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The Kramers–Fokker–Planck operator in the semiclassical limit.

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0. Introduction.

In this talk we describe the main results and ideas from a recent joint work [HeSjSt] with F. Hérau and C. Stolk. Following earlier works by many authors (Bouchut-Dolbeault, Talay, Villani-Desvillettes, Rey-Bellet-Thomas, Eckmann-Hairer, Eckman-Pillet-Rey-Bellet), F. Hérau and F. Nier [HeNi] used more traditional methods of partial differenial equations to study the Kramers-Fokker-Planck operator

$$K=y\cdot\partial_x-\frac{1}{m}V'(x)\cdot\partial_y-\gamma\partial_y\cdot(\frac{1}{m\beta}\partial_y+y),\ x,y\in\mathbf{R}^n, \tag{0.1}$$

and the long time behaviour of the corresponding evolution problem

$$\begin{cases}\partial_t f+Kf=0 \text{ on } [0,+\infty[\times\mathbf{R}^{2n},\\ f_{|t=0}=f_0.\end{cases} \tag{0.2}$$

Here x denotes the position, y the velocity, m the mass of the particles, $\gamma>0$ is the friction, $\beta=(kT)^{-1}$ where $T>0$ is the temperature and k is a constant. $f(t,x,y)$ is the particle density at time t and we notice that $\iint f(t,x,y)dxdy$ is independent of t under reasonable general assumptions.

The first order part, $y\cdot\partial_x-\frac{1}{m}V'(x)\cdot\partial_y$ is equal to the Hamilton vector field $H_{q/m}=m^{-1}(\partial_y q\cdot\partial_x-\partial_x q\cdot\partial_y)$ where $q=my^2/2+V(x)$. The Maxwellian

$$M(x,y)=e^{-\beta q(x,y)} \tag{0.3}$$

is annihilated by K. Following a tradition in the subject, Hérau and Nier studied rather the conjugated operator

$$\widetilde{P}=M^{-\frac{1}{2}}KM^{\frac{1}{2}}=y\cdot\partial_x-\frac{1}{m}V'(x)\cdot\partial_y-\frac{\gamma m}{4}(y-\frac{2}{m\beta}\partial_y)(y+\frac{2}{m\beta}\partial_y). \tag{0.4}$$

Choose for simplicity $m=2$, and replace V by $2V$. Then with $h=1/\beta$, we get

$$\frac{1}{\beta}\widetilde{P}=y\cdot h\partial_x-V'(x)\cdot h\partial_y+\frac{\gamma}{2}(y-h\partial_y)\cdot(y+h\partial_y)=:P \tag{0.5}$$

and the evolution problem becomes

$$(h\partial_t+P)u=0,\ u_{|t=0}=u_0. \tag{0.6}$$

Herau–Nier [HeNi] assumed some symbol behaviour for V and some polynomial growth at ∞ for $|V(x)|$ and $|V'(x)|$. They showed that P is globally hypoelliptic in a

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suitable sense and that the eigenvectors in $\mathcal{S}'$ belong to $\mathcal{S}$. Moreover P is m-accretive (a result considerably generalized by Helffer–Nier [HelNi]), implying that the evolution problem (0.6) is wellposed for $u_0 \in L^2(\mathbf{R}^{2n})$. They also showed that the spectrum $\sigma(P)$ of P is contained in a set of the form $\mathrm{Re}\, z \geq \max(\frac{1}{C}|\mathrm{Im}\, z|^{1/N} - C, 0)$ (with C depending on the parameters) and away from such a region they obtained the estimate $\|(z-P)^{-1}\| \leq C|z|^{-\epsilon}$. This implies results about the return to equilibrium:

