What is the semiclassical limit of non-Hermitian time evolution?

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- Graefe, RS: Phys. Rev. A **83** (2011), 060101.
- Graefe, RS: J. Phys. A **45** (2012) 244033

Non-Hermitian time evolution

$$\mathrm{i}\hbar\partial_t\psi = \mathcal{H}(t)\psi \ , \quad \operatorname{Im}\mathcal{H} = \frac{1}{2\mathrm{i}}(\mathcal{H} - \mathcal{H}^*) \neq 0$$

- Systems with loss/gain: $\mathcal{H} = -\hbar^2\Delta + V(t,x)$, $\operatorname{Im} V(t,x) \neq 0$
- absorbing potentials: $\operatorname{Im} V \leq 0$
- complex scaling: complex eigenvalues/Resonances, escape rates, ...
- If $\operatorname{Im}\mathcal{H} \leq 0$ and $\mathcal{H}$ t-independent: semigroup theory
- PT-symmetry: $V^*(-x) = V(x)$, balance between gain and loss, e.g., lasers. Eigenvalues are real or come in pairs E, E^*.
- non-hermiticity at principal symbol level, unlike damped wave equation.

Existence of time evolution

$$\Lambda := -\hbar^2\Delta^2 + |x|^2 + 1,$$
$$H^m_\Lambda := \{\psi\,;\ \|\psi\|_{H^m_\Lambda} := \|\Lambda^m\psi\|_{L^2} < \infty\}$$

Definition

$\mathcal{H}(t) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n)$ *is of type* Λ *if*

(i) $\Lambda^{-1/2}\mathcal{H}(t)\Lambda^{-1/2} \in \mathcal{B}$ ($\mathcal{B}$*: set of bounded operators on* L^2*)*

(ii) $\mathrm{i}\hbar^{-1}[\Lambda, \mathcal{H}(t)]\Lambda^{-1} \in \mathcal{B}$

(iii) $\mathrm{Im}\,\mathcal{H}(t) \leq g(t)$, *for some continuous* $g : \mathbb{R} \to \mathbb{R}$.

Examples:

- $-\hbar^2\Delta + V(x)$ is of type Λ if $\mathrm{Im}\, V(x) \leq C$ and

$$|V(x)| \leq C\langle x\rangle^2\ , \quad |\nabla V(x)| \leq C\langle x\rangle\ .$$

- $V(x) = \mathrm{i}x^3$ not of type Λ.

$$\mathrm{i}\partial_t \mathcal{U}(t,s) = \mathcal{H}(t)\mathcal{U}(t,s)\ , \quad \mathcal{U}(s,s) = I$$

Theorem (RS, 2013)

Assume $\mathcal{H}$ is of type Λ, then $\mathcal{U}(t,s) : H^m_\Lambda \to H^m_\Lambda$ exists with

$$\|\mathcal{U}(t,s)\psi\|_{H^m_\Lambda} \leq C\mathrm{e}^{c_m|t-s|+\frac{1}{\hbar}\int_s^t g(t')\,\mathrm{d}t'}\|\psi\|_{H^m_\Lambda}$$

and

$$\|\mathcal{U}(t,s)\psi\|_{L^2} \leq C\mathrm{e}^{\frac{1}{\hbar}\int_s^t g(t')\,\mathrm{d}t'}\|\psi\|_{L^2}\ .$$

Remarks:

- $\mathcal{H}(t)$ time-dependent, so resolvent methods do not work.
- instead proof works by approximating $\mathcal{H}$ by $\mathcal{H}_\varepsilon = (1+\varepsilon\Lambda^{1/2})^{-1}\mathcal{H}(t)(1+\varepsilon\Lambda^{1/2})^{-1}$
- Can replace Λ by $\mathrm{Op}[\lambda]$ for any order function λ with $\lambda \in S(\lambda)$.

