Κύματα, Πιθανότητες και Αναμνήσεις

Επιστημονικό συνέδριο προς τιμήν του
Ομότιμου Καθηγητή Ε.Μ.Π.
Γεράσιμου Αθανασούλη

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Λύσεις κυματοπακέτων γιά την εξίσωση Schrodinger του φασικού χώρου

Γεώργιος Μακράκης (Παν. Κρήτης & ΙΥΜ-ΙΤΕ)

Wavepacket solutions of the phase-space Schrödinger equation

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The problem: What we want to do & why

Scope: We want to construct wave packet (i.e. localized) solutions of the phase space Schrödinger equation (PSSE), the phase-space image of the usual ($\sim$ living in physical space time) Schrödinger equation (SE) under the wave packet transform

Where PSSE appears: *phase-space representations of QM* applied to: quantum chemistry, quantum optics/paraxial propagation, atomic optical trapping, laser cooling, etc. ref

Why PSSE is mathematically challenging: It is a linear, but non local, pseudo-differential equation, living in phase space, which is the natural space to describe wave propagation

What we have done so far (...small progress...)

We have constructed a formal asymptotic solution in four steps:

(1) We derived an approximate Fourier integral representation of the solution of PSSE, in terms of anisotropic Gaussian wave packets

(2) By Stationary Complex Phase Theorem, we obtained an Ansatz of the solution, in the form of a WKB function with complex phase

(3) We derived a Hamilton-Jacobi type equation for the complex phase and the corresponding transport equation for the complex amplitude

(4) We constructed the wavepacket solution from beam-like solutions of the equations in step 3, by using Maslov's complex WKB method

The Schrödinger equation (SE)

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t}-\widehat{H}\right)\psi(\boldsymbol{x},t;\hbar) &= 0\ ,\quad t\in[0,T]\ ,\\ \psi(\boldsymbol{x},t=0;\hbar) &= \psi_0(\boldsymbol{x};\hbar)\in L^2(\mathbb{R}^d)\end{aligned}$$

The Hamiltonian operator $\widehat{H}=\mathrm{Op}_{\mathbf{w}}(H)$ is the Weyl quantization of the real-valued and smooth Hamiltonian function $H(\boldsymbol{q},\boldsymbol{p})$, acting as

$$\widehat{H}\psi(\boldsymbol{x},t;\hbar):=\left(\frac{1}{2\pi\hbar}\right)^d\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}e^{\frac{i}{\hbar}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{q})}H\left(\frac{\boldsymbol{x}+\boldsymbol{q}}{2},\boldsymbol{p}\right)\psi(\boldsymbol{q},t;\hbar)\,d\boldsymbol{q}d\boldsymbol{p}$$

Wave packet transform

The wavepacket transform of $\psi \in L^2(\mathbb{R}^d, \mathbb{C}; d\boldsymbol{x})$ is defined by

$$(\mathcal{W}\psi)(\boldsymbol{q}, \boldsymbol{p}, t; \hbar) := \left(2\pi\hbar\right)^{-d/2} \int_{\mathbb{R}^d} \bar{G}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x}; \hbar)\psi(\boldsymbol{x}, t; \hbar)\, d\boldsymbol{x}$$

where

$$G_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x}; \hbar) = (\pi\hbar)^{-d/4} \exp \frac{i}{\hbar}\left(\frac{\boldsymbol{p}\cdot\boldsymbol{q}}{2} + \boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{q}) + \frac{i}{2}|\boldsymbol{x}-\boldsymbol{q}|^2\right) .$$

The map

$$\mathcal{W} : L^2(\mathbb{R}^d, \mathbb{C}; d\boldsymbol{x}) \to L^2(\mathbb{R}^{2d}, \mathbb{C}; d\boldsymbol{q}d\boldsymbol{p}) \ \ |\psi \mapsto \Psi = \mathcal{W}\psi$$

is not a bijection.

Wave packet transform

The image of $\mathcal{W}$ is the *Fock-Bargmann space*

$$\mathfrak{F} = \Big\{ \Psi : \int |\Psi|^2 \, d\boldsymbol{q} d\boldsymbol{p} < +\infty \ \text{ and }$$

$$\left(\left(\frac{\boldsymbol{q}}{2} - i\hbar \frac{\partial}{\partial \boldsymbol{p}} \right) - i \left(\frac{\boldsymbol{p}}{2} + i\hbar \frac{\partial}{\partial \boldsymbol{q}} \right) \right) \Psi = \mathbf{0} \Big\}$$

Thus, only Gaussian-weighted square, integrable analytic functions in the variable $(\boldsymbol{q} - i\boldsymbol{p}) \in \mathbb{C}^d$, satisfying the Cauchy-Riemann relations

$$\left(\frac{\partial}{\partial \boldsymbol{q}} - i \frac{\partial}{\partial \boldsymbol{p}} \right) \left(e^{\frac{1}{2\hbar}(i\boldsymbol{p}\cdot\boldsymbol{q} + |\boldsymbol{p}|^2)} \Psi \right) = \mathbf{0} \ ,$$

are *admissible* phase space wave functions.

The phase space Schrödinger equation (PSSE)

The conjugation $\widehat{\mathcal{H}} = \mathcal{W}\widehat{H}\mathcal{W}^{-1}$ of $\widehat{H}$ with the wave packet transform $\mathcal{W}$, leads to the *phase space Schrödinger equation*

$$\Big(i\hbar\frac{\partial}{\partial t} - \widehat{\mathcal{H}}\Big)\Psi(\boldsymbol{q},\boldsymbol{p},t;\hbar) = 0 \ , \quad t \in [0,T] \ ,$$

$$\Psi(\boldsymbol{q},\boldsymbol{p},t=0;\hbar) = \Psi_0(\boldsymbol{q},\boldsymbol{p};\hbar) \in \mathfrak{F} \ ,$$

governing the evolution of the phase space wavefunction (pswf)

$$\begin{aligned}\Psi(\boldsymbol{q},\boldsymbol{p},t;\hbar) \quad &:= \quad (\mathcal{W}\psi)(\boldsymbol{q},\boldsymbol{p},t;\hbar) \\ &= \quad \Big(2\pi\hbar\Big)^{-d/2}\int_{\mathbb{R}^d} \bar{G}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x};\hbar)\psi(\boldsymbol{x},t;\hbar)\,d\boldsymbol{x}\end{aligned}$$

Approximate phase space wave fucntion

By using the resolution of identity

$$\left(\frac{1}{2\pi\hbar}\right)^d \int G_{(\boldsymbol{q},\boldsymbol{p})} \langle G_{(\boldsymbol{q},\boldsymbol{p})}, \bullet \rangle \, d\boldsymbol{q} d\boldsymbol{p} = \mathbb{I}_{L^2} \bullet \quad ,$$

and the approximate solution $G^{\mathcal{Z}}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x}, t; \hbar)$ of the problem

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t} - \widehat{H}\right)\psi(\boldsymbol{x}, t; \hbar) &= 0 \ , \quad t \in [0, T] \ , \\ \psi(\boldsymbol{x}, t = 0; \hbar) &= \psi_0(\boldsymbol{x}; \hbar) = \bar{G}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x}; \hbar) \ , \end{aligned}$$

the approximation understood in the sense

$$\left\| \left(i\hbar \frac{\partial}{\partial t} - \widehat{H}\right) G^{\mathcal{Z}}_{(\boldsymbol{q},\boldsymbol{p})}(\bullet, t; \hbar) \right\|_{L^2(\mathbb{R}^d)} = O(\hbar^{3/2}) \ , \quad \hbar \to 0^+$$

for the fixed time interval $[0, T]$ gz

Approximate phase space wave function

we construct the approximate pswf

$$\boxed{\Psi \sim \psi^{\mathcal{Z}}(\boldsymbol{q},\boldsymbol{p},t;\hbar) = \int \mathcal{K}^{\mathcal{Z}}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{\eta},\boldsymbol{\xi},t;\hbar)\Psi_0(\boldsymbol{\eta},\boldsymbol{\xi};\hbar)\, d\boldsymbol{\eta} d\boldsymbol{\xi}}$$

where

$$\mathcal{K}^{\mathcal{Z}}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{\eta},\boldsymbol{\xi},t;\hbar) := \left(\frac{1}{2\pi\hbar}\right)^d \int \bar{G}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x};\hbar)\, G^{\mathcal{Z}}_{(\boldsymbol{\eta},\boldsymbol{\xi})}(\boldsymbol{x},t;\hbar)\, d\boldsymbol{x}\ .$$

is the approximate phase space propagator (Green's fucntion).

