Tunnel effect for Krammers-Fokker-Planck type operators: return to equilibrium and applications

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Qmath10 conference, Brasov 2007
The Fokker-Planck operator:

\[ P = y \cdot h \partial_x - V'(x) \cdot h \partial_y + \gamma (-h \partial_y + y/) \cdot (h \partial_y + y/2) \]

position \( x \in \mathbb{R}^d \), velocity \( y \in \mathbb{R}^d \), friction coefficient \( \gamma \).

Some natural 1/2 classical questions arise:

- Eigenvalues, resolvent estimate
- Return to the equilibrium for the heat problem
- Tunnel effect (in the case of multiple critical points for \( V \))
- Intrinsic structure \( \rightarrow \) supersymmetry

Intensive work last years: Helffer, Nier, Lebeau, Bismut...
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(Linearized) Kinetic equations $X_0 - L$,
- Krammers-Fokker-Planck
- Linear Boltzmann (not local)
- Linearized Boltzmann, Landau, ...
- Probabilistic models, other models

Related questions and structures:
- Hypoellipticity
- Hypocoercivity and trend to the equilibrium
- Supersymmetry and inner structures (KFP-like)
- Boundary, potentials, non-linear problems, perturbative study...

Villani, Mouhot, Guo, Schmeiser, Talay, Eckmann, Rey-bellet, Hairer...
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Very constructive interaction

P.D.E
- 1/2 classical methods
- $\phi$ dO methods
- supersymmetry ...

Kinetic
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Hérau, Hitrik, Sjöstrand
Tunnel effect for KFP
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Assumptions and main result

Back to the Fokker-Planck operator

\[ P = y \cdot h \partial_x - V'(x) \cdot h \partial_y + \gamma(-h \partial_y + y/2) \cdot (h \partial_y + y/2) \]

We impose on the potential \( V \) the following:

- \( \partial^\alpha V = O(1) \) for \( |\alpha| \geq 2 \),
- \( |\nabla V| \geq 1/C \), for \( |x| \geq C \) with \( C \) sufficiently large
- \( V \) has 3 critical points: 2 local minima and 1 critical point of index 1

Then \( P \) has 2 eigenvalues in the disc \( D(0, C/h) \) for \( h \) sufficiently small, \( \mu_0 = 0 \) and \( \mu_1 \), with \( \mu_1 \) of the form

\[ \mu_1 = h \left( a_1(h) e^{-2S_1/h} + a_{-1}(h) e^{-2S_{-1}/h} \right), \quad S_j = V(x_j) - V(x_0). \]
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"Simple well" : $V$ has precisely 1 local minimum and $V(x) \to \infty$ then from [HHS07], $P$ has only 1 eigenvalue $\mu_0 = 0$ in the disc $D(0, C/h)$ for $h \ll 1$.

"A well and the sea" : $V$ has precisely 1 local minimum $x_1$ and 1 critical point $x_0$, then $P$ has only 1 eigenvalue $\mu_1$ in the disc $D(0, C/h)$.

$$\mu_1 = ha_1(h)e^{-2S_1/h}, \quad S_1 = V(x_1) - V(x_0).$$

"multiple wells" : Serious hope to get similar results as in the Witten case (see recent work about linear algebra by le peutrec in the Witten case).

Main problem : resolvent estimates, spectral projectors not selfadjoint...
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Heat problem

Analyse of $e^{-tP/h}$.

- In the case without "tunneling effect" (e.g. the simple well case), the return to equilibrium is of order of magnitude 1.
- What is this rate in the case of tunneling effect ("double well" and "a well and the sea").

Main result

In the double well case, Let $\Pi_j$ the spectral projection associated to $\mu_j$, then

$$\Pi_j = O(1), \quad h \to 0.$$ 

and uniformly as $t \geq 0$, and $h \to 0$,

$$e^{-tP/h} = \Pi_0 + e^{-t\mu_1/h} \Pi_1 + O(1)e^{-t/C}, \quad C > 0, \quad \text{in } L^2(L^2, L^2).$$
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Sketch of proof
Eigenvalues [HHS07] : let \( p \) be the symbol of KFP and \( \rho_{0,j} \) be the symbol of the quadratic approximation at \( \rho_j \) critical point. The spectrum of \( P \) in \( D(0, Bh) \) is discrete and equal to

\[
\lambda_{j,k}(h) \sim h \left( \mu_{j,k} + h^{1/N_{j,k}} \mu_{j,k,1} + h^{2/N_{j,k}} \mu_{j,k,2} + \ldots \right),
\]

