

Semiclassical Theory of the Koopman-van Hove Equation

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Motivation: Can wavefunctions live directly on phase space?

- **Can we represent classical mechanics using the same framework as quantum mechanics?**

B. O. Koopman & J. von Neumann 1932

Bernard Koopman



John von Neumann



- **How do canonical symplectic transformations act on complex (wave) function spaces?**

L. van Hove 1951

Leon van Hove



- **What is the mathematical structure behind quantization?**
Pre-quantization before geometric quantization!

B. Kostant 1972

Bertram Kostant



Motivation: Can wavefunctions live directly on phase space?

- **Is there a classical or semiclassical wavefunction? and, if so, ...**
- **Can we couple quantum & classical systems self-consistently?**
E. C. G. Sudarshan 1976 → D. Bondar, F. Gay-Balmaz, C. Tronci PRSA 2019
- **How can we use quantum computers to simulate classical dynamics?**
I. Joseph PRR 2020, et al POP 2023
- **Complete quantum algorithm for simulating advection-diffusion and Koopman-von Neumann dynamics!**
I. Novikau & I. Joseph 2024 arxiv

EC George Sudarshan



Ceasare Tronci



Ivan Novikau



I. Joseph, Semiclassical Theory and the Koopman-van Hove (KvH) Equation

<https://arxiv.org/abs/2306.01865>

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<https://doi.org/10.1088/1751-8121/ad0533>

- **Can wavefunctions live directly on phase space?**
 - **KvH equation** combines conservation of probability with nontrivial phase evolution in classical phase space
 - **Wigner-Weyl transform** applies to density matrices, not wavefunctions
- **Semiclassical derivation of KvH equation**
 - **Hamilton-Jacobi + Amplitude Transport equations = KvH** on configuration space
 - **Natural Injection:** KvH on configuration space $\rightarrow$ KvH on phase space
 - **Natural Projection:** *semiclassical KvH* on phase space $\rightarrow$ KvH on configuration space
- **KvH eigensystem for harmonic oscillator**
 - For Integrable systems, KvH spectrum = cartesian product of classical & semiclassical spectra
 - JWKB analysis eliminates classical spectrum and leads to **quantization** of the semiclassical spectrum
- **Semiclassical theory has much to say about decoherence!**

Classical dynamics has a natural linear representation on function spaces

- Consider a set of ODEs for $z(\tau) \in \mathbb{R}^{2d}$

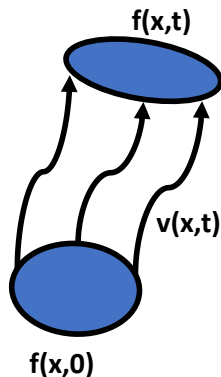
$$dz/d\tau = \mathbf{V}(\tau, z)$$

- Advection of a passive scalar $\theta(\tau, z)$

$$d\theta/d\tau = (\partial_\tau + \mathbf{V} \cdot \nabla) \theta = 0$$

- Along trajectory $z_\tau = \mathcal{T}_\tau(z_0)$, we have

$$\theta_\tau = \mathcal{T}_\tau \theta_0 \quad \theta_\tau(z_\tau) = \theta_0 \circ \mathcal{T}_\tau^{-1} \circ z_\tau = \theta_0(z_0)$$



Classical dynamics has a natural linear representation in terms of conservation of probability

- **Advection of a volume-form: Liouville's equation for probability density function (PDF)**

- Assume $\mathbf{f}(\tau, z) = f(\tau, z) \mathbf{d}z^1 \wedge \mathbf{d}z^2 \cdots \wedge \mathbf{d}z^{2d}$

$$d\mathbf{f}/d\tau := (\partial_\tau + \mathcal{L}_{\mathbf{V}})\mathbf{f} = 0 \quad \longleftrightarrow \quad df/d\tau + f\nabla \cdot \mathbf{V} = (\partial_\tau + \nabla \cdot \mathbf{V})f = 0$$