Semiclassical limit if $\operatorname{Im}\mathcal{H} = 0$: WKB vs Ehrenfest

WKB : $\psi = a\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S}$ insert in Schrödinger, $\mathcal{H} = \mathrm{Op}[H]$:

- $\partial_t S(t,x) + H(\nabla S(t,x), x) = 0$, Hamilton Jacobi, solved using Hamiltonian trajectories:

$$\dot{z} = \Omega \nabla H(z)\,, \quad \Omega = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \quad z = (p,q) \qquad (1)$$

- transport equation along (1) for $a(t,x)$

Ehrenfest theorem: If $\psi(x)$, $\hat{\psi}(\xi)$ localised near q and p, then

$$Z(t) = (P(t), Q(t))\,, \quad P(t) := \frac{\langle \psi(t), \hat{p}\psi(t)\rangle}{\|\psi(t)\|^2}\,, \quad Q(t) := \frac{\langle \psi(t), x\psi(t)\rangle}{\|\psi(t)\|^2}$$

satisfies (1) approximately.

If $\operatorname{Im} H \neq 0$: complex trajectories from (1), but $Z(t) \in \mathbb{R}^n \times \mathbb{R}^n$

Coherent states and their geometry

$$\psi_Z^B(x) = \frac{(\det \operatorname{Im} B)^{1/4}}{(\pi\hbar)^{n/4}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[P\cdot(x-Q)+\frac{1}{2}(x-Q)\cdot B(x-Q)]}$$

- $Z = (P, Q) \in \mathbb{R}^n \times \mathbb{R}^n$, $B \in M_n(\mathbb{C})$ symmetric, $\operatorname{Im} B > 0$
- Wignerfunction

$$W(z) = \frac{1}{(\pi\hbar)^n} \mathrm{e}^{-\frac{1}{\hbar}(z-Z)\cdot G(z-Z)}$$

$G = \begin{pmatrix} I & 0 \\ -\operatorname{Re} B & I \end{pmatrix} \begin{pmatrix} [\operatorname{Im} B]^{-1} & 0 \\ 0 & \operatorname{Im} B \end{pmatrix} \begin{pmatrix} I & -\operatorname{Re} B \\ 0 & I \end{pmatrix}$ symplectic metric: $G\Omega G = \Omega$, ψ pure state with minimal uncertainty.

- Expectation values and variance:

$$\langle \hat{A} \rangle_\psi = A(Z) + O(\hbar) \qquad (\Delta \hat{A})_\psi^2 = \frac{\hbar}{2} \nabla A(Z) \cdot G^{-1} \nabla A(Z) + O(\hbar^2)$$

Non-Hermitian Ehrenfest Theorem: coherent states

$$W(t,z) \approx \frac{\mathrm{e}^{-\frac{\alpha(t)}{\hbar}}}{(\pi\hbar)^n} \mathrm{e}^{-\frac{1}{\hbar}(z-Z(t))\cdot G(t)(z-Z(t))}$$

up to $O(\sqrt{\hbar})$, if

$$\dot{Z} = \Omega\nabla \operatorname{Re} H(Z) + G^{-1}\nabla \operatorname{Im} H(Z)$$

$$\dot{G} = \operatorname{Re} H''(Z)\Omega G - G\Omega \operatorname{Re} H''(Z) - \operatorname{Im} H''(Z) + G\Omega^T \operatorname{Im} H''(Z)\Omega G$$

$$\dot{\alpha} = -2 \operatorname{Im} H(Z) - \frac{\hbar}{2} \operatorname{tr}[\operatorname{Im} H''(Z) G^{-1}]$$

- Expand $H(z)$ up to second order around $z = Z(t)$ (following Hermitian case, Hepp '74, Heller '74). Exact if H quadratic.
- Hamiltonian and gradient part of dynamics of $Z(t)$, coupled dynamics for $Z(t)$ and metric $G(t)$