Recall that \( \mu_{j,k} \) are all numbers in \( D(0, B) \) of the form

\[
\mu_{j,k} = \frac{1}{i} \sum_{\ell=1}^{n} \left( \nu_{j,k,\ell} + \frac{1}{2} \right) \lambda_{j,\ell}, \quad \nu_{j,k,\ell} \in \mathbb{N},
\]

for some \( j \in \{1, \ldots, N\} \). Here \( \lambda_{j,\ell} \), \( 1 \leq \ell \leq n \), are the eigenvalues of the Hamilton map of the quadratic part of \( p \) at \( \rho_j \in \mathcal{C} \), for which \( \text{Im} \lambda_{j,\ell} > 0 \).
A coercive estimate

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Crucial estimate:

Lemma

Let $B \geq 0$ and $\Pi_B$ the corresponding spectral projector, then for all $u \in \text{Ran}(1 - \Pi_B)$,

$$\left\| e^{-tP/h}u \right\| = O(1) e^{-t/C}, \quad C = C(B)$$

difficulties:

- $\Pi_B$ not selfadjoint,
- $\text{Re} \langle Pu, u \rangle \geq Ch \| u \|^2$ not true
- $\text{Re} \langle Pu, u \rangle_\epsilon \geq Ch \| u \|^2_\epsilon$ true with a modified norm!
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Exists Global FIO $A_\varepsilon$ exploiting the hypoelliptic properties of $P$ such that $\|u\|_\varepsilon \overset{\text{def}}{=} \|A_\varepsilon u\| \sim \|u\|$. 

**Study of** $P_\varepsilon = A_\varepsilon^{-1} P_\varepsilon A_\varepsilon$ in $L^2$:

We already know [HHS07] that for all $u$

$$\text{Re } ((P_\varepsilon + K_\varepsilon)u, u) \geq ch \|u\|^2$$

where $K_\varepsilon$ is (micro-)localized near the critical points. Sufficient to prove $\|K_\varepsilon u\| \ll h \|u\|$.

- Building a selfadjoint operator $Q$ (an harmonic oscillator) adapted to the evs $\leq B$.
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\[ p = p_2 + ip_1 + p_0 \]

where

\[ p_2 = \sum b_{j,k} \xi_j \xi_k, \quad p_1 = \sum c_j(x) \xi_j, \quad p_0 = p_0(x) \]

with the following assumptions:

- positivity \( p_2 \) and \( p_0 \geq 0 \),
- growth \( |\partial^\alpha b| + |\partial^{\alpha+1} c| + |\partial^{\alpha+2} p_0| = O(1), \quad |\alpha| \geq 0 \),
- finite critical set \( \{(x_l,0) \text{ with } p_0(x_l) = 0, \ c(x_l) = 0\} \),

and if \[ <p> = \frac{1}{T} \int_{[-T,T]} (p_0 + p_2 / <\xi>^2) dt, \]

- local dynamic \( <p> \sim |\rho - \rho_j|^2 \) near \( \rho_j \)
- global dynamic \( <p> \geq C \) away.
General form

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They are defined through:

- An invertible real $d \times d$ matrix $A = B + C$, $B$ sym., $C$ skew.
- A morse function $\phi$ where $\partial^\alpha \phi$ and $\partial^\alpha < B \nabla \phi, \nabla \phi >$ are $O(1)$.

The Witten Hodge Laplacian is

$$
\sum -\hbar^2 \sum \partial_j B_{j,k} \partial_k + \sum \partial_j \phi B_{j,k} \partial_k \phi - \hbar \text{tr}(B \phi'')
+ \sum \partial_j \phi C_{j,k} \partial_k + \sum \partial_j C_{j,k} \partial_k \phi
$$

Principal symbol: $p = \langle B \xi, \xi \rangle + 2i \langle C \nabla \phi, \xi \rangle + \langle B \nabla \phi, \nabla \phi \rangle$, Of Witten Hodge Laplacian type: $-\Delta_A = d^A_\phi \ast d_\phi$ on $k$–forms.
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Return to equilibrium

With the supersymmetric structure: reduce the problem of exp. small evs to a finite dimensional problem.