If V is positive near ∞, then 0 is the only eigenvalue with $\mathrm{Re}\, z = 0$, and $e_0 = CM^{1/2}$ is the corresponding eigenfunction. If V is negative near ∞, all eigenvalues have real part > 0. In the two cases we get respectively,

$$\|u(t) - (u|e_0)e_0\| \leq e^{-\tau_1 t} \times \text{a polynomial in } t, t^{-1},$$
$$\|u(t)\| \leq e^{-\tau_1 t} \times \text{a polynomial in } t, t^{-1},$$

where here and in the following $\|\cdot\|$ denotes the L^2-norm if nothing else is indicated explicitly. They also obtained very interesting estimates on the decay rate $\tau_1 > 0$, in terms of the first non-vanishing eigenvalue of the Witten Laplacian in degree 0:

$$(-\partial_x + \frac{1}{2}\partial_x V_\beta)\cdot(\partial_x + \frac{1}{2}\partial_x V_\beta), \quad V_\beta(x) = \beta V(\beta^{-\frac{1}{2m}}x).$$

Recently, there has been a lot of interest in the notion of *pseudospectrum* of matrices and differential operators, introduced by L.N. Trefethen. Roughly, this is the set of points in the complex spectral plane, where the resolvent is large, and in the semiclassical limit we can also view it approximately as the set of values of the semiclassical symbol of the operator. See works of L.N. Trefethen, E.B. Davies, M. Zworski and others, [Tr], [Da1,2], [Zw], [DeSjZw]. There have also been interesting recent works about evolution problems associated to non-self-adjoint operators in more or less explicit relation to the pseudospectrum ([TanZw], [BuZw], [Da3], [Hi2]). For the KFP-operator, the pseudospectrum is (in the first approximation) the right half-plane, while Hérau–Nier show in this case that the actual spectrum avoids a parabolic neighborhood of the imaginary axis. In this direction, there is a general result by Dencker, Sjöstrand and Zworski [DeSjZw], valid in the semi-classical limit, which can be viewed as an adaptation of general subellipticity results of Yu. Egorov and L. Hörmander (see [Hö]), and of which we recall a very much simplified version:

Theorem 0.1. *Let $P = P^w(x, hD_x; h)$ be the h-Weyl quantization of $P(x,\xi;h)$ belonging to a suitable symbol-class and with leading part $p(x,\xi) = p_1(x,\xi) + ip_2(x,\xi)$. Then the spectrum $\sigma(P)$ is contained in $p(\mathbf{R}^{2n}_{x,\xi}) + D(0, o(1))$, $h \to 0$, where $D(z,r) \subset \mathbf{C}$ denotes the open disc of radius r and center z.*

Assume also that $p_1 \geq 0$. Let $z_0 \in i\mathbf{R}$ be away from the set of accumulation points of $p(x,\xi)$ at $(x,\xi) = \infty$ and assume that

$$p(\rho) = z_0 \Rightarrow H^2_{p_2} p_1(\rho) > 0. \tag{0.7}$$

Then when $h > 0$ is sufficiently small, the resolvent $(P - z_0)^{-1}$ exists as a bounded operator in $L^2(\mathbf{R}^n)$ and $\|(P-z_0)^{-1}\| = \mathcal{O}(h^{-2/3})$. In particular $D(z_0, h^{2/3}/C) \cap \sigma(P) = \emptyset$, for some $C > 0$.

1. The new results.

We now state the results obtained with F. Hérau and C. Stolk in [HeSjSt]. We consider P in (0.5) in the semi-classical limit $(h \to 0)$ with $\gamma > 0$ fixed and make the following assumptions about V:

$$V \in C^\infty(\mathbf{R}^n; \mathbf{R}),\ \partial^\alpha V = \mathcal{O}(1),\ |\alpha| \geq 2. \tag{H1}$$

$$|V'(x)| \geq 1/C, \text{when} |x| \geq C \text{ for some } C > 0. \tag{H2}$$

$$V \text{ is a Morse function.} \tag{H3}$$

In the following results it is tacitly assumed that $0 < h \leq h_0$ for some fixed sufficiently small $h_0 > 0$. Our first result is about the location of the spectrum.

Theorem 1.1. *There exists a constant $C > 0$ such that for $h > 0$ small enough, the spectrum of P is contained in*

$$\{z \in \mathbf{C};\ \mathrm{Re}\, z \geq \frac{1}{C} \min(|\mathrm{Im}\, z|, h^{\frac{2}{3}} |\mathrm{Im}\, z|^{\frac{1}{3}}) - C_N h^N\}, \tag{1.1}$$

for every $N \in \mathbf{N}$.