Example: Anharmonic oscillator with damping

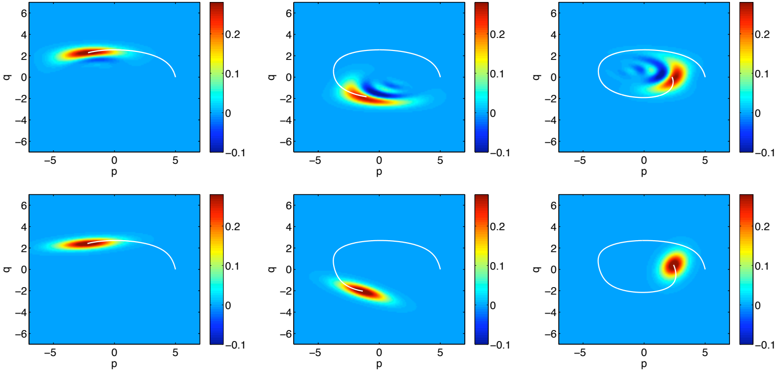

Figure: Normalised exact Wigner function (top row) and the semiclassical approximation (bottom row) at different times ($t = 0,\ 1,\ 2.5,\ 4$). The white line shows the motion of the center.

$$\mathrm{Re}\, H = \frac{1}{2}(p^2 + q^2) + \frac{1}{8}q^4\,, \quad \mathrm{Im}\, H = -\frac{1}{10}(p^2 + q^2)\,,\ \hbar = 1$$

Some complex symplectic geometry

- positive Lagrangian subspace $L \subset T^*\mathbb{C}^n$: $h(z, z') := \frac{\mathrm{i}}{2}\Omega(z, \bar{z}')$ is positive on L.
- $J : T^*\mathbb{R}^n \to T^*\mathbb{R}^n$ is a Ω-compatible complex structure if $G = \Omega J$ is symmetric and positive definite, and $J^2 = -I$.
- Siegel upper half space
  $\Sigma_n := \{B \in M_n(\mathbb{C})\,;\ B^T = B\,,\ \mathrm{Im}\, B > 0\}$:
  $L_B := \{(Bx, x)\,;\ x \in \mathbb{C}^n\}$ is positive Lagrangian iff $B \in \Sigma_n$.

These three sets can be identified:

- define $P_J : T^*\mathbb{C}^n \to T^*\mathbb{R}^n$ by $P_J(x + iy) := x + Jy$ then $L_J := \ker P_J$ is positive Lagrangian.
- If $L = L_B$, then $J = \begin{pmatrix} -\mathrm{Re}\, B & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} [\mathrm{Im}\, B]^{-1} & 0 \\ 0 & \mathrm{Im}\, B \end{pmatrix} \begin{pmatrix} I & -\mathrm{Re}\, B \\ 0 & I \end{pmatrix}$ is a complex structure such that $L_B = \ker P_J$

Relation to complex trajectories: Quadratic case

$$\psi_z^B(x) = \frac{(\det \operatorname{Im} B)^{1/4}}{(\pi\hbar)^{n/4}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[p\cdot(x-q)+\frac{1}{2}(x-q)\cdot B(x-q)]}\,, \quad z = (p,q) \in \mathbb{C}^n \times \mathbb{C}^n$$

- Complex Structure: $J := -\Omega G_B\,, \qquad J^2 = -I$
- Heller, Huber, Littlejohn '88; Graefe, RS '12: complex centre $z = \operatorname{Re} z + \mathrm{i} \operatorname{Im} z$ equivalent to real centre $Z = \operatorname{Re} z + J \operatorname{Im} z$:

$$\psi_z^B(x) = C_z \psi_Z^B(x)$$

- Exner '83, Hörmander '95: $\psi(t,x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma(t)} \psi_{z(t)}^{B(t)}(x)$, *$z(t)$ complex Hamiltonian trajectory*
- Graefe, RS '12: If $z(t))$ complex Hamiltonian trajectory, then $Z(t) = P_J(z) = \operatorname{Re} z(t) + J(t) \operatorname{Im} z(t)$ is Ehrenfest trajectory.