In particular build the corresponding eigenfunctions for $-\Delta^{(0)}_A$ and $-\Delta^{(1)}_A$, as in the treatment by Helffer-Sjöstrand [HS80'].

\[ e_j(x) = h^{-n/4} c_j(h) e^{\frac{1}{\hbar}(\phi(x) - \phi(x_j))} \]

Back to the double well case: 2 minima, therefore 2 exp. small evs (0 and $\mu_1$).

- Express explicitly the projectors $\Pi_k$ for each exp. small eigenvalue.
- Write $e^{-tP/\hbar} = e^{-tP/\hbar}(\Pi_0 + \Pi_1 + \Pi_{(2-B)} + (1 - \Pi_B))$
- Use the former result for the last term, and the 2 first (the third one is easy with resolvent estimates from [HHS07]).
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Return to equilibrium

With the supersymmetric structure: reduce the problem of exp. small evs to a finite dimensional problem. In particular build the corresponding eigenfunctions for $-\Delta_A^{(0)}$ and $-\Delta_A^{(1)}$, as in the treatment by Helffer-Sjostrand [HS80’].

\[ e.g. \quad e_j(x) = h^{-n/4} c_j(h) e^{\frac{1}{\hbar}(\phi(x) - \phi(x_j))} \]

Back to the double well case: 2 minima, therefore 2 exp. small evs (0 and $\mu_1$).

- Express explicitly the projectors $\Pi_k$ for each exp. small eigenvalue.
- Write $e^{-tP/h} = e^{-tP/h}(\Pi_0 + \Pi_1 + \Pi_{(2-B)} + (1 - \Pi_B))$
- Use the former result for the last term, and the 2 first (the third one is easy with resolvent estimates from [HHS07]).
Examples of KFP type operators
Some problem may come from Probability. Let

\[ dx(t) = b(x(t))dt + \sigma dw \]

where \( w \) is a \( d \)-dimensional process, \( \sigma \) a constant matrix and \( \partial^\alpha b = O(1) \). Then there exists a unique solution (in an \( L^2 \) adapted space) for \( x_0 \perp w \).

Define the associated semi group by

\[ \mathbb{E}(\phi(x(t))) = T^t\phi(x_0) \]

This is a strongly semi-group (on \( C_\infty \), we can work also on \( L^2 \)) whose infinitesimal generator is

\[ L = \nabla \cdot D \nabla + b(x) \cdot \nabla \quad \text{with} \quad D = \frac{1}{2} \sigma \sigma^t \]
Some problem may come from Probability. Let

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This is a strongly semi-group (on \( C_\infty \), we can work also on \( L^2 \)) whose infinitesimal generator is

\[ L = \nabla \cdot D \nabla + b(x) \cdot \nabla \quad \text{with} \quad D = \frac{1}{2} \sigma \sigma^t \]
Its formal adjoint is

$$L^* = \nabla.D\nabla - \nabla.b(x)$$

and is the infinitesimal generator of $(T^t)^*$ (at least its closure in an $L^2$ setting).

This means that if $\mu_0 = f_0 dx$ is the a.c. measure of probability of $x_0$, then $\mu_t = f(t, .) dx$ is the one of $x(t)$ and $\partial_t f - L^* f = 0$, ie

$$\begin{cases} 
\partial_t f + (-\nabla.D\nabla + \nabla.b)f = 0 \\
 f|_{t=0} = f_0
\end{cases}$$

An invariant measure will be associated to a time-independent function $M$. What remains in particular cases is

- exhibit the Maxwellian $M$,
- do a conjugation, a $1/2$ classical scaling
- recognize a supersymmetric structure
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This means that if \(\mu_0 = f_0 \, dx\) is the a.c. measure of probability of \(x_0\), then \(\mu_t = f(t, .) \, dx\) is the one of \(x(t)\) and \(\partial_t f - L^* f = 0\), i.e.

\[
\begin{aligned}
\partial_t f + (-\nabla.D\nabla + \nabla.b)f &= 0 \\
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\end{aligned}
\]