The next result gives an estimate for the resolvent away from the set in (1.1).

Theorem 1.2. *For $\mathrm{Re}\, z \leq (2C)^{-1} \min(|\mathrm{Im}\, z|, h^{2/3}|\mathrm{Im}\, z|^{1/3}) - h$, we have*

$$\|(z - P)^{-1}\| \leq \widetilde{C} / \min(|z|, h^{2/3}|z|^{1/3}). \tag{1.2}$$

The next result is about the spectrum inside any h-neighborhood of 0.

Theorem 1.3. *Let $C > 0$. Then (for h small enough depending on C) the spectrum in $D(0, Ch)$ is discrete and the eigenvalues are of the form $\lambda_k = \mu_k h + \mathcal{O}(h^{1/N_0})$. Here μ_k denote the eigenvalues of the quadratic approximations of $P_{h=1}$ at the finitely many critical points of V.*

Here, if x_0 is a critical point of V, the corresponding quadratic approximation of $P_{h=1}$ is the operator

$$P_0 = y \cdot \partial_x - (V_0''(x_0)(x - x_0)) \cdot \partial_y + \frac{\gamma}{2}(y - \partial_y) \cdot (y + \partial_y),$$

and since this is the Weyl-quantization of a quadratic form the eigenvalues can be calculated explicitly [Ri], [Sj1]. (The calculation in [Ri] is formal and in [Sj1] there is an assumption about ellipticity near infinity, that is not satisfied here, but we show in [HeSjSt], how to pass to a new exponentially weighted space without changing the eigenvalues and for which we do have the required ellipticity assumption.) From the explicit formulae for these eigenvalues, we know that they are confined to an angle $|\arg z| \leq \theta_0 < \pi/2$, that 0 is an eigenvalue iff x_0 is a local minimum of V and when it is an eigenvalue it is simple. Moreover the eigenvalues are all real ($\theta_0 = 0$) precisely when all the eigenvalues of the Hessian matrix $V''(x_0)$ are $\leq \gamma^2/4$.

Our last result concerns the large time asymptotics for the evolution problem. Thanks to a recent result of F. Nier and B. Helffer, we know that P is a so called m-accretive operator and this implies in our case that the semi-group $e^{-tP/h}$ is well defined for $t \geq 0$ and that $\|e^{-tP/h}\| \leq 1$.

Theorem 1.4. *Choose $a > 0$ with $a \neq \operatorname{Re}\mu_k$ for all k. Let $\lambda_j(h)$, $j = 0, 1, ..., N-1$, be the eigenvalues of the preceding theorem with $\operatorname{Re}\mu_j < a$. Assume for simplicity that the corresponding μ_j are distinct and simple. Then $\lambda_j(h)$ are also simple and $\mu_j h$ is the leading term in a complete asymptotic expansion of $\lambda_j(h)$ in integer powers of h. Let*

$$\Pi_{\lambda_j} = \frac{1}{2\pi i}\int_{|z-\lambda_j|=\epsilon h}(z-P)^{-1}dz = \mathcal{O}(1),\ 0 < \epsilon \ll 1,$$

be the corresponding spectral projection. Then in $\mathcal{L}(L^2(\mathbf{R}^{2n}), L^2(\mathbf{R}^{2n}))$, we have

$$e^{-tP/h} = \sum_{0}^{N-1} e^{-t\lambda_j/h}\Pi_{\lambda_j} + \mathcal{O}(e^{-ta}),\ t \geq 0. \tag{1.3}$$

For other non-self-adjoint evolution problems, various asymptotic results about the long time behaviour of the associated evolution problems have been given in [TaZw], [BuZw], [Hi2], [Da3]. In many of these results, the possible exponential growth of the resolvent inside the pseudospectrum implies that the final estimates are not as sharp as the result in Theorem 1.4, where we use the resolvent estimates of Theorem 1.2.

