Return to equilibrium, non-self-adjointness and symmetries

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based on joint works with F. Hérau and M. Hitrik

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0. Introduction

Consider differential operators $P = P(x, hD; h)$ on $\mathbf{R}^n$ or on a compact n-dimensional manifold. $D_x = \frac{1}{i}\frac{\partial}{\partial x}$, $h \to 0$. h can be Planck's constant or the temperature. Assume $0 \in \sigma(P)$ is a simple eigenvalue and e_0 a corresponding eigenfunction. Also assume that $\sigma(P) \subset \{z \in \mathbf{C};\ \Re z \geq 0\}$. The following problems are "equivalent" or at least closely related:

- Return to equilibrium: Study how fast $e^{-tP/h}u$ converges to a multiple of e_0 when $t \to +\infty$.
- Study the gap between 0 and $\sigma(P) \setminus \{0\}$.

Such problems appear when P is the Schrödinger operator, the Kramers-Fokker-Planck operator and for systems of coupled oscillators. Related problems appear in dynamical systems. The equivalence is clear when P is self-adjoint.

Simplifying feature for Kramers-Fokker-Planck: the presence of a supersymmetric structure (showing that we have a non-self-adjoint Witten Laplacian) observed by J.M. Bismut and Tailleur–Tanase-Nicola–Kurchan and also a reflection symmetry.
This also applies to a chain of two anharmonic oscillators between heatbaths in the case the temperatures are equal.
New result: Not always the case when the temperatures are different, so we then need a more direct tunneling approach.
Contrary to the case of Schrödinger operators and the ordinary Witten Laplacians, our operators are non-self-adjoint and non-elliptic.

1. Schrödinger operators and Witten Laplacians

Consider

$$P = -h^2\Delta + V(x), \quad 0 \le V \in C^\infty(M), \tag{1}$$

$M = \mathbf{R}^n$ or $=$ a compact Riemannian manifold. $\liminf_{x\to\infty} V > 0$ in the first case. Assume that $V^{-1}(0)$ is finite $= \{U_1, ..., U_N\}$, where $V''(U_j) > 0$. B. Simon (1983), B. Helffer–Sj (1984) showed that the eigenvalues in any interval $[0, Ch]$ have complete asymptotic expansions in powers of h:

$$\lambda_{j,k} = \lambda_{j,k}^{(0)} h + o(h), \tag{2}$$

where $\lambda_{j,k}^{(0)}$ are the eigenvalues of the quadratic approximations $-\Delta + \frac{1}{2}\langle V''(U_j)x, x\rangle$.

If u is a corresponding normalized eigenfunction:

$$|u(x;h)| \leq C_{\epsilon,K} e^{-\frac{1}{h}(d(x)-\epsilon)},\ x \in K \Subset M, \quad d(x) = d(x, \cup_1^N U_j), \tag{3}$$

Agmon distance, associated to the metric to $V(x)dx^2$.

Double well case: Assume $N = 2$, $V \circ \iota = V$, where ι is an isometry with $\iota^2 = 1$, $\iota(U_1) = U_2$. The eigenvalues form exponentially close pairs. The two smallest eigenvalues E_0, E_1 satisfy

$$E_1 - E_0 = h^{\frac{1}{2}} b(h) e^{-d(U_1,U_2)/h},\ b(h) \sim \sum_0^\infty b_j h^j,\ b_0 > 0. \tag{4}$$

1D: Harrel, Combes-Duclos-Seiler, multi-D: B.Simon, B.Helffer-Sj. The precise formula (4) is due to Helffer–Sj with an additional non-degeneracy assumption on the minimizing Agmon geodesics from U_1 to U_2.

Multi-well case: Helffer-Sj: similar result using an interaction matrix. Sometimes quite explicit, sometimes less when non-resonant wells are present.