An invariant measure will be associated to a time-independant function \(M\). What remains in particular cases is

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- do a conjugation, a 1/2 classical scaling
- recognize a supersymetric structure
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\[
\begin{cases}
\partial_t f + (-(\nabla . D) . \nabla + \nabla . b)f = 0 \\
 f|_{t=0} = f_0
\end{cases}
\]

An invariant measure will be associated to a time-independent function \(M\). What remains in particular cases is

- exhibit the Maxwellian \(M\),
- do a conjugation, a 1/2 classical scaling
- recognize a supersymmetrical structure
Witten case

\[ W : dx = -\gamma \partial_x V dt + \sqrt{2\gamma T} dw \]

- Parameters: \( D = \sigma^* \sigma / 2 = \gamma T \) and \( b(x) = -\gamma \partial_x V \).
- Density: \( \partial_t f - \gamma \partial_x (T \partial_x + \partial_x V) f = 0 \).
- Let \( t = h \) and \( \times h : h\partial_t f - \gamma h \partial_x (h\partial_x + \partial_x V) f = 0 \).
- Maxwellian: \( \mathcal{M} = e^{-V / h} \).
- Conjugation \( f = \mathcal{M}^{1/2} h : h\partial_t u + \gamma (-h\partial_x + \partial_x V / 2). (h\partial_x + \partial_x V / 2) u = 0 \).
- Supersymmetry: \( A = \gamma I, \phi(x) = V(x) / 2 \).
- Potential: \( V \) Morse and \( \partial^\alpha V(x) = O(1) \) when \( |\alpha| = 2 \) and \( O(<x>^{-1}) \) when \( |\alpha| \geq 3 \).
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  \[ \partial^\alpha V(x) = \mathcal{O}(1) \text{ when } |\alpha| = 2 \text{ and } \mathcal{O}(< x >^{-1}) \text{ when } |\alpha| \geq 3. \]
**Witten case**

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\textbf{Witten case}

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Fokker-Planck case

\[
\text{KFP : } \begin{cases} 
    dx = y dt \\
    dy = -\gamma y dt - \partial_x V dt + \sqrt{2\gamma} T dw
\end{cases}
\]

- Parameters : \( D = \begin{bmatrix} 0 & 0 \\ 0 & \gamma T \end{bmatrix} \) and \( b(x) = \begin{bmatrix} y \\ -\gamma y - \partial_x V \end{bmatrix} \).
- Density, scaling :
  \( h \partial_t f - \gamma h \partial_y (h \partial_y + y) f + y h \partial_x f - \partial_x V h \partial_y f = 0 \).
- Maxwellian : \( M = C^{-1} e^{(-V(x)+y^2/2)/\hbar} \).
- Conjugation :
  \( h \partial_t u + \gamma (-h \partial_y + y/2) (h \partial_y + y/2) u + \gamma y h \partial_x u - \partial_x V h \partial_y u = 0 \).
- Supersymmetry : \( A = \begin{bmatrix} 0 & -I \\ I & \gamma \end{bmatrix} \) and \( \phi(x, \nu) = V(x)/2 + y^2/4 \).
- Potential : \( V \) Morse and \( \partial^\alpha V(x) = O(1) \).
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\begin{aligned}
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- Maxwellian:
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- Conjugation:
  \( h \partial_t u + \gamma (h \partial_y + y/2)(h \partial_y + y/2)u + \gamma y h \partial_x u - \partial_x V h \partial_y u = 0. \)

- Supersymmetry:
  \( A = \begin{bmatrix} 0 & -I \\ I & \gamma \end{bmatrix} \) and \( \phi(x, v) = V(x)/2 + y^2/4. \)

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Fokker-Planck case

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h \partial_t f - \gamma h \partial_y . (h \partial_y + y) f + y h \partial_x f - \partial_x V h \partial_y f = 0.
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- **Maxwellian**: \( \mathcal{M} = C^{-1} e^{(-V(x)+y^2/2)/h} \).

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Fokker-Planck case

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\begin{align*}
\frac{dx}{dt} &= y dt \\
\frac{dy}{dt} &= -\gamma y dt - \partial_x V dt + \sqrt{2\gamma} T dw 
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- **Parameters**: \( D = \begin{bmatrix} 0 & 0 \\ 0 & \gamma T \end{bmatrix} \) and \( b(x) = \begin{bmatrix} y \\ -\gamma y - \partial_x V \end{bmatrix} \).

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KFP \begin{cases}
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\end{cases}.

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Chains case

\[
\begin{align*}
    dx_1 &= y_1 \, dt \\
    dy_1 &= -\partial_{x_1} V dt + z_1 \, dt \\
    dz_1 &= -\gamma z_1 \, dt + \gamma x_1 \, dt - \sqrt{2\gamma T_1} \, dw_1 \\
    dz_2 &= -\gamma z_1 \, dt + \gamma x_2 \, dt - \sqrt{2\gamma T_2} \, dw_2 \\
    dy_2 &= -\partial_{x_2} V dt + z_2 \, dt \\
    dx_2 &= y_2 \, dt.
\end{align*}
\]

where \( V(x_1, x_2) = V_p(x_1) + V_p(x_2) + V_c(x_1 - x_2) \).

- Parameters: \( D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \gamma T \end{bmatrix} \) and \( b(x) = \begin{bmatrix} y \\ -\partial_x V + z \\ \gamma(x - z) \end{bmatrix} \).
- Scaling \( T_1 = \alpha_1 h, \ T_2 = \alpha_2 h, \) and \( \times h : \)

\[
\begin{align*}
    h\partial_t f + \gamma\alpha_1(-h\partial_{z_1})(h\partial_{z_1} + (z_1 - x_1)/\alpha_1)f \\
    + \gamma\alpha_2(-h\partial_{z_2})(h\partial_{z_2} + (z_2 - x_2)/\alpha_2)f \\
    + (y\partial_x f - (\partial_x V - z)\partial_y)f = 0.
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    dx_1 &= y_1 \, dt \\
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    dz_2 &= -\gamma z_2 \, dt + \gamma x_2 \, dt - \sqrt{2\gamma T_2} \, dw_2 \\
    dy_2 &= -\partial_{x_2} V dt + z_2 \, dt \\
    dx_2 &= y_2 \, dt.
\end{align*}
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where \( V(x_1, x_2) = V_p(x_1) + V_p(x_2) + V_c(x_1 - x_2) \).

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- Scaling: \( T_1 = \alpha_1 h, \ T_2 = \alpha_2 h, \) and \( \times h : \)

\[
    
    h \partial_t f + \gamma \alpha_1 (-h \partial_{z_1}). (h \partial_{z_1} + (z_1 - x_1)/\alpha_1) f \\
    + \gamma \alpha_2 (-h \partial_{z_2}). (h \partial_{z_2} + (z_2 - x_2)/\alpha_2) f \\
    + (y \partial_x f - (\partial_x V - z) \partial_y) f = 0.
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\[
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\text{Ch :} & \\
\begin{cases}
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    dx_2 &= y_2 \, dt.
\end{cases}
\end{align*}
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where \( V(x_1, x_2) = V_p(x_1) + V_p(x_2) + V_c(x_1 - x_2) \).

- Parameters: \( D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \gamma T \end{bmatrix} \) and \( b(x) = \begin{bmatrix} y \\ -\partial_x V + z \\ \gamma(x - z) \end{bmatrix} \).

- Scaling \( T_1 = \alpha_1 h \), \( T_2 = \alpha_2 h \), and \( \times h : \)

\[
\begin{align*}
    h \partial_t f + \gamma \alpha_1 (-h \partial_z_1). (h \partial_z_1 + (z_1 - x_1)/\alpha_1) f \\
    + \gamma \alpha_2 (-h \partial_z_2). (h \partial_z_2 + (z_2 - x_2)/\alpha_2) f \\
    + (y \partial_x f - (\partial_x V - z) \partial_y) f = 0.
\end{align*}
\]
Chains case

\[ \begin{align*}
\text{Ch} : \quad & d x_1 = y_1 \ dt \\
& d y_1 = - \partial x_1 \ V dt + z_1 \ dt \\
& d z_1 = - \gamma z_1 \ dt + \gamma x_1 \ dt - \sqrt{2 \gamma T_1} \ dw_1 \\
& d z_2 = - \gamma z_1 \ dt + \gamma x_2 \ dt - \sqrt{2 \gamma T_2} \ dw_2 \\
& d y_2 = - \partial x_2 \ V dt + z_2 \ dt \\
& d x_2 = y_2 \ dt.
\end{align*} \]

where \( V(x_1, x_2) = V_p(x_1) + V_p(x_2) + V_c(x_1 - x_2) \).

- Parameters: \( D = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \gamma T \end{bmatrix} \) and \( b(x) = \begin{bmatrix} y \\ - \partial_x V + z \\ \gamma (x - z) \end{bmatrix} \).

- Scaling \( T_1 = \alpha_1 h, \ T_2 = \alpha_2 h, \) and \( \times h : \)

\[
\begin{align*}
& h \partial_t f + \gamma \alpha_1 (-h \partial z_1). (h \partial z_1 + (z_1 - x_1)/\alpha_1) f \\
& \hspace{1cm} + \gamma \alpha_2 (-h \partial z_2). (h \partial z_2 + (z_2 - x_2)/\alpha_2) f \\
& \hspace{1cm} + (y \partial_x f - (\partial_x V - z) \partial_y) f = 0.
\end{align*}
\]
Difficult to exhibit a Maxwellian (although existence OK under additional conditions [EPR99])

- Maxwellian: \( \mathcal{M}_\alpha = C^{-1} e^{-\left(V(x)+y^2/2+z^2/2-\alpha^2x\right)/\alpha h} \).

- Conjugation:

\[
\begin{align*}
  h\partial_t u & + \gamma_1 \left( -h\partial_{z_1} + \frac{1}{2\alpha}(z_1 - x_1) \right) \cdot \left( h\partial_{z_1} + \left( \frac{1}{\alpha_1} - \frac{1}{2\alpha} \right) (z_1 - x_1) \right) u \\
  & + \gamma_2 \left( -h\partial_{z_2} + \frac{1}{2\alpha}(z_2 - x_2) \right) \cdot \left( h\partial_{z_2} + \left( \frac{1}{\alpha_2} - \frac{1}{2\alpha} \right) (z_2 - x_2) \right) u \\
  & + (y h\partial_x f - (\partial_x V - z) h\partial_y) u = 0.
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Difficult to exhibit a Maxwellian (although existence OK under additional conditions \([\text{EPR99}]\)) Restriction to the case of same temperature for the baths.

- Maxwellian: \(\mathcal{M}_\alpha = C^{-1} e^{-\left(V(x) + y^2/2 + z^2/2 - zx\right)/\alpha h}\).
- Conjugation:

\[
\begin{align*}
&h\partial_t u \\
&+ \gamma \alpha_1 \left( -h\partial_{z_1} + \frac{1}{2\alpha_1}(z_1 - x_1) \right) \cdot \left( h\partial_{z_1} + \left( \frac{1}{\alpha_1} - \frac{1}{2\alpha_1} \right)(z_1 - x_1) \right) u \\
&+ \gamma \alpha_2 \left( -h\partial_{z_2} + \frac{1}{2\alpha_2}(z_2 - x_2) \right) \cdot \left( h\partial_{z_2} + \left( \frac{1}{\alpha_2} - \frac{1}{2\alpha_2} \right)(z_2 - x_2) \right) u \\
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+ (y\hbar \partial_x f - (\partial_x V - z)\hbar \partial_y) u & = 0.
\end{align*}
\]
Supersymmetry: \( A = \alpha \begin{bmatrix} 0 & \text{Id} & 0 \\ -\text{Id} & 0 & 0 \\ 0 & 0 & \gamma \text{Id} \end{bmatrix} \) and
\[ \phi_\alpha = \left( V(x) + y^2/2 + z^2/2 - zx \right)/2/\alpha. \]

Potential: \( V \) Morse, \( \partial^\alpha V(x) = \mathcal{O}(1) \) and for example, \( V_p \) of double well type and \( V_c \) of simple well type.
Supersymmetry: \( A = \alpha \begin{bmatrix} 0 & \text{Id} & 0 \\ -\text{Id} & 0 & 0 \\ 0 & 0 & \gamma \text{Id} \end{bmatrix} \) and

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