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Construction of approximate initial data

We assume WKB initial data for the Schrödinger equation (SE)

$$\psi_0(\boldsymbol{x};\hbar) = \psi_0^{\hbar}(\boldsymbol{x}) := R_0(\boldsymbol{x})\, e^{\frac{i}{\hbar} S_0(\boldsymbol{x})} \ , \quad \hbar \ll 1 \ ,$$

$$S_0 \in C^{\infty}(\mathbb{R}^d, \mathbb{R}), \ \det\left(\frac{\partial^2 S_0}{\partial \boldsymbol{x}^2}\right) \neq 0 \, , R_0 \in C_0^{\infty}(\mathbb{R}^d, \mathbb{R}) \, , \ \int_{\mathbb{R}^d} R_0^2 \, d\boldsymbol{x} = 1 \, ,$$

and, by using the Stationary Complex Phase Theorem, we approximate $\Psi_0 = \mathcal{W}\psi_0$ for $\hbar \ll 1$ scpf

$$\Psi_0(\boldsymbol{q},\boldsymbol{p};\hbar) \sim \Psi_0^{\hbar}(\boldsymbol{q},\boldsymbol{p}) := \chi_0(\boldsymbol{q},\boldsymbol{p};\hbar))\exp\left(\frac{i}{\hbar}\theta_0(\boldsymbol{q},\boldsymbol{p})\right)$$

Construction of approximate initial data

The amplitude χ_0 and the phase θ_0 are given by

$$\chi_0(\boldsymbol{q},\boldsymbol{p};\hbar) = (\pi\hbar)^{-d/4} \frac{R_0(\boldsymbol{z}(\boldsymbol{q},\boldsymbol{p}))}{\sqrt{\det\left(\mathbf{I} - i\,\frac{\partial^2 S_0}{\partial \boldsymbol{z}^2}(\boldsymbol{z}(\boldsymbol{q},\boldsymbol{p}))\right)}}$$

$$\theta_0(\boldsymbol{q},\boldsymbol{p}) = S_0(\boldsymbol{z}(\boldsymbol{q},\boldsymbol{p})) - \boldsymbol{p}\cdot\Big(\boldsymbol{z}(\boldsymbol{q},\boldsymbol{p}) - \boldsymbol{q}\Big) + \frac{i}{2}\Big(\boldsymbol{z}(\boldsymbol{q},\boldsymbol{p}) - \boldsymbol{q}\Big)^2 - \frac{\boldsymbol{p}\cdot\boldsymbol{q}}{2}$$

- $S_0(\boldsymbol{z})$ and $R_0(\boldsymbol{z})$ are the *almost analytic extensions* to the complex variable $\boldsymbol{z} = \boldsymbol{x} + i\boldsymbol{y} \in \mathbb{C}^d$ of $S_0(\boldsymbol{x})$ and $R_0(\boldsymbol{x})$
- $\boldsymbol{z} = \boldsymbol{z}(\boldsymbol{q},\boldsymbol{p})$ is the complex solution of

$$\frac{\partial S_0(\boldsymbol{z})}{\partial \boldsymbol{z}} - \boldsymbol{p} + i(\boldsymbol{z} - \boldsymbol{q}) = \mathbf{0}$$

Fourier integral representation of the ps wavefunction

By using the approximate initial data, we further approximate

$$\boxed{\Psi^{\mathcal{Z}} \sim \Psi^{\hbar}(\boldsymbol{q},\boldsymbol{p},t) = \left(\frac{1}{2\pi\hbar}\right)^{d} \int \varphi(\boldsymbol{\eta},\boldsymbol{\xi},t;\hbar)\, e^{\frac{i}{\hbar}F(\boldsymbol{q},\boldsymbol{p},\boldsymbol{\eta},\boldsymbol{\xi},t)}\, d\boldsymbol{\eta} d\boldsymbol{\xi}}$$

where

$$F(\boldsymbol{q},\boldsymbol{p},\boldsymbol{\eta},\boldsymbol{\xi},t) = \theta_0(\boldsymbol{\eta},\boldsymbol{\xi}) + A(\boldsymbol{\eta},\boldsymbol{\xi},t) + \frac{\boldsymbol{\xi}\cdot\boldsymbol{\eta} - \boldsymbol{\xi}_t\cdot\boldsymbol{\eta}_t}{2}$$

$$+\frac{1}{2}(\boldsymbol{q},\boldsymbol{p})\cdot \mathbf{J}(\boldsymbol{\eta}_t,\boldsymbol{\xi}_t) + \frac{1}{2}\begin{pmatrix} \boldsymbol{q}-\boldsymbol{\eta}_t \\ \boldsymbol{p}-\boldsymbol{\xi}_t \end{pmatrix}^{T} \mathcal{Q}(\boldsymbol{\eta},\boldsymbol{\xi},t) \begin{pmatrix} \boldsymbol{q}-\boldsymbol{\eta}_t \\ \boldsymbol{p}-\boldsymbol{\xi}_t \end{pmatrix}$$

and

$$\varphi(\boldsymbol{\eta},\boldsymbol{\xi},t;\hbar) = (\pi\hbar)^{-d/4}\left(\det \frac{\partial(\boldsymbol{\eta}_t - i\boldsymbol{\xi}_t)}{\partial(\boldsymbol{\eta} - i\boldsymbol{\xi})}\right)^{-1/2} \chi_0(\boldsymbol{z}(\boldsymbol{\eta},\boldsymbol{\xi}));\hbar)$$

