Non-Hermitian propagation of coherent states

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MOPNET 5
UCL, 13.9.2011

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, decay, damping, pumping, ...
- 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 $\Gamma = 0$: oscillatory states and Ehrenfest

Oscillatory states : $\psi(t,x) = a(t,x)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S(t,x)}$ 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, 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 $Z(t) \in \mathbb{R}^n \times \mathbb{R}^n$

Wignerfunctions and their evolution

$$W(p,q) := \frac{1}{(2\pi\hbar)^n}\int \psi(q+x/2)\psi^*(q-x/2)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}x\cdot p}\,\mathrm{d}x$$

If $\hat{A} := A(\hat{p},q)$ (Weyl quantisation), then

$$\langle\psi,\hat{A}\psi\rangle = \int W(z)A(z)\,\mathrm{d}z\ , \quad z=(p,q)$$

If $\mathrm{i}\hbar\partial_t\psi = [\hat{H}-\mathrm{i}\hat{\Gamma}]\psi$ then using semiclassical symbol calculus one finds up to terms of order $\hbar^3|\partial^3 W|(|\partial^3 H|+|\partial^3\Gamma|)$:

$$\hbar\partial_t W(t,z) = -\bigg(-\frac{\hbar^2}{4}\Delta_\Gamma - \hbar\nabla H\cdot\Omega\nabla_z + 2\Gamma\bigg)W(t,z) \qquad (2)$$

- $\Delta_\Gamma := \nabla_z\Omega^T\Gamma''(z)\Omega\nabla_z$, “symplectic Laplace Beltrami”
- $\Gamma = 0$: Liouville equation, transport along $z(t)$

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:

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

- 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

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

  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

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

is an approximate solution to (2) (up to $O(\sqrt{\hbar})$) if

$$\dot{Z} = \Omega\nabla H(Z) - G^{-1}\nabla\Gamma(Z)$$

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

$$\dot{\alpha} = 2\Gamma(Z) + \frac{1}{2}\mathrm{tr}[\Gamma''(Z)G^{-1}]$$

- Expand $H(z), \Gamma(z)$ up to second order around $Z(t)$ (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: PT-symmetric potential

$$H = \frac{1}{2}(p^2 + q^2) \ , \ \Gamma = cq$$

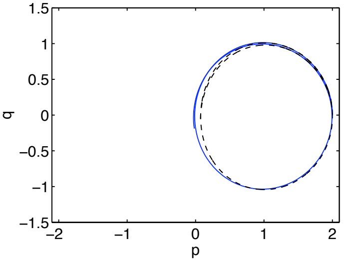
then $H'' = I$, $\Gamma'' = 0$ and $G = I$ is a solution. Equations for (p, q):

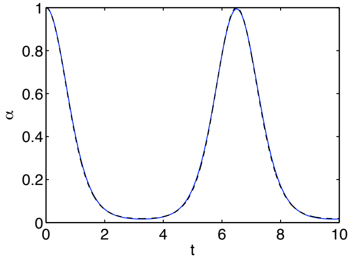
$$\dot{p} = -q \ , \quad \dot{q} = p - c$$

Shift of p: $p' = p - c$ gives shifted harmonic oscillator

$$\dot{p}' = -q \ , \quad \dot{q} = p'$$

Example: $\Gamma = 5\tanh(q/5)$
upper panel: $Z(t)$
lower panel: $\alpha(t)$





Example: Anharmonic oscillator with damping

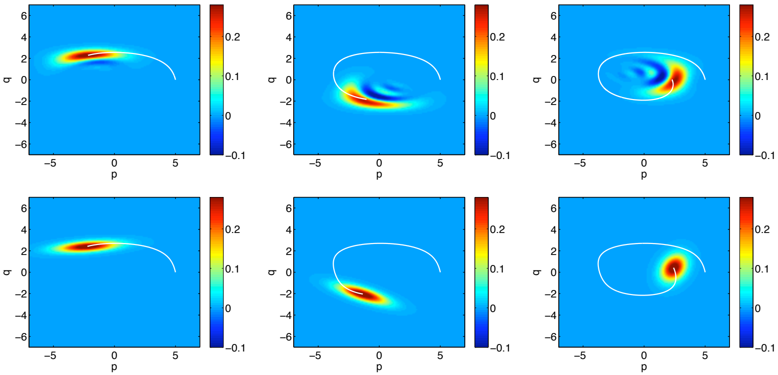


Figure: Normalised exact Wigner function (top row) and the semiclassical approximation (bottom row) at different times ($t = 0$, 1, 2.5, 4). The white line shows the motion of the center.

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

Quadratic case: the relation to complex trajectories

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

Theorem

Let $H(z), \Gamma(z)$ quadratic. Let $S \in M_{2n}(\mathbb{C})$ be solution to

$$\dot{S} = \Omega(H'' - \mathrm{i}\Gamma'')S \;, \quad S(0) = I$$

and set $z(t) = S(t)z$ and $B(t) := (S_{pp}B + S_{pq})(S_{qp}B + S_{qq})^{-1}$, then there exist a $\sigma(t)$ such that

$$\psi(t,x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma(t)}\psi_{z(t)}^{B(t)}(x)$$

is a solution to the Schrödinger equation.

$z(t)$ **complex, but** $Z(t)$ **real, what is the relation?**

The complex structure

$J := -G_B\Omega$ is a Ω-compatible complex structure, i.e.,

$$J^2 = -I \ , \quad \text{and} \quad G_B^{-1} = \Omega J \quad \text{is symmetric and positive}$$

Theorem (E.M. Graefe and RS '11)

For $\mathbf{z} = \operatorname{Re}\mathbf{z} + \mathrm{i}\operatorname{Im}\mathbf{z} \in \mathbb{C}^n \times \mathbb{C}^n$ *set* $\mathbf{Z} = \operatorname{Re}\mathbf{z} + \mathbf{J}\operatorname{Im}\mathbf{z} \in \mathbb{R}^n \times \mathbb{R}^n$*, then there exist a* $\sigma_J(z)$ *such that*

$$\psi_z^B(x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\sigma_J(z)}\psi_Z^B(x) \ .$$

Quadratic case:

If z *satisfies* $\dot{z} = \Omega(\nabla H - \mathrm{i}\nabla\Gamma)$

then $\dot{Z} = \Omega(\nabla H - J\nabla\Gamma) = \Omega\nabla H - G^{-1}\nabla\Gamma$

where $\dot{G} = H''\Omega G - G\Omega H'' + \Gamma'' - G\Omega^T\Gamma''\Omega G$.

Huber, Heller and Littlejohn '88: complex centre not unique.

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

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

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

$\dot{Z} = \Omega\nabla H(Z) - G_B^{-1}\nabla\Gamma(Z)$, with G_B 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 $J = -G\Omega$:

$$i \to J$$

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