$$\mathrm{i} \rightarrow J$$

Geometry: Global case

- Donaldson: (M, ω, J) Kähler, $H : M \to \mathbb{C}$, is there a natural way to define Hamiltonian symplectomorphism for complex H?
- Burns, Lupercio and Uribe (2013): Embed M in symplectic complexification X with complex Lagrangian fibration

$$\Pi : X \to M \ , \quad L_m := \Pi^{-1}(m) \ \text{ complex Lagrangian}$$

$$\Phi_H^t : M \to X \text{ Hamiltonian flow of } H,\ L_{m(t)}(t) = \Phi_h^t(L_m),$$

$$\Pi_t : X \to M \ , \quad L_{m(t)}(t) := \Pi_t^{-1}(m(t))$$

  - there exits a complex structure $J_t : TM \to TM$ such that Π_t is holomorphic with respect to J_t.
  - we have

$$\dot{m} = X_{\mathrm{Re}\, H} + J_t X_{\mathrm{Im}\, H} \ .$$

These are equivalent to previous Ehrenfest dynamics.

Relation to complex trajectories: WKB

Assume $H = |p|^2/2 + V(x)$ real analytic, propagated state:

$$\psi(t,x) = A(t,x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}$$

- $\partial_t S(t,x) + H(\nabla S(t,x), x) = 0$
- $A(t,x)$ satisfies transport equation.
- Cauchy Kovalevskaya gives local existence of S, A.

Main observation:

$$|\psi(t,x)|^2 = |A(t,x)|^2\mathrm{e}^{-\frac{2}{\hbar}\operatorname{Im} S(t,x)}$$

main contribution to $\psi(t,x)$ come from **local minima** of $\operatorname{Im} S(t,x)$.

How do critical points of $\operatorname{Im} S(t,x)$ evolve in time?

Evolution of critical points $(H = \frac{1}{2}|p|^2 + V(x))$

- Assume $S(t,x)$ solves $\partial_t S + \frac{1}{2}|\nabla S(t,x)|^2 + V(t,x) = 0$
- Define $Q(t)$, $t \in [0,T]$, by $\nabla \operatorname{Im} S(t, Q(t)) = 0$ and set

$$P(t) := \nabla S(t, Q(t)) \; , \mathbf{B}(t) = S''(t, Q(t))$$

Theorem

The functions $(P(t), Q(t), \mathbf{B}(t))$ *satisfy*

$$\dot{P} - \operatorname{Re}\mathbf{B}\dot{Q} = -\operatorname{Re}\mathbf{B}P - \nabla \operatorname{Re} V(t,Q)$$

$$\operatorname{Im}\mathbf{B}\dot{Q} = \operatorname{Im}\mathbf{B}P - \nabla \operatorname{Im} V(t,Q)$$

$$\dot{\mathbf{B}} = -V''(t,Q) - \mathbf{B}^T\mathbf{B} \; .$$

If $\operatorname{Im}\mathbf{B}(t)$ *is invertible then this system is equivalent to the previous Ehrenfest system.*

local minima vs global behaviour

Lemma

Assume Im $B_0 > 0$ *and* Im $V'' \leq 0$, *then* Im $B(t) > 0$.

- If Im $V'' \leq 0$ local minima propagate.
- behaviour of $\psi(t, x)$ is dominated by smallest local minimum.
  $=>$ Problem is not local.
- If Im $S_0 = 0$, but Im V a Morse function, then Im $S(t, x)$ develops local minima.

Questions:

- How are local minima created or destroyed?
- What happens for general Im V''?

Summary and Outlook

- We studied Schrödinger equation with non-Hermitian Hamiltonian.
- Two different semiclassical dynamics emerging:
  - Ehrenfest Theorem: Mixed Hamiltonian and gradient flow with coupled time dependent metric.
  - Hamilton-Jacobi: Hamiltonian flow in complex phase space
- Relation given by projection using complex structure $J = -\Omega G$:

$$i \to J$$

- Ehrenfest dynamics describes dynamics of critical points of solutions to Hamilton Jacobi.
- Open problems:
  - Accurate remainder estimates: suitable function spaces and a-priori estimates.
  - Explore underlying complex symplectic geometry.