Narrow beam approximation of $\Psi^\hbar$ and the Ansatz

Applying Stationary Complex Phase Theorem to the Fourier integral for $\Psi^\hbar$ we get a narrow beam approximation of the form

$$\boxed{\Psi^\hbar_B(\boldsymbol{X},t) = \chi(\boldsymbol{X},t;\hbar)\, e^{\frac{i}{\hbar}\Phi(\boldsymbol{X},t)} \;, \quad \boldsymbol{X} = (\boldsymbol{q},\boldsymbol{p})}$$

We use this approximation as an Ansatz to built an approximate solution of PSSE. It follows that this Ansatz solves approximately the PSSE

$$i\hbar\frac{\partial \Psi^\hbar_B}{\partial t} - \widehat{\mathcal{H}}\Psi^\hbar_B = O(\hbar^2)\,, \;\; \Psi^\hbar_B(\boldsymbol{X},0) = \Psi^\hbar_0(\boldsymbol{X},0) = \chi_0(\boldsymbol{X};\hbar)e^{\frac{i}{\hbar}\theta_0(\boldsymbol{X})}$$

pswo

The Ansatz

provided that the complex phase Φ solves the Hamilton-Jacobi equation

$$\frac{\partial \Phi}{\partial t} + \mathcal{H}\Big(\boldsymbol{X}, \frac{\partial \Phi}{\partial \boldsymbol{X}}\Big) = 0 \ , \quad \Phi(\boldsymbol{X}, 0) = \theta_0(\boldsymbol{X}) \ ,$$

and the complex amplitude χ solves the transport equation

$$\frac{\partial \chi}{\partial t} - \mathbf{J}\frac{\partial H}{\partial \boldsymbol{X}}\Big(\frac{\boldsymbol{X}}{2} - \mathbf{J}\frac{\partial \Phi}{\partial \boldsymbol{X}}\Big) \cdot \frac{\partial \chi}{\partial \boldsymbol{X}} - \frac{1}{2}\,\mathrm{tr}\,\mathbf{J}\frac{\partial^2 \Phi}{\partial \boldsymbol{X}^2}\mathbf{J}\frac{\partial^2 H}{\partial \boldsymbol{X}^2}\Big(\frac{\boldsymbol{X}}{2} - \mathbf{J}\frac{\partial \Phi}{\partial \boldsymbol{X}}\Big)\chi = 0 \ ,$$

$$\chi(\boldsymbol{X}, 0; \hbar) = \chi_0(\boldsymbol{X}; \hbar)$$

Construction of the wavepacket solution of PSSE

By using Maslov's complex WKB method we construct

- the phase Φ

$$\Phi(\boldsymbol{X},t) = \Big\{\theta_0(\boldsymbol{X}_0(\boldsymbol{\alpha})) + \frac{1}{2}\mathbf{J}\boldsymbol{X}_t(\boldsymbol{\alpha}) \cdot (\boldsymbol{X} - \boldsymbol{X}_t(\boldsymbol{\alpha})) + A_w(\boldsymbol{X}_0(\boldsymbol{\alpha}), t) + \frac{1}{2}(\boldsymbol{X} - \boldsymbol{X}_t(\boldsymbol{\alpha})) \cdot \tilde{\mathcal{Q}}(\boldsymbol{\alpha}, t)(\boldsymbol{X} - \boldsymbol{X}_t(\boldsymbol{\alpha}))\Big\}_{\boldsymbol{\alpha}=\boldsymbol{\alpha}(\boldsymbol{X},t)}$$

psg

where

- A_w is the symmetrized phase space action

$$A_w(\boldsymbol{X}_0(\boldsymbol{\alpha}),t) = A(\boldsymbol{X}_0(\boldsymbol{\alpha}),t) - \frac{\boldsymbol{p}_t(\boldsymbol{\alpha}) \cdot \boldsymbol{q}_t(\boldsymbol{\alpha}) - \boldsymbol{p}_0(\boldsymbol{\alpha}) \cdot \boldsymbol{q}_0(\boldsymbol{\alpha})}{2} .$$

Construction of the wavepacket solution of PSSE

- $\tilde{\mathcal{Q}}$ solves a certain Riccati equation, and it is such that on any compact set $\mathcal{K}$ outside some neighborhood Δ_t of Λ_t

$$\boxed{\mathrm{Im}\,\Phi(\boldsymbol{X},t) > C(\mathcal{K}) > 0}$$

- $\boldsymbol{\alpha} = \boldsymbol{\alpha}(\boldsymbol{X},t)$ is the unique solution of the system

$$(\boldsymbol{X} - \boldsymbol{X}_t(\boldsymbol{\alpha})) \cdot \frac{\partial \boldsymbol{X}_t}{\partial \alpha_j}(\boldsymbol{\alpha}) = 0 \ , \quad j = 1, \dots, d$$

i.e., to every point $\boldsymbol{X}$ not belonging to, but in proximity to Λ_t, there exists a unique nearest point $\boldsymbol{X}_t(\boldsymbol{\alpha}(\boldsymbol{X},t))$ on Λ_t.

Construction of the wavepacket solution of PSSE

- the amplitude χ

$$\chi(\boldsymbol{X}, t; \hbar) = \left\{ \frac{\chi_0(\boldsymbol{X}_0(\boldsymbol{\alpha}); \hbar)}{\sqrt{\det \mathbf{C}(\boldsymbol{\alpha}, t)}} \right\}_{\boldsymbol{\alpha}=\boldsymbol{\alpha}(\boldsymbol{X},t)}$$

it has compact support

where the matrix $\mathbf{C}(\boldsymbol{X}, \boldsymbol{P}, t)$ is derived from the variational system in double phase space

$$\frac{d}{dt}\begin{pmatrix} \mathbf{C} \\ \mathbf{D} \end{pmatrix} = \begin{pmatrix} \mathcal{H}_{\boldsymbol{PX}} & \mathcal{H}_{\boldsymbol{PP}} \\ -\mathcal{H}_{\boldsymbol{XX}} & -\mathcal{H}_{\boldsymbol{XP}} \end{pmatrix} \begin{pmatrix} \mathbf{C} \\ \mathbf{D} \end{pmatrix}$$

$$\mathbf{C}(\boldsymbol{X}_0(\boldsymbol{\alpha}), \boldsymbol{P}_0(\boldsymbol{\alpha}), 0) = \mathbf{I} \text{ and } \mathbf{D}(\boldsymbol{X}_0(\boldsymbol{\alpha}), \boldsymbol{P}_0(\boldsymbol{\alpha}), 0) = \frac{\partial^2 \theta_0}{\partial \boldsymbol{X}^2}(\boldsymbol{X}_0(\boldsymbol{\alpha})) \, .$$

Construction of the wavepacket solution of PSSE

The constructed solution

$$\Psi_B^\hbar(\boldsymbol{X}, t) = \chi(\boldsymbol{X}, t; \hbar)\, e^{\frac{i}{\hbar}\Phi(\boldsymbol{X},t)} \ , \quad \boldsymbol{X} = (\boldsymbol{q}, \boldsymbol{p})$$

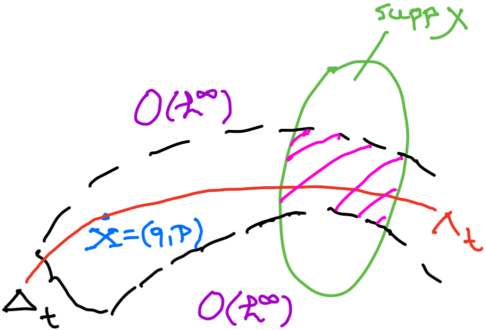
is a wavepacket moving in phase space thanks to the properties

$$\mathrm{Im}\,\Phi(\boldsymbol{X}, t) > C(\mathcal{K}) > 0$$

and

χ **has compact support**

Schematic description of the wavepacket in phase space



Some final remarks

- The accuracy of the approximation have been systematically studied for linear and quadratic potential (even in these simple cases the application of stationary complex phase formula is non trivial due to the needed almost analytic continuations)
- Open problem: Construction of eigenfunctions of PSSE which do not belong to the Fock-Bargmann space, i.e. "generalized eiagenfunctions" needed to built scattering solutions
- Most of the results are described in
  - *Asymptotic approximations for the phase space Schrödinger equation*, J. Phys. A: Math. & Theor., 2022
  - *Construction of the Van Vleck formula using the wave packet transform*, submitted

Thank you very much for your attention!!

References

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Explicit form of $G^{\mathcal{Z}}$

The explicit form of $G^{\mathcal{Z}}$ is

$$G^{\mathcal{Z}}_{(\boldsymbol{q},\boldsymbol{p})}(\boldsymbol{x},t;\hbar) = (\pi\hbar)^{-d/4} a(\boldsymbol{q},\boldsymbol{p},t)$$

$$\times \exp \frac{i}{\hbar}\left(\frac{\boldsymbol{p}\cdot\boldsymbol{q}}{2} + A(\boldsymbol{q},\boldsymbol{p},t) + \boldsymbol{p}_t\cdot(\boldsymbol{x}-\boldsymbol{q}_t) + \frac{1}{2}(\boldsymbol{x}-\boldsymbol{q}_t)\cdot\mathcal{Z}(\boldsymbol{x}-\boldsymbol{q}_t)\right) ,$$

where

- $(\boldsymbol{q}_t\ ,\boldsymbol{p}_t)$: the solution of the Hamiltonian system

$$\frac{d\boldsymbol{q}_t}{dt} = \frac{\partial H}{\partial \boldsymbol{p}} , \quad \frac{d\boldsymbol{p}_t}{dt} = -\frac{\partial H}{\partial \boldsymbol{q}} , \qquad (\boldsymbol{q}_0,\boldsymbol{p}_0) = (\boldsymbol{q},\boldsymbol{p}) ,$$

Explicit form of $G^{\mathcal{Z}}$

- $\mathcal{Z}$: solution of the Riccati equation

$$\frac{d\mathcal{Z}}{dt} + \mathcal{Z}\, H_{\boldsymbol{pp}}\, \mathcal{Z} + H_{\boldsymbol{qp}}\, \mathcal{Z} + \mathcal{Z}\, H_{\boldsymbol{pq}} + H_{\boldsymbol{qq}} = \mathbf{0} \ , \qquad \mathcal{Z}(0) = i\,\mathbb{I}$$

- a: amplitude

$$a(\boldsymbol{q}, \boldsymbol{p}, t) = \exp\left(-\frac{1}{2} \int_0^t \left\{ \mathrm{tr}\Big(H_{\boldsymbol{pp}}\, \mathcal{Z}(\boldsymbol{q}, \boldsymbol{p}, \tau) \Big) + H_{\boldsymbol{pq}} \right\} d\tau \right)$$

- $A(\boldsymbol{q}, \boldsymbol{p}, t)$: phase space action along the trajectory $(\boldsymbol{q}_t, \boldsymbol{p}_t)$

$$A(\boldsymbol{q}, \boldsymbol{p}, t) = \int_0^t \boldsymbol{p}_\tau \cdot \frac{d\boldsymbol{q}_\tau}{d\tau}\, d\tau - H(\boldsymbol{q}, \boldsymbol{p})\, t \ .$$

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Explicit form of $\mathcal{K}^{\mathcal{Z}}$

By direct Gaussian integration

$$\mathcal{K}^{\mathcal{Z}}(\boldsymbol{q},\boldsymbol{p},\boldsymbol{\eta},\boldsymbol{\xi},t)=\left(\frac{1}{2\pi\hbar}\right)^{d}\left(\det\frac{\partial(\boldsymbol{\eta}_t-i\boldsymbol{\xi}_t)}{\partial(\boldsymbol{\eta}-i\boldsymbol{\xi})}\right)^{-1/2}$$

$$\times\exp\frac{i}{\hbar}\left\{A(\boldsymbol{\eta},\boldsymbol{\xi},t)+\frac{\boldsymbol{\xi}\cdot\boldsymbol{\eta}-\boldsymbol{\xi}_t\cdot\boldsymbol{\eta}_t}{2}+\frac{1}{2}(\boldsymbol{q},\boldsymbol{p})\cdot\mathbf{J}(\boldsymbol{\eta}_t,\boldsymbol{\xi}_t)\right.$$

$$\left.+\frac{1}{2}\begin{pmatrix}\boldsymbol{q}-\boldsymbol{\eta}_t\\ \boldsymbol{p}-\boldsymbol{\xi}_t\end{pmatrix}^{T}\mathcal{Q}\begin{pmatrix}\boldsymbol{q}-\boldsymbol{\eta}_t\\ \boldsymbol{p}-\boldsymbol{\xi}_t\end{pmatrix}\right\}$$

where

$$\mathcal{Q}(\boldsymbol{\eta},\boldsymbol{\xi},t)=\begin{pmatrix} i\mathbf{I}-i(\mathbf{I}-i\mathcal{Z})^{-1} & \frac{1}{2}\mathbf{I}-(\mathbf{I}-i\mathcal{Z})^{-1}\\ \frac{1}{2}\mathbf{I}-(\mathbf{I}-i\mathcal{Z})^{-1} & i(\mathbf{I}-i\mathcal{Z})^{-1}\end{pmatrix}$$

kzback

Stationary Complex Phase Formula

Theorem. (Nazaikinksii et al., Melin & Sjostrand)Consider the oscillatory integral

$$\left(\frac{1}{2\pi\hbar}\right)^{m/2}\int_{\mathbb{R}^m} e^{-\frac{1}{2\hbar}\boldsymbol{x}\cdot\mathbf{M}\boldsymbol{x}+\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}}\,d\boldsymbol{x}=\frac{1}{\sqrt{\det\mathbf{M}}}\exp\left(-\frac{1}{2\hbar}\boldsymbol{p}\cdot\mathbf{M}^{-1}\boldsymbol{p}\right).$$

$I(\boldsymbol{p};\hbar)$, with $s\geqslant 1$, amplitude $a:\mathbb{R}^m\to\mathbb{C}$ and phase $\Phi:\mathbb{R}^n\times\mathbb{R}^m\to\mathbb{C}$ of class C^s in $\boldsymbol{p}$, where a is compactly supported and Φ possesses an everywhere non-negative imaginary part on $\mathrm{supp}\,a$, so that, for given $\boldsymbol{p}\in\mathbb{R}^n$, the equations

$$\mathrm{Im}\,\Phi(\boldsymbol{p},\boldsymbol{x})=0\ ,\quad \frac{\partial\Phi}{\partial\boldsymbol{x}}(\boldsymbol{p},\boldsymbol{x})=\mathbf{0}$$

have at most a single solution on $\mathrm{supp}\,a$,

Stationary Complex Phase Formula

while the Hessian matrix

$$\frac{\partial^2 \Phi}{\partial \boldsymbol{x}^2}(\boldsymbol{p}, \boldsymbol{x})$$

is non-singular for all $(\boldsymbol{p}, \boldsymbol{x}) \in \mathbb{R}^n \times \operatorname{supp} a$.
Then, for all $r = 0, \ldots, s$, the following estimate holds as $\hbar \to 0^+$

$$I(\boldsymbol{p}; \hbar) = \frac{{}^r a(\boldsymbol{p}, \boldsymbol{z}(\boldsymbol{p}))}{\sqrt{\det - \frac{\partial^2 \, {}^r\Phi}{\partial \boldsymbol{z}^2}(\boldsymbol{p}, \boldsymbol{z}(\boldsymbol{p}))}} e^{\frac{i}{\hbar} \, {}^r\Phi(\boldsymbol{p}, \boldsymbol{z}(\boldsymbol{p}))} \left(1 + o(\hbar)\right)$$

where $\sqrt{\bullet}$ is the principal branch of the square root function, the left superscript r denotes the r-analytic extensions of a function to the complex variable $\boldsymbol{z} = \boldsymbol{x} + i\boldsymbol{y}$,

Stationary Complex Phase Formula

and $\boldsymbol{z} = \boldsymbol{z}(\boldsymbol{p})$ is the unique complex solution of the equation

$$\frac{\partial\ ^{r}\Phi}{\partial \boldsymbol{z}}(\boldsymbol{p}, \boldsymbol{z}) = \boldsymbol{0}\ .$$

In addition, there exists $c > 0$ such that for all $\boldsymbol{p} \in \mathbb{R}^n$

$$\mathrm{Im}\,\Phi(\boldsymbol{p}, \boldsymbol{z}(\boldsymbol{p})) \geqslant c\,|\mathrm{Im}\,\boldsymbol{z}(\boldsymbol{p})|^2\ .$$

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Phase space Weyl operator

The action of $\widehat{\mathcal{H}} = \mathcal{W}\widehat{H}\mathcal{W}^{-1}$ on the phase space wavefunction Ψ is given in integral form by

$$\widehat{\mathcal{H}}\Psi(\boldsymbol{X}) = \left(\frac{1}{2\pi\hbar}\right)^{2d} \int e^{\frac{i}{\hbar}\boldsymbol{P}\cdot(\boldsymbol{X}-\boldsymbol{Y})} \mathcal{H}(\boldsymbol{X},\boldsymbol{P})\left(\frac{\boldsymbol{X}+\boldsymbol{Y}}{2},\boldsymbol{P}\right)\Psi(\boldsymbol{Y})\, d\boldsymbol{Y}\, d\boldsymbol{P}$$

where the Weyl symbol

$$\mathcal{H}(\boldsymbol{X},\boldsymbol{P}) := H\left(\frac{\boldsymbol{q}}{2}-\boldsymbol{v},\frac{\boldsymbol{p}}{2}+\boldsymbol{u}\right) = H\left(\frac{\boldsymbol{X}}{2} - \mathbf{J}\boldsymbol{P}\right),\ \ \boldsymbol{X} = (\boldsymbol{q},\boldsymbol{p})\,,\, \boldsymbol{P} = (\boldsymbol{u},\boldsymbol{v})$$

of the operator $\widehat{\mathcal{H}}$ is defined on the doubled phase space pswoback

Some phase space geometry

$$L_t = \left\{ \boldsymbol{X} = \boldsymbol{X}_t(\boldsymbol{\alpha}),\ \boldsymbol{P} = \boldsymbol{P}_t(\boldsymbol{\alpha}) = \frac{1}{2}\mathbf{J}\boldsymbol{X}_t(\boldsymbol{\alpha})\ ,\quad \boldsymbol{\alpha} \in \mathbb{R}^d \right\}$$

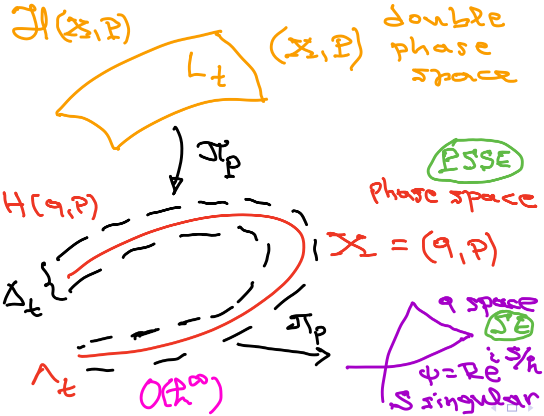
is the solution of the Hamiltonian system

$$\frac{d\boldsymbol{X}}{dt} = \frac{\partial \mathcal{H}}{\partial \boldsymbol{P}}\ ,\quad \frac{d\boldsymbol{P}}{dt} = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{X}}\ ,\quad t \geqslant 0$$

generated by the Hamiltonian $\mathcal{H}(\boldsymbol{X}, \boldsymbol{P}) = H\left(\frac{1}{2}\boldsymbol{X} - \mathbf{J}\boldsymbol{P}\right)$ in double phase space $(\boldsymbol{X} = (\boldsymbol{q}, \boldsymbol{p}), \boldsymbol{P} = (\boldsymbol{u}, \boldsymbol{v})) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$, with initial conditions

$$\boldsymbol{X}|_{t=0} = \boldsymbol{X}_0(\boldsymbol{\alpha}) \in \Lambda_0\ ,\quad \boldsymbol{P}|_{t=0} = \boldsymbol{P}_0(\boldsymbol{\alpha}) := \frac{\partial \theta_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0(\boldsymbol{\alpha})) = \frac{1}{2}\mathbf{J}\boldsymbol{X}_0(\boldsymbol{\alpha})\ ,$$

Some phase space geometry



Some phase space geometry

where Λ_0 is the Lagrangian manifold generated by the phase of the initial data for (SE),

$$\Lambda_0 := \left\{ \boldsymbol{X}_0 = (\boldsymbol{q}, \boldsymbol{p}) \in \mathbb{R}^{2d} \mid \boldsymbol{p} = \frac{\partial S_0}{\partial \boldsymbol{x}}(\boldsymbol{q}) \right\} ,$$

described in appropriately chosen parametrization

$$\boldsymbol{X}_0 = \boldsymbol{X}_0(\boldsymbol{\alpha}) \ , \boldsymbol{\alpha} \in \mathbb{R}^d .$$

It is helpful to observe that the projection of L_t to the phase space is

$$\Lambda_t = \left\{ \boldsymbol{X} = \boldsymbol{X}_t(\boldsymbol{\alpha}) \ , \quad \boldsymbol{\alpha} \in \mathbb{R}^d \right\} ,$$

that is, the image of Λ_0 under the Hamiltonian flow in phase space. psgback