Non-Hermitian propagation of coherent states

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- E. M. Graefe, M. Höning, and H. J. Korsch: J. Phys. A 43 (2010) 075306
- Graefe, RS: Phys. Rev. A **83** (2011), 060101.
- Graefe, RS: J. Phys. A **45** (2012) 244033

Schrödinger equation with complex Hamiltonian

$$\mathrm{i}\hbar\partial_t\psi = [\hat{H} - \mathrm{i}\hat{\Gamma}]\psi$$

$\hat{H}$, $\hat{\Gamma}$ hermitian, e.g., complex potential $V(x)$, damping $-\gamma\hbar^2\Delta$

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \mathrm{Re}\, V(x) \qquad \hat{\Gamma} = -\gamma\hbar^2\Delta + \mathrm{Im}\, V(x)$$

- $\|\psi\|$ not conserved: modelling open systems, loss and gain.
- scattering resonances: complex scaling, absorbing potentials
- spectrum and pseudo-spectrum, PT symmetric operators
- optical waveguides with absorbing and active materials, PT symmetric waveguides

What type of classical dynamics emerges in the limit $\hbar \to 0$?

Semiclassical limit if $\Gamma = 0$: WKB vs Ehrenfest

WKB : $\psi(t,x) = a(t,x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}$ insert in Schrödinger:

- $\partial_t S(t,x) + H(\nabla S(t,x), x) = 0$, 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: $\psi(x)$, $\hat{\psi}(\xi)$ 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 $\Gamma \neq 0$: 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

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

- $G_B = \begin{pmatrix} I & 0 \\ -\operatorname{Re} B & I \end{pmatrix} \begin{pmatrix} (\operatorname{Im} B)^{-1} & 0 \\ 0 & \operatorname{Im} B \end{pmatrix} \begin{pmatrix} I & -\operatorname{Re} B \\ 0 & I \end{pmatrix}$
- Expectation values and variance:

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

- G symplectic metric: $G_B \Omega G_B = \Omega$, ψ pure state with minimal uncertainty.

Coherent states: Background and Applications

- Schrödinger '27: Follow classical trajectories for harmonic oscillator
- Ground state of harmonic oscillator: approximate groundstate of anharmonic oscillator, normal forms
- Gaussian beams, Babich et.al.
- Time evolution if $\Gamma = 0$: Hepp '74, Heller '74, Maslov '70's, Hagedorn '80, Combescure Robert '97, ... : If $Z(t)$ satisfies Hamiltons equations then

$$\psi(t,x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma(t)}\psi^{B(t)}_{Z(t)}(x) + O_{L^2}(\sqrt{\hbar}) \ ,$$

  where $B(t)$ is related to linearized flow around $Z(t)$.
- Wide applications in chemistry: expansion into coherent states, Initial value representations (IVR's), Herman Kluk propagator, etc
- Numerical propagation schemes: Lubich '09, Runborg, ...
- Pseudo-spectrum: Dencker, Sjöstrand and Zworski '04 (following Hörmander)

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

$$\dot{Z} = \Omega\nabla H(Z) - G^{-1}\nabla\Gamma(Z)$$
$$\dot{G} = H''(Z)\Omega G - G\Omega H''(Z) + \Gamma''(Z) - G\Omega^T\Gamma''(Z)\Omega G$$
$$\dot{\alpha} = 2\Gamma(Z) + \frac{\hbar}{2}\mathrm{tr}[\Gamma''(Z)G^{-1}]$$

- Expand $H(z), \Gamma(z)$ up to second order around $z = Z(t)$ (following Hermitian case). Exact if H, Γ quadratic.
- Hamiltonian and gradient part of dynamics of $Z(t)$, coupled dynamics for $Z(t)$ and metric $G(t)$

Example: Anharmonic oscillator with damping

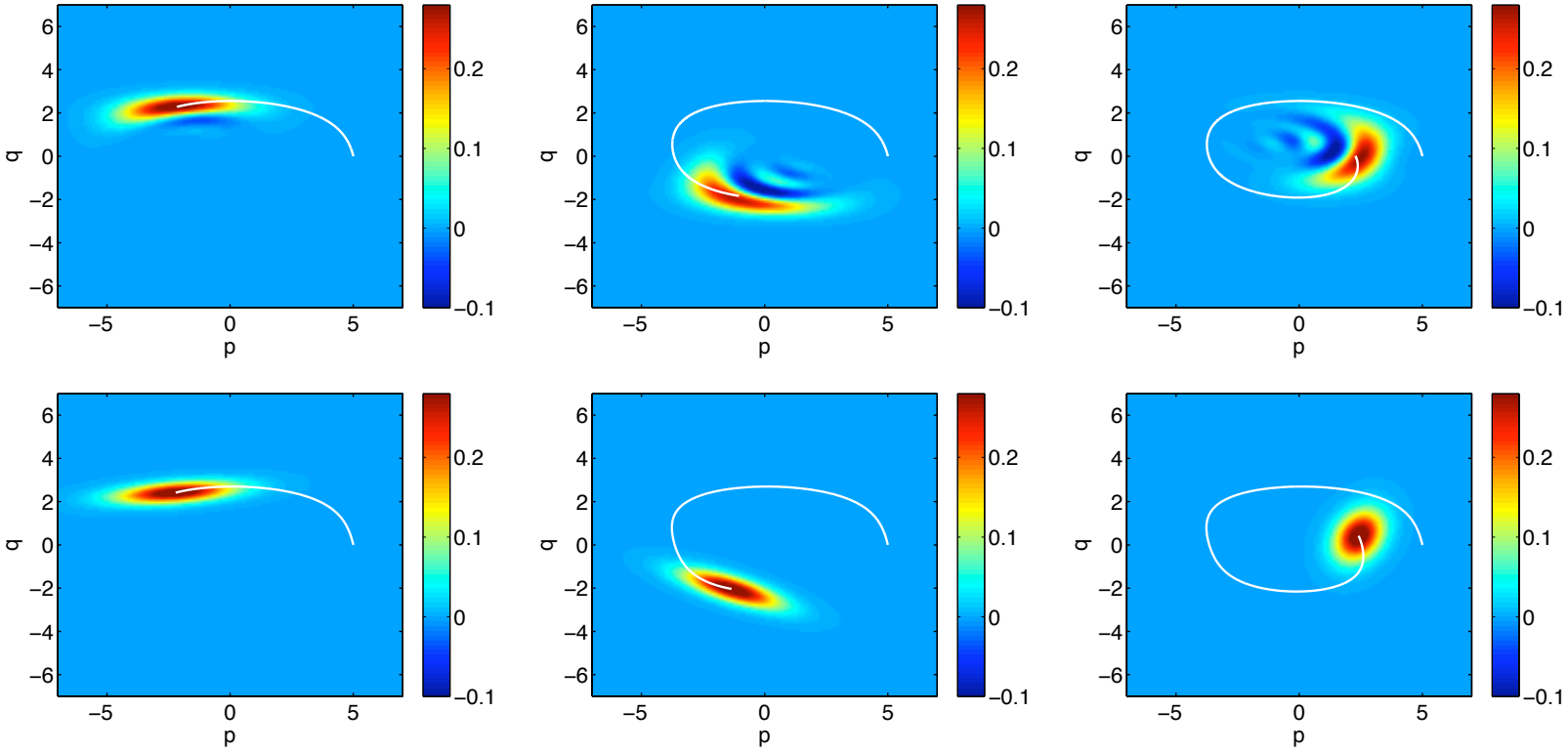

Figure: Normalised exact Wigner function (top row) and the semiclassical approximation (bottom row) at different times ($t = 0$, 1, 2.5, 4). The white line shows the motion of the center.

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

Example: Damped Harmonic Oscillator

Let $\alpha \in \mathbb{C}$ with $|\alpha| = 1$ and $\operatorname{Im}\alpha, \operatorname{Re}\alpha > 0$, $\omega > 0$, and take

$$\hat{H} - \mathrm{i}\hat{\Gamma} = \frac{\bar{\alpha}^2}{2}\hat{p}^2 + \frac{\omega}{2}\hat{q}^2$$

Then $G = \begin{pmatrix} (\omega \operatorname{Re}\alpha)^{-1} & \operatorname{Im}\alpha(\operatorname{Re}\alpha)^{-1} \\ \operatorname{Im}\alpha(\operatorname{Re}\alpha)^{-1} & \omega[\operatorname{Re}\alpha + \operatorname{Im}\alpha(\operatorname{Re}\alpha)^{-2}] \end{pmatrix}$ is a sol. with $\dot{G} = 0$, and an attractor, and

$$\dot{P} = -\omega^2 Q - 2\omega \operatorname{Im}\alpha \; P \;, \quad \dot{Q} = P$$

hence we get the *underdamped* oscillator

$$\ddot{Q} + 2\omega \operatorname{Im}\alpha \, \dot{Q} + \omega^2 Q = 0 \;, \quad 0 \leq \operatorname{Im}\alpha < 1$$

Relation to complex trajectories: Quadratic case:

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

- Exner '83, Hörmander '95: H quadratic, then $\psi(t,x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma(t)}\psi_{z(t)}^{B(t)}(x)$, $z(t)$ *complex Hamiltonian trajectory*
- Complex Structure:

$$J := -\Omega G_B\,, \qquad J^2 = -I$$

- Heller, Huber, Littlejohn '88; Graefe, RS '12: complex centre z equivalent to real centre $Z = \operatorname{Re} z + J \operatorname{Im} z$.

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

- Graefe, RS '12: If $z(t)$ complex Hamiltonian trajectory, then $Z(t) = \operatorname{Re} z(t) + J(t) \operatorname{Im} z(t)$ is Ehrenfest trajectory.

Relation to complex trajectories: general case

propagated state: $\psi(t,x) = a(t,x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}$.

$$\partial S(t,x) + H(\nabla S(t,x),x) - \mathrm{i}\Gamma(\nabla S(t,x),x) = 0$$

$a(t,x)$ satisfies transport equation. Expectation values

$$\begin{aligned}\langle\psi(t),\hat{A}\psi(t)\rangle &= \int A(\nabla S(t,x),x)|a(t,x)|^2\mathrm{e}^{-\frac{2}{\hbar}\operatorname{Im}S(t,x)}\,\mathrm{d}x + O(\hbar)\\ &= \|\psi(t)\|^2 A(Z(t)) + O(\hbar)\end{aligned}$$

main contribution from stationary point $Q(t)$:

$$\nabla \operatorname{Im} S(t,Q(t)) = 0\ , \quad \text{then} \quad P(t) := \nabla S(t,Q(t)) \in \mathbb{R}^n$$

and $Z(t) := (P(t),Q(t)) \in \mathbb{R}^n \times \mathbb{R}^n$ satisfies

$$\dot{Z} = \Omega\nabla H(Z) - G_B^{-1}\nabla\Gamma(Z)\ , \quad \text{with } G_B \text{ defined by } B(t) = S''(t,Q(t))$$

Summary and Outlook

- We studied Schrödinger equation with non-Hermitian Hamiltonian $\hat{H} - \mathrm{i}\hat{\Gamma}$.
- 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 $J = -\Omega G$:

$$i \longrightarrow J$$

- Open problems:
  - Accurate remainder estimates: suitable function spaces and a-priori estimates.
  - Explore underlying complex symplectic geometry.