\gamma_{ev} u\rangle_{L^2(\partial X, |p_1| dq' dp;\mathfrak{f})}}\,.$$

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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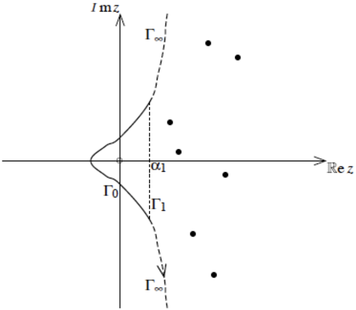
Questions

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" ?



Compactness of the resolvent ? Discrete spectrum ? Exponential decay ppties of

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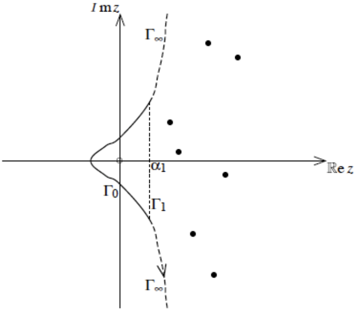

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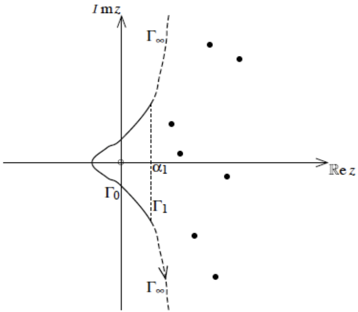

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Some related works and motivations

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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.

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

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

$$u \in L^2(Q; \mathcal{H}^1) \quad , \quad P_{\pm,Q,g} u \in L^2(X, dqdp; \mathfrak{f}),$$
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the operator $K_{\pm,A,g} - \frac{d}{2}$ is maximal accretive and

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

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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 $\lambda \in \mathbb{R}$.

Subelliptic estimates when $\mathrm{Re}\, A \geq c_A > 0$

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.

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

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

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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 $(-p_1, p')$;
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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 $\mathfrak{e}$

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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 $\overline{d}^X_\eta$ the "codifferential" defined by

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

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

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

Hypoelliptic Laplacian $\qquad \mathcal{U}^2_{\mathcal{H}}=(d^X_{\mathcal{H}}+\overline{d}^X_{\eta,\mathcal{H}})^2\,.$

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 $e^i=dq^i$, $\hat{e}_j=dp_j-\Gamma^{\ell}_{ij}p_\ell dq^i$, consider the weight operator

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

Then $\langle p\rangle^{-\widehat{\deg}}\circ\mathcal{U}^2_{\mathcal{H}}\circ\langle p\rangle^{+\widehat{\deg}}$ 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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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 $\bigwedge T^*_xX$, $x=(q,p)$.
Call d^X the differential on X and $\overline{d}^X_\eta$ the "codifferential" defined by

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

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

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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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$$\mathbf{j}_k(e^I \hat{e}_J) = (-1)^k (-1)^{|\{1\}\cap I| + |\{1\}\cap J|} e^I \hat{e}_J \,,$$

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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Starting from $\mathcal{D} = \left\{ u \in \mathcal{C}_0^\infty(\overline{X}; \bigwedge T^* X) \,, \gamma_{odd} u = 0 \right\}$, the closure of $C + \langle p \rangle^{-\widehat{\deg}} \circ \mathcal{U}_{\mathcal{H}}^2 \circ \langle p \rangle^{+\widehat{\deg}}$ is maximal accretive. The fiber bundle version of Theorem 1 and its corollaries are valid.

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Strategy

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

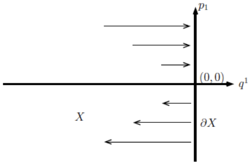

Fig.1: The boundary $\partial X = \{q^1 = 0\}$ and the vector field $p_1\partial_{q^1}$ are represented. For the absorbing case, the boundary condition says $\gamma u(p_1) = 0$ for $p_1 < 0$ and corresponds to the case ($j = 1$ and $A = 1$).

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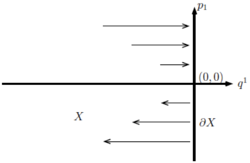

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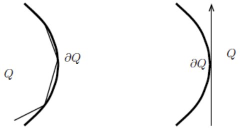

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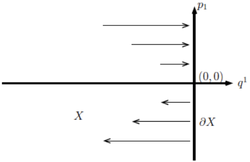

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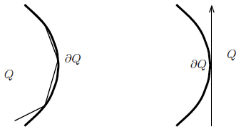

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Pb 1 solved by introducing adapted Fourier series and a quantization of the function $\mathrm{sign}(p_1)$.
Pb 2 solved by introducing a dyadic partition of unity in the p-variable and by using the 2nd resolvent formula for the corresponding semiclassical problems $(h = 2^{-j})$.

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...