If V has only one local minimum, then we have a unique eigenvalue $\lambda_j =: \lambda_0$ which is $\mathcal{O}(h^\infty)$ and the real parts of the other eigenvalues are bounded from below by h/C. Then (1.3) gives a fairly precise result about the so called return to equilibrium, namely about the exponential rate of convergence of $e^{-tP/h} - e^{t\lambda_0/h}\Pi_{\lambda_0}$ to zero. (In the case of a global minimum, we have $\lambda_0 = 0$ and Π_{λ_0} is then the projection onto the equilibrium state.) If V has 2 or more local minima and say is positive near infinity, then there are several eigenvalues that are $\mathcal{O}(h^\infty)$ (and they are probably exponentially small) but only one of them is 0. In this situation, Hérau–Nier [HelNi] obtain interesting estimates on the rate of return to equilibrium by establishing a relation with a corresponding Witten Laplacian for V. It would be most interesting to make a direct semi-classical study in this case and possibly clarify some tunnel effect between the local minima of V. Finally we recall that our results concern the conjugated Kramers–Fokker-Planck operator (0.5), and it would be most interesting to know about similar ones for the operator in (0.1).

2. Methods and ideas of the proofs

The semiclassical principal symbol of P is

$$p = p_1 + ip_2, \tag{2.1}$$

where

$$p_2 = y \cdot \xi - V'(x) \cdot \eta,\ p_1 = \frac{\gamma}{2}(y^2 + \eta^2). \tag{2.2}$$

The critical ponts of p are of the form $(x, y; \xi, \eta) = (x_j, 0; 0, 0)$, where x_j are the critical points of V; $V'(x_j) = 0$. Let $\mathcal{C}$ be the set of critical points of p. Notice that we also have $p_{|\mathcal{C}} = 0$.

If $p_1(x, y; \xi, \eta) = 0$ ($\Leftrightarrow y = \eta = 0$), then

$$\begin{aligned} H_{p_2}p_1 &= -\gamma(\xi \cdot \eta + V'(x) \cdot \eta) = 0 \\ H_{p_2}^2 p_1 &= \gamma(\xi^2 + V'(x)^2 - \eta \cdot V''(x) \cdot y) = \gamma(\xi^2 + V'(x)^2), \end{aligned}$$

and the last quantity is positive precisely when $(x, 0; 0, 0) \notin \mathcal{C}$. Near $\mathcal{C}$, we introduce $\delta(\rho) = \operatorname{dist}(\rho, \mathcal{C})$. Then $H_{p_2}^2 p_1 \sim \delta^2$ on $\{p_1 = 0\}$, and it follows from the assumption (H3), that

$$p_1 + \epsilon H_{p_2}^2 p_1 \sim \delta^2, \tag{2.3}$$

in a fixed bounded set when $\epsilon > 0$ is small and fixed.

In a compact set disjoint from $\mathcal{C}$ the analysis is very much similar to that of [DeSjZw] in the special case of Theorem 0.1, but new difficulties appear because of the critical points and also because we need nice uniform control all the way to ∞.

Consider a region $h^{\frac{1}{2}} \leq \delta \leq \mathcal{O}(1)$. (We only explain some ideas of the proof and not the actual constructions which finally became a little different.) Here $H := \{\rho;\ H_{p_2}p_1(\rho) = 0\}$ is a smooth hypersurface where p_1 is small, and if ρ is an arbitrary point, we represent it as $\rho = \exp tH_{p_2}(\rho')$, for $\rho' \in H$. We now want to pass to an exponentially weighted space (defined using an FBI-transform), and roughly this space is the set of functions of the form $u = e^{\epsilon G(x,y,hD;h)/h}\widetilde{u}$, $\widetilde{u} \in L^2$. Following now standard constructions in the microlocal approach to resonances, the principal symbol of P, acting on the new space is $\widetilde{p}(\rho) = p(\exp i\epsilon H_G(\rho))$ which is approximately equal to $p(\rho) - i\epsilon H_p G(\rho)$. The new feature here (and also in [DeSjZw]) is that we want the new space to have a norm which is uniformly equivalent to the ordinary L^2-norm, when h tends to 0 and this forces us to impose the condition $G = \mathcal{O}(h)$.

Now put

$$G(\rho) = h\chi\left(\frac{\lambda p_1(\rho')}{\delta(\rho')^2}\right) g\left(\frac{t}{\beta(\rho'; h)}\right), \tag{2.4}$$

where χ is a standard cut-off that we forget about and $g \in C_0^\infty(\mathbf{R}, \mathbf{R})$ is such that $g(t) = t$ for $|t| < 1$. Then, we get for $\widetilde{p} = \widetilde{p}_1 + i\widetilde{p}_2$,

$$\widetilde{p}_1 \approx p_1 + \epsilon H_{p_2} G \geq \frac{1}{C}\delta^2 t^2 + \epsilon \begin{cases} h/\beta, & |t| \leq \beta, \\ \mathcal{O}(h/\beta), & |t| > \beta. \end{cases} \tag{2.5}$$

Choose $\beta > 0$ with $\delta^2\beta^2 = h/\beta$, ie $\beta = h^{1/3}\delta^{-2/3}$. Then we get $\widetilde{p}_1 \geq C^{-1}(\delta h)^{2/3}$ if we fix $\epsilon > 0$ sufficiently small. On the other hand, $\widetilde{p}_2 = \mathcal{O}(\delta^2)$, so the values of $\widetilde{p}$ from this region of phase space are contained in the set $\{z \in \mathbf{C}; \operatorname{Re} z \geq C^{-1}h^{2/3}|\operatorname{Im} z|^{1/3}\}$.

Now consider the region $\delta \leq h^{1/2}$. Take

$$G = \int k(t/T) p_1 \circ \exp(t H_{p_2}) dt \ (= \mathcal{O}(h)), \tag{2.6}$$

where $k(s)$ is the odd function which satisfies, $k(t) = \frac{1}{2} - t$ for $0 < t < \frac{1}{2}$, $k(t) = 0$ for $t \geq \frac{1}{2}$. Then $H_{p_2} G = p_1 - \langle p_1 \rangle_T$, where

$$\langle p_1 \rangle_T = \frac{1}{T} \int_{-T/2}^{T/2} p_1 \circ \exp(t H_{p_2}) dt.$$

It follows that in this region (and with the new function $G = G_T$), that $\widetilde{p_1}(\rho) \sim \delta^2$, $\widetilde{p}_2 = \mathcal{O}(\delta^2)$.

By suitably gluing together the two functions G we get a new function G, defined in any fixed bounded subset of phase space, such that G/h is bounded and such that

$$\widetilde{p}_1 \geq \frac{1}{C} \min(\delta^2, (\delta h)^{2/3}), \ \widetilde{p}_2 = \mathcal{O}(\delta^2). \tag{2.7}$$

In these geometrical considerations, we can replace "h" by "Ah" for some large A. This has the effect of increasing the neighborhood of the critical set where G is a more standard weight-function and and allows us to justify the quadratic approximation in that set. Using FBI-transforms and associated techniques from [Sj2], [Sj3], [DeSjZw], as well as a special study near infinity exploiting Hörmander's Weyl calculus [Hö], we get the theorems 1.1 and 1.2.

As for Theorem 1.3, we choose A very large depending on the constant C, if we want to determine asymptotically the eigenvalues in $D(0, Ch)$. In the region $\delta(\rho) = \mathcal{O}((Ah)^{1/2})$, we can assume the weight G to be quadratic near each point of $\mathcal{C}$, and we can replace P up to a small error by its quadratic approximation, which becomes elliptic near infinity in the quadratically weighted space. For the quadratic approximations, we know the eigenvalues explicitly ([Sj1]), and by applying also techniques and ideas from [HelSj], we get the theorem. One can also get complete asymptotic expansions in (fractional) powers of h.

The proof of Theorem 1.4 is more standard, just write down a Cauchy integral formula,

$$e^{-tP/h} = \frac{1}{2\pi i} \int_\gamma e^{-tz/h} (z - P)^{-1} dz, \tag{2.8}$$

where γ is the boundary of the set appearing in Theorem 1.2, oriented in the direction of decreasing $\operatorname{Im} z$, then in an h-neighborhood of $z = 0$ we push the contour to the right and add the corresponding residue terms.

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