The Witten complex

Let M be a compact Riemannian manifold, $\phi : M \to \mathbf{R}$ a Morse function, $d : C^\infty(M; \wedge^\ell T^*M) \to C^\infty(M; \wedge^{\ell+1} T^*M)$ the de Rahm complex.
Witten complex:

$$d_\phi = e^{-\frac{\phi}{h}} \circ hd \circ e^{\frac{\phi}{h}} = hd + d\phi^\wedge.$$

Witten (Hodge) Laplacian:

$$\Box_\phi = d_\phi^* d_\phi + d_\phi d_\phi^*$$

Restriction to ℓ-forms

$$\Box_\phi^{(\ell)} = -h^2 \Delta^{(\ell)} + |\phi'|^2 + hM_\phi^{(\ell)}, \quad M_\phi^{(\ell)} = \text{ smooth matrix.}$$

Matrix Schrödinger operator with the critical points of ϕ as potential wells.

Let $C^{(\ell)}$ be the set of critical points of index ℓ. The result (2) applies to $\Box_\phi^{(\ell)}$.

Proposition

- *If $U_j \in C^{(\ell)}$, then the smallest of the $\lambda_{j,k}^{(0)}$ is zero.*
- *If $U_j \notin C^{(\ell)}$, the all the $\lambda_{j,k}^{(0)}$ are > 0.*

Thus $\Box_\phi^{(\ell)}$ has precisely $\sharp C^{(\ell)}$ eigenvalues that are $o(h)$ and using the intertwining relations, $\Box_\phi^{(\ell+1)} d_\phi = d_\phi \Box^{(\ell)}$ and similarly for d_ϕ^*, one can show that they are actually exponentially small.

In principle it should be possible to analyze the exponentially small eigenvalues by applying the interaction matrix approch (Helffer-Sj) to $\Box_\phi^{(\ell)}$, but we run into the problem of tunneling through non-resonant wells, and it turned out to be better to make a corresponding analysis directly for d_ϕ and d_ϕ^*.

Let $\mathcal{B}^{(\ell)}$ be the spectral subspace generated by the eigenvalues of $\square_\phi^{(\ell)}$ that are $o(h)$, so that $\dim \mathcal{B}^{(\ell)} = \# C^{(\ell)}$. Then hd_ϕ splits into the exact sequence:

$$\mathcal{B}^{(0)\perp} \to \mathcal{B}^{(1)\perp} \to \ldots \to \mathcal{B}^{(n)\perp}$$

and the finite dimensional complex:

$$\mathcal{B}^{(0)} \to \mathcal{B}^{(1)} \to \ldots \to \mathcal{B}^{(n)}. \tag{5}$$

Witten (Simon, Helffer-Sj): analytic proof of the Morse inequalities. Tunneling analysis (Helffer-Sj) gives an analytic proof of

Theorem

The Betti numbers can be obtained from the orientation complex.

More recently Bovier–Eckhoff–Gayrard–Klein, Helffer-Klein-Nier studied the non-vanishing exponentially small eigenvalues in degeree 0. Le Peutrec-Nier-Viterbo have recent results also in higher degree.

2. The Kramers-Fokker-Planck operator (Hérau-Hitrik-Sj)

$$P = \underbrace{y \cdot h\partial_x - V'(x) \cdot h\partial_y}_{\text{skew-symmetric}} + \underbrace{\frac{\gamma}{2}(y - h\partial_y) \cdot (y + h\partial_y)}_{\geq 0 \text{ dissipative part}} \text{ on } \mathbf{R}^{2d}_{x,y}. \quad (6)$$

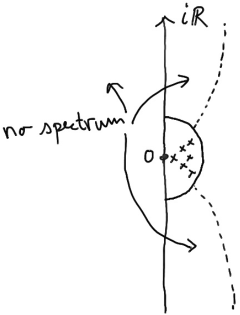
$h > 0$ is the temperature and we will work in the low temperature limit. $\gamma > 0$ is the friction.
We will assume that $V \in C^\infty(\mathbf{R}^d; \mathbf{R})$,

$$\partial^\alpha V = \mathcal{O}(1) \text{ when } |\alpha| \geq 2, \quad |V'(x)| \geq \frac{1}{C} \text{ for } |x| \geq C, \quad (7)$$

and also for simplicity that $V(x) \to +\infty$, when $x \to \infty$.

- P is maximally accretive, it has a unique closed extension $L^2 \to L^2$ from $\mathcal{S}(\mathbf{R}^{2d})$.
- The spectrum $\sigma(P)$ of P is contained in the closed half-plane $\Re z \geq 0$.
- If $V(x) \to +\infty$ when $|x| \to \infty$, then $e_0(x,y) := e^{-(y^2/2+V(x))/h} \in \mathcal{N}(P)$ so $0 \in \sigma(P)$ and this is the only eigenvalue on $i\mathbf{R}$. The problem of return to equilibrium is then to study how fast $e^{-tP/h}u$ converges to a multiple of e_0 when $t \to +\infty$ "$\Leftrightarrow$" Study the gap between 0 and "the next eigenvalue".
- The problem of return to equilibrium is originally posed in other spaces.

Freidlin-Wentzel: probabilistic methods.
Desvillettes, Villani, Eckmann, Hairer, Hérau, F. Nier, Helffer-Nier: classical PDE (pre-microlocal analysis) methods.
Hérau-Nier showed a global hypoellipticity result and in particular that there is no spectrum in a parabolic neighborhood of $i\mathbf{R}$ away from a disc around the origin and that the spectrum in that disc is discrete:



They also showed very interesting estimates relating the first spectral gap of P with that of the Witten Laplacian $d_V^* d_V$ on 0-forms.

Assume that

$$V \text{ is a Morse function with } n_0 \text{ local minima.} \tag{8}$$

Hérau–Sj–C. Stolk: The spectrum in any band $0 \leq \Re z < Ch$ is discrete and the eigenvalues are of the form

$$\mu h + o(h), \text{ complete asymptotic expansion.} \tag{9}$$

μ are the eigenvalues of the quadratic approximations of P at $(x_c, 0)$, where x_c are the critical points of V, explicitly known (H. Risken, HeSjSt). Sometimes the μ are real, sometimes not, but in all cases they belong to a sector $|\Im\mu| \leq \Re\mu$.
There are precisely n_0 eigenvalues with $\mu = 0$ and they are $\mathcal{O}(h^\infty)$ (HeSjSt).

NB: More difficult than in the Schrödinger case:

- P is non-self-adjoint and non-elliptic.
- Quite advanced microlocal analysis seems to be necessary.
- The difficulties become worse when considering exponential decay and tunneling.

Important supersymmetric observation by J.M. Bismut, Tailleur–Tanase-Nicola–Kurchan: P is equal to a "twisted" Witten Laplacian in degree 0: $d_\phi^{A,*} d_\phi$ which uses a non-symmetric sesquilinear product on L^2.

2.1. A result

The result is analogous to those of Bovier–Eckhoff–Gayrard–Klein, Helffer-Klein-Nier, Nier, Le Peutrec in the case of the Witten Laplacian. Recall that $\phi(x,y) = y^2/2 + V(x)$ and let $n = 2d$. Critical points of ϕ of index 1: saddle points. If $s \in \mathbf{R}^{2d}$ is such a point then for $r > 0$ small, $\{(x,y) \in B(s,r);\ \phi(x,y) < \phi(s)\}$ has two connected components. We say that s is a separating saddle point (ssp) if these components belong to different components in $\{(x,y) \in \mathbf{R}^{2n};\ \phi(x,y) < \phi(s)\}$.

Consider $\phi^{-1}(]-\infty,\sigma[)$ for decreasing σ. For $\sigma=+\infty$ we get $\mathbf{R}^n$ which is connected. Let m_1 be a point of minimum of ϕ and write $E_{m_1}=\mathbf{R}^n$. When decreasing σ, $E_{m_1}\cap\phi^{-1}(]-\infty,\sigma[)$ remains connected and non-empty until one of the following happens:

a) We reach $\sigma=\phi(s)$, where s is one or several ssps in E_{m_1}. Then $\phi^{-1}(]-\infty,\sigma[)\cap E_{m_1}$ splits into several connected components.

b) We reach $\sigma=\phi(m_1)$ and the connected component dissappears: $\phi^{-1}(\sigma)\cap E_{m_1}=\emptyset$.

In case a) one of the components contains m_1. For each of the other components, E_k we choose a global minimum $m_k\in E_k$ of $\phi_{|E_k}$ and write $E_k=E_{m_k}$, $\sigma=\sigma(m_k)$. Then continue the procedure with each of the connected components (including the one containing m_1).

Put $S_k=\sigma(m_k)-\phi(m_k)>0$, $S_1=+\infty$.

Theorem (Hérau-Hitrik-Sj, J. Inst. Math. Jussieu 2011)

- *The* n_0 *eigenvalues that are* $o(h)$*, are real and exponentially small:*

$$\lambda_j \asymp h e^{-2S_j/h}.$$

- *If we assume, after relabelling, that* $S_{k_2} > \max_{j\geq 3} S_{k_j}$ *and that* $\partial E_{m_{k_2}}$ *contains only one ssp, then the smallest non-vanishing eigenvalue is of the form*

$$\lambda_2 = h|b_2(h)|^2 e^{-2S_{k_2}/h},\ b_2 \sim b_{2,0} + h b_{2,1} + ..,\ b_{2,0} \neq 0. \quad (10)$$

- *Under an even stronger generic assumption, all the* $\lambda_2, \lambda_3, .., \lambda_{n_0}$ *are as in (10).*

2.2 Reflection symmetry

Let $\kappa : (x, y) \mapsto (x, -y)$ and define $U_\kappa : L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ by $U_\kappa u = u \circ \kappa$:

$$U_\kappa^2 = 1,\ U_\kappa^* = U_\kappa,$$

$$P^* U_\kappa = U_\kappa P.$$

Introduce the non-degenerate non-positive Hermitian form

$$(u|v)_\kappa := (U_\kappa u|v)_{L^2},\ \text{giving a Krein space structure.}$$

P is formally self-adjoint for $(\cdot|\cdot)_\kappa$:

$$(Pu|v)_\kappa = (U_\kappa Pu|v) = (P^* U_\kappa u|v) = (U_\kappa u|Pv) = (u|Pv)_\kappa.$$

Proposition

Let $E^{(0)} \subset L^2(\mathbf{R}^n)$ be the spectral subspace corresponding to $\lambda_1, ..., \lambda_{n_0}$. Then $(\cdot|\cdot)_\kappa$ is positive definite on $E^{(0)} \times E^{(0)}$ and hence a scalar product there.

$P : E^{(0)} \to E^{(0)}$ is self-adjoint, so $\lambda_1, ..., \lambda_{n_0}$ are real.

2.3 The supersymmetry

The supersymmetric structure of the KFP operator was observed by J.M. Bismut and Tailleur–Tanase-Nicola–Kurchan.
Let $A : (\mathbf{R}^n)^* \to \mathbf{R}^n$ be linear and invertible. For $u, v \in \wedge^k (\mathbf{R}^n)^*$, put

$$(u|v)_A = \langle \wedge^k A u | v \rangle$$

and extend the definition to square integrable k-forms by integration:

$$(u|v)_A = \int (u(x)|v(x))_A dx.$$

Adjoint: $(Qu|v)_A = (u|Q^{A,*} v)_A$.
If $\phi \in C^\infty(\mathbf{R}^n)$, put $d_\phi = e^{-\phi/h} \circ hd \circ e^{\phi/h}$. Twisted Witten Laplacian:

$$\Box_A := d_\phi^{A,*} d_\phi + d_\phi d_\phi^{A,*}, \text{ NB: } \Box_A^{(0)}(e^{-\phi/h}) = 0.$$

Example

Let

$$\mathbf{R}^n = \mathbf{R}^{2d}_{x,y}, \quad A = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & \gamma \end{pmatrix}, \quad \phi(x,y) = \frac{y^2}{2} + V(x).$$

Then

$$\Box_A^{(0)} = \mathrm{KFP}.$$

3. Supersymmetric structures, some generalities

Let M be $\mathbf{R}^n$ or a compact manifold of dimension n, equipped with a smooth strictly positive volume density $\omega(dx)$.
$\delta : C^\infty(M; \wedge^{k+1} TM) \to C^\infty(M; \wedge^k TM)$ be the adjoint of the de Rahm complex.
Let $A(x) : T_x^* M \to T_x M$ depend smoothly on $x \in M$. We have the bilinear product

$$(u|v)_A = (\wedge^k Au|v)_{L^2(\omega(dx))}, \; u, v \in C_0^\infty(M; \wedge^k T_x^* M).$$

When A is pointwise bijective we have formal adjoints, and for the restriction of the de Rahm operator to zero forms, we get

$$d^{A,*} = \delta A^{\mathrm{t}}.$$

Let P be a second order real differential operator on M. In local coordinates,

$$P = -\sum \partial_{x_j} B_{j,k}(x) \partial_{x_k} + \sum v_j(x) \partial_{x_j} + v_0, \tag{11}$$

where $(B_{j,k})$ is symmetric. Viewing P as acting on 0 forms, we ask whether there is a smooth map $A(x)$ as above, such that

$$P = d^{A,*} d = \delta A^{\mathrm{t}} d, \tag{12}$$

either locally or globally on M.

Proposition

- *In order to have (12), it is necessary that*

$$P(1) = 0 \textit{ and } P^*(1) = 0. \tag{13}$$

- *If (13) holds and the δ-complex is exact in degree 1 for smooth sections, we can find a smooth matrix A such that (12) holds. Moreover, $A = B + C$, where C antisymmetric.*

More generally, we assume that there exist smooth strictly positive functions $e^{-\phi}$ and $e^{-\psi}$ in the kernels of P and P^* respectively:

$$P(e^{-\phi}) = 0, \; P^*(e^{-\psi}) = 0. \tag{14}$$

This is a necessary condition for having

$$P = d_{\psi}^{A,*} d_{\phi}. \tag{15}$$

and also sufficient if we assume that the δ complex is exact in degree 1.

4. Chains of harmonic oscillators and absence of supersymmetry

We consider a chain of two oscillators coupled to two heat baths:

$$\widetilde{P}_W = \frac{\gamma}{2}\sum_{j=1}^{2}\alpha_j(-h\partial_{z_j})(h\partial_{z_j}+\frac{2}{\alpha_j}(z_j-x_j))+y\cdot h\partial_x-(\partial_x W(x)+x-z)\cdot h\partial_y.$$

- $(x_j, y_j) \in \mathbf{R}^{2n}$ are the coordinates of a classical particle,
- $\frac{y^2}{2} + W(x) + x^2/2$ is the classical Hamiltonian,
- $z_j \in \mathbf{R}^n$ correspond to each of the heat baths,
- $T_j = \alpha_j h/2 > 0$ are the temperatures in the baths,
- $\gamma > 0$ is the friction.

Eckmann–Pillet–Rey-Bellet (99)

The supersymmetric approach can be applied in two cases:

- Equilibrium case: The exterior temperatures are equal so that $\alpha_1 = \alpha_2 =: \alpha$.
- The decoupled case: $W = W_0(x) = W_1(x_1) + W_2(x_2)$

In each case we have an explicit function $\phi_0(x, y, z)$ such that

$$P_W := e^{\phi_0/h} \widetilde{P}_W e^{-\phi_0/h} = d_{\phi_0}^{A,*} d_{\phi_0},$$
$$P_W(e^{-\phi_0/h}) = 0, \; P_W^*(e^{-\phi_0/h}) = 0$$

In the first case (before observing the reflection symmetry) we had obtained an analogue of the above theorem for KFP in the case when W is a Morse function with two local minima and one saddle point.

In the decoupled case we have

$$\phi_0(x,y,z) = \sum_1^2 \frac{1}{\alpha_j}\left(\frac{y_j^2}{2} + W_j(x_j) + \frac{(x_j - z_j)^2}{2}\right).$$

$$\begin{aligned} P_{W_0} &= e^{\phi_0/h}\widetilde{P}_{W_0} e^{-\phi_0/h} \\ &= \frac{\gamma}{2}\sum_1^2 \alpha_j\left(-h\partial_z + \frac{1}{\alpha_j}(z_j - x_j)\right)\left(h\partial_z + \frac{1}{\alpha_j}(z_j - x_j)\right) \\ &\qquad + y\cdot h\partial_x - (\partial_x W_0(x) + x - z)\cdot h\partial_y, \end{aligned}$$

$$P_{W_0}(e^{-\phi_0/h}) = 0,\ P^*_{W_0}(e^{-\phi_0/h}) = 0.$$

Symbol:

$$q_{W_0}(x,y,z;\xi,\eta,\zeta) = \frac{\gamma}{2}\sum_1^2 \alpha_j(\zeta_j^2 - \frac{1}{\alpha_j}(z_j - x_j)^2)$$
$$+ y\cdot\xi - (\partial_x W_0(x) + x - z)\cdot\eta,$$

To leading order,

$$P_{W_0} = -q_{W_0}(x,y,z;-h\partial_x,-h\partial_y,-h\partial_z).$$

Eiconal equation:

$$q_{W_0}(x,y,z;\partial_x\phi_0,\partial_y\phi_0,\partial_z\phi_0) = 0$$

Now perturb $\widetilde{P}_{W_0}$ by replacing W_0 by $W = W_0 = W_0 + \delta W$, so we get $\widetilde{P}_W = \widetilde{P}_{W_0} - \partial_x\delta W(x)\cdot h\partial_y$,
$P_W = P_{W_0} - \partial_x\delta W(x)\cdot(h\partial_y - \partial_y\phi_0)$.

The following recent result that we have obtained with F. Hérau and M. Hitrik shows that the supersymmetric method breaks down for some perturbations:

Theorem

Take $\gamma = 1$ and assume that $\alpha_1 \neq \alpha_2$, $\alpha_j > 0$. Let $W_1(x_1)$ be a Morse function with two local minima m_1, m_2 and a saddle point s_0, tending to $+\infty$ when $x_1 \to \infty$. Let $W_2(x_2)$ be a positive definite quadratic form. Let $3 \leq m \in \mathbf{N}$. There exists $C^\infty(\mathbf{R}^{2n}) \ni \delta W = \mathcal{O}(|x_2|^m)$ arbitrarily small, vanishing near M_j and S_0, such that the eiconal equation $q_{W_0+\delta W}(x, y, z, \partial_x \phi, \partial_y \phi, \partial_z \phi) = 0$ has no smooth solution on $\mathbf{R}^{3n}$ with $\phi(\widetilde{M}_1) = 0$, $\phi'(\widetilde{M}_1) = 0$, $\phi''(\widetilde{M}_1) > 0$. Here, $M_j = (m_j, 0)$, $S_0 = (s_0, 0)$, $\widetilde{M}_1 = (M_1, 0, M_1)$.

Consequence: In general for coupled oscillators, there is no simple way of writing $P_W = d_{\psi}^{A,*} d_\phi$ with a smooth h-independent function ϕ.