- **Along trajectory $z_\tau = \mathcal{T}_\tau(z_0)$, we now multiply by the Jacobian**

$$\mathbf{f}_\tau = \mathbf{T}_\tau \mathbf{f}_0 \qquad f_\tau(z_\tau) = \mathcal{J}_\tau^0 f_0(z_0) \qquad \mathcal{J}_\tau^0 = \det \left(\frac{\partial z_0}{\partial z_\tau} \right)$$

The Koopman-von Neumann (KvN) equation evolves probability **amplitudes**

- KvN evolves the square root of a volume form

- Assume $|\psi|^2 = f$ so that $\psi = f^{1/2}e^{i\theta} = \psi(\tau, z)\sqrt{dz^1 \wedge dz^2 \cdots \wedge dz^{2d}}$ and $\psi = f^{1/2}e^{i\theta} \in \mathbb{C}$

$$d\psi/d\tau := (\partial_\tau + \mathcal{L}_V)\psi = 0 \quad \longleftrightarrow$$

$$\boxed{i\hbar \left(d\psi/d\tau + \frac{1}{2}\psi \nabla \cdot \mathbf{V} \right) = i\hbar \left(\partial_\tau + \frac{1}{2}\{\mathbf{V} \cdot \nabla + \nabla \cdot \mathbf{V}\} \right) \psi = 0}$$

- Along trajectory $z_\tau = \mathcal{T}_\tau(z_0)$, we now multiply by sqrt Jacobian

$$\psi_\tau = \mathcal{T}_\tau \psi_0 \qquad \psi_\tau(z_\tau) = (\mathcal{J}_\tau^0)^{1/2} \psi_0(z_0) \qquad \mathcal{J}_\tau^0 = \det \left(\frac{\partial z_0}{\partial z_\tau} \right)$$

The Koopman-van Hove (KvH) equation evolves **wavefunctions** that have phase dynamics

- KvH also evolves the complex phase $\psi = f^{1/2} e^{i\theta}$

- Phase has nontrivial dynamics

$$\hbar d\theta/d\tau = \hbar (\partial_\tau + \mathbf{V} \cdot \nabla) \theta = L(\tau, \mathbf{z})$$

- Feynman's prescription for path integral chooses $L(\tau, \mathbf{z}) = \mathbf{classical Lagrangian}$

$$\hbar d\theta/d\tau = L(\tau, \mathbf{z}) = \mathbf{p} \cdot \nabla_{\mathbf{p}} H(\tau, \mathbf{z}) - H(\tau, \mathbf{z})$$

- Combining phase evolution with Liouville equation for f yields KvH

$$d\psi/d\tau := (\partial_\tau + \mathcal{L}_{\mathbf{V}})\psi = iL\psi/\hbar \quad \longleftrightarrow$$

$$i\hbar \left(d\psi/d\tau + \frac{1}{2}\psi(\nabla \cdot \mathbf{V}) \right) = i\hbar \left(\partial_\tau + \frac{1}{2}\{\mathbf{V} \cdot \nabla + \nabla \cdot \mathbf{V}\} \right) \psi = -L\psi$$

- Does this actually agree with semiclassical theory? $\psi_\tau(z_\tau) = (\mathcal{J}_\tau^0)^{1/2} \psi_0(z_0) e^{i \int_0^\tau L d\tau / \hbar}$

Important Questions!

- Is there a semiclassical derivation of the KvH and/or KvN equations?
- If so, does the physics agree with semiclassical theory?
- How accurate is KvN or KvH?
- What about quantization conditions?
- What about decoherence?

Semiclassical analysis for generalized Schrödinger equation follows JWKB theory

- Consider asymptotic JWKB analysis for generalized Schrödinger equation

$$i\hbar\partial_\tau\psi = \hat{H}(\tau, \hat{x}, \hat{p})\psi$$

- Position $\hat{x} = x \in \mathbb{R}^d$ and momentum $\hat{p} = -i\hbar\partial_x$ operators satisfy CCR: $[\hat{x}, \hat{p}] = i\hbar$
- “Local” JWKB ansatz for wavefunction:

$$\psi = Re^{i\theta} = e^{i(\theta_0 + \epsilon\theta_1 + \epsilon^2\theta_2)} = e^{i\theta_0} R_1 R_2 \dots$$

- Asymptotic expansion: $1 \gg \epsilon$ implies $d\theta_0 \gg d\log R_1 \gg d\log R_2 \dots$
- Lowest order phase defines **classical action** $S = \hbar\theta_0$
- Lowest order approximation to $\hat{p} \log \psi$ defines **classical momentum** $p := \partial_x S = \hbar\partial_x \theta_0$
- Variational principle yields asymptotic JWKB result: $H := \hat{H}(\tau, x, p)$

$$\mathcal{A}[\psi, \psi^\dagger; \tau, x] = \int \psi^\dagger (i\hbar\partial_\tau - \hat{H}) \psi dx d\tau \simeq - \int \psi^\dagger (\partial_\tau S + H) \psi dx d\tau + \dots$$

Semiclassical theory yields Hamilton-Jacobi equation & Hamilton's equations

- At 0th order, we obtain the **Hamilton-Jacobi equation (HJE)** for the phase $\psi = R \exp(i\bar{\theta}/\hbar)$

$$\hbar \partial_\tau \theta = \partial_\tau S = -H(\tau, x, p) \qquad p(\tau, x) := \partial_x S$$

- **Group velocity** derived from stationary phase approximation $dS = p \cdot dx - H d\tau$

$$\dot{x} := dx/d\tau = -\partial_p \partial_\tau S = \partial_p H|_x$$

- **Generalized forces** for evolution of momentum $p = \partial_x S$ derived using chain rule

$$\dot{p} := \frac{d}{d\tau} p(\tau, x) = \partial_\tau p + \dot{x} \cdot \partial_x p = -\partial_x H|_{\tau, p(x)} + \partial_p H|_x \cdot \partial_x p = -\partial_x H|_p$$

- **Infinitesimal HJE:** classical action is driven by the classical Lagrangian L

$$\frac{d}{d\tau} S(\tau, x) = \partial_\tau S + \dot{x} \cdot \partial_x S = -H + \partial_p H|_x \cdot p =: L$$

Semiclassical theory yields a nonlinear KvH equation on **configuration space**

- At 1st order, we obtain a conservation law for probability $f = |\psi|^2 = R^2$

$$df/d\tau = -f(\partial_x \cdot \dot{x}) \quad \longleftrightarrow \quad (\partial_\tau + \partial_x \cdot \dot{x}) f = 0$$

- This implies the amplitude transport equation (ATE) for the amplitude $R = f^{1/2}$

$$dR/d\tau = -\frac{1}{2}R(\partial_x \cdot \dot{x}) \quad \longleftrightarrow \quad \left(\partial_\tau + \frac{1}{2}\{\partial_x \cdot, \dot{x}\}\right) R = 0$$

- Combining HJE and ATE generates the KvH equation ... but on configuration space!

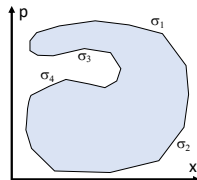
$$\hbar d\psi/d\tau = -\frac{1}{2}\hbar\psi(\partial_x \cdot \dot{x}) + iL\psi \quad \longleftrightarrow \quad \hbar \left(\partial_\tau + \frac{1}{2}\{\partial_x \cdot, \dot{x}\}\right) \psi = iL\psi$$

- Configuration space KvH is **nonlinear in phase dynamics** due to dependance of $\dot{x}(\tau, x, p)$ on $p = \partial_x S$

There is a natural injection of configuration space into **phase space**

- Solving for the trajectories requires solving for both position and momentum given initial data $x(\tau = 0), p(\tau = 0)$

$$\dot{x} = \partial_p H(\tau, x, p) \qquad \dot{p} = -\partial_x H(\tau, x, p)$$



- A general solution of the HJE, $S(\tau, x, J)$, depends on d constants of the motion J

$$\dot{J} := dJ/d\tau = 0$$

$$d/d\tau = \partial_\tau + \dot{z} \cdot \partial_z = \partial_\tau + \dot{x} \cdot \partial_x + \dot{J} \cdot \partial_J = \partial_\tau + \dot{x} \cdot \partial_x$$

- For general solutions, the phase and amplitude are naturally functions of phase space $z = \{x, J\}$ and so is the wavefunction $\psi(\tau, z)$

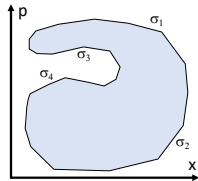
$$d\psi/d\tau = \left(\partial_\tau + \frac{1}{2} \{ \dot{z} \cdot, \partial_z \} \right) \psi = \left(\partial_\tau + \frac{1}{2} \{ \dot{x} \cdot, \partial_x \} \right) \psi = iL\psi/\hbar$$

General asymptotic solution is a superposition of terms in the local asymptotic form

- **Local asymptotic solution has issues near classical turning points, caustics, etc.**
 - Multiple trajectories can have the same final position, when starting from different initial data $x(\tau = 0)$, $p(\tau = 0)$
- **Linearity of Schrödinger's equation $\longrightarrow$ wavefunction = superposition of solutions**
- Thus, we can postulate a superposition of local asymptotic solutions on different branches σ

$$\psi(\tau, x) = \sum_{\sigma} R_{\sigma} e^{iS_{\sigma}/\hbar}$$

- Configuration space HJE is weakly nonlinear: only affects phase $\partial_{\tau} S = -H(\tau, x, \partial_x S)$



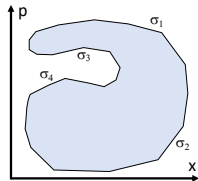
- **If we include the ability to form superpositions in phase space, then we arrive at a natural projection from phase space to configuration space**

$$\psi(\tau, x) = \sum_{\sigma} \int R_{\sigma} e^{iS_{\sigma}/\hbar} d^d p = \sum_{\sigma} \int R_{\sigma} e^{iS_{\sigma}/\hbar} (\det \partial p / \partial J) d^d J$$

A modified semiclassical KvH equation **naturally** projects onto configuration space

- Natural projection from phase space $\longrightarrow$ configuration space

$$\psi(\tau, x) = \int \psi^{\text{SC}}(\tau, x, p) d^d p = \sum_{\sigma} \int \psi_{\sigma}^{\text{SC}}(\tau, x, p) |\det \partial p / \partial J| d^d J$$



- This requires ψ^{SC} to be a volume form in p and the square root of a volume form in x

$$\psi^{\text{SC}}(\tau, \mathbf{z}) = \psi^{\text{SC}} d p^1 \wedge d p^2 \cdots \wedge d p^d \wedge \sqrt{d x^1 \wedge d x^2 \cdots \wedge d x^d}$$

- Modified amplitude transport for $R^{\text{SC}} = |\psi^{\text{SC}}|$

$$dR^{\text{SC}}/d\tau = -R^{\text{SC}} \left(\partial_p \cdot \dot{p} + \frac{1}{2} \partial_x \cdot \dot{x} \right) \longleftrightarrow \left(\partial_{\tau} + \partial_p \cdot \dot{p} + \frac{1}{2} \{ \partial_x \cdot, x \} \right) R^{\text{SC}} = 0$$

- Modified semiclassical KvH equation on phase space

$$\hbar d\psi^{\text{SC}}/d\tau = iL\psi^{\text{SC}} \longleftrightarrow \boxed{i\hbar \left(\partial_{\tau} + \partial_p \cdot \dot{p} + \frac{1}{2} \{ \partial_x \cdot, \dot{x} \} \right) \psi^{\text{SC}} = -L\psi^{\text{SC}}}$$

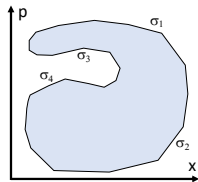
Orthonormality & completeness are different in phase space vs. configuration space

- Configuration space inner product

$$\langle \phi | \psi \rangle = \int \phi^*(x) \psi(x) d^d x$$

- Phase space inner product $z = \{x, p\}$

$$\langle \langle \Phi | \Psi \rangle \rangle = \int \Phi^*(z) \Psi(z) d^{2d} z$$



- Phase space eigenfunctions should still use configuration space inner product
- While we require $\psi(x) \in L^2$, we only require $\psi^{\text{SC}}(z) \in L^1$, e.g. Dirac delta function in J

On phase space, ψ^{SC} vanishes near turning points instead of blowing up

- **Standard KvH** $\psi(\tau, z)$ is continuous in phase space
→ jumps in configuration space

$$R(\tau, z) \sim \text{constant}$$

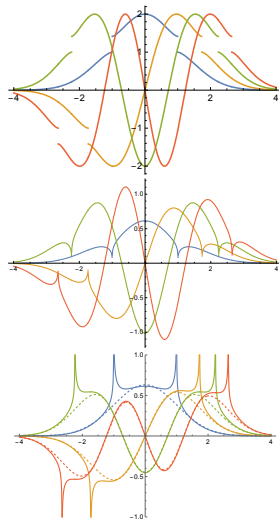
$$R(\tau, x) \sim \text{piecewise continuous}$$

- **Semiclassical KvH** $\psi^{\text{SC}}(\tau, z)$ has $1/\sqrt{\text{Van Vleck det}}$ for the amplitude

$$R^{\text{SC}}(\tau, z) \sim (\det \partial J / \partial p)^{1/2} \sim p^{1/2}$$

- **For JWKB**, $\psi(\tau, x)$, integrating over $d^d p = |\det \partial p / \partial J| d^d J$ multiplies by Van Vleck so the total has $\sqrt{\text{Van Vleck det}}$

$$R(\tau, x) \sim (\det \partial p / \partial J)^{1/2} \sim p^{-1/2}$$



KvH analysis and JWKB analysis can be made to agree, but requires care!

- **Semiclassical analysis has some subtleties**

- **Jeffreys-Wentzel-Kramers-Brillouin (JWKB)** phase matching conditions = boundary conditions at classical turning points & mode coupling points
- **Einstein-Brillouin-Keller (EBK)** quantization: $J/\hbar = n + \mu/4$ where $\mu \in \mathbb{N}$ is the Maslov index
- Tunneling requires extending analysis to complex phase space
- Completeness & orthonormality relations defined in configuration space

- **KvH analysis has both classical and semiclassical parts to the physics**

- Classical spectrum should be eliminated to reproduce JWKB
- JWKB boundary conditions should be applied to get correct phases, Maslov index, & EBK quantization conditions
- Completeness & orthonormality relations usually considered on phase space, but should actually be defined in configuration space!

For integrable systems, the KvH spectrum is complete over phase space

- An integrable system has action-angle coordinates $\dot{J} = 0$ and $\dot{\theta} = \vec{\Omega}(J) = \vec{\partial}_J H(J)$
- Standard KvH eigenfunctions on phase space have the form

$$\phi_{\vec{J}, \vec{m}}(\tau, z) = R_{\vec{J}, \vec{m}} \exp \left(i \left[\vec{m} \cdot (\vec{\theta} - \vec{\Omega} \tau) + S/\hbar \right] \right)$$

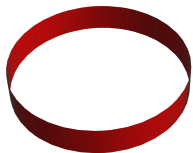
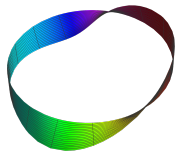
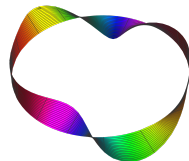
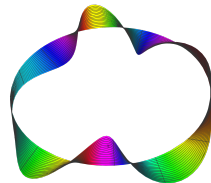
- **Classical spectrum** arises from amplitude transport: $\partial_\tau \psi + \vec{\Omega} \cdot \vec{\partial}_\theta \psi = 0 \quad \longrightarrow \quad \omega = \vec{m} \cdot \vec{\Omega}$
- **Semiclassical spectrum** arises from Hamilton-Jacobi equation: $\hbar \omega = -\partial_\tau S = H(J)$
- KvH eigenfunctions $\phi_{\vec{J}, \vec{m}}(\tau, z)$ are complete over phase space
 - Classical spectrum is complete over θ , while semiclassical spectrum is complete over J
 - The classical & semiclassical spectra are **continuous** due to the ability to choose **non-integer** values of $\vec{m}$

The KvH spectrum is quantized by eliminating classical spectrum!

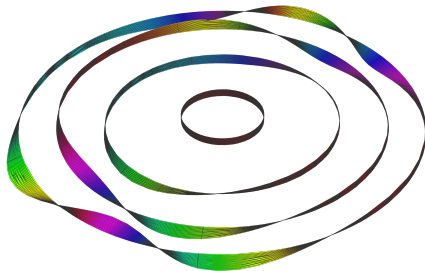
- Phase space KvH eigenfunctions are overcomplete in configuration space
- JWKB theory uses HJE and eliminates ATE:
asymptotic expansion eliminates classical spectrum by requiring $\vec{m} = 0$
 - Eliminates classical spectrum
 - Semiclassical spectrum becomes discrete
 - Eliminates completeness in phase space
 - Retains completeness in configuration space
- Quantization conditions for J demand continuity of the phase around closed loops
 - Standard KvH yields Bohr-Sommerfeld quantization: $J/\hbar = n \in \mathbb{N}$
 - Semiclassical KvH uses JWKB BCs for the phase across turning points which yields
 - Einstein-Brillouin-Keller (EBK) quantization: $J/\hbar = n + \mu/4$ where μ is the Maslov index

Harmonic Oscillator: Standard KvH $\longrightarrow$ Bohr-Sommerfeld quantization

- $n = 0$

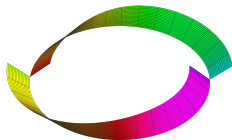
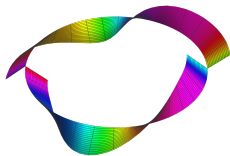
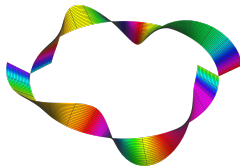
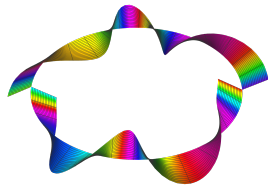
 $n = 1$  $n = 2$  $n = 3$  $\dots$

- Superposition of semiclassical eigenfunctions including $n = 0, \dots, 3$**

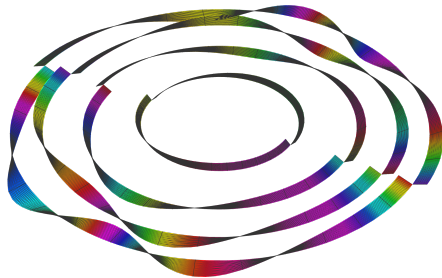


Harmonic Oscillator: Semiclassical KvH $\rightarrow$ Einstein-Brillouin-Keller quantization

- $n = 0$

 $n = 1$  $n = 2$  $n = 3$  $\dots$

- Superposition of semiclassical eigenfunctions including $n = 0, \dots, 3$**



Semiclassical theory provides an explanation for the Copenhagen interpretation

- **Why does classical probability theory arise from quantum theory?**

- Why are superpositions forbidden classically but required quantumly ?

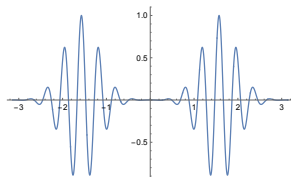
- **Lowest order semiclassical theory only has local observables and local observables $\longrightarrow$ classical probability**

- Lowest order semiclassical theory treats all observables as local in phase space $|z\rangle = |x, p\rangle$
- Born's rule implies that probability is classical in the eigenbasis of the observable $\hat{O} |z\rangle = O(z) |z\rangle$

$$\langle \hat{O} \rangle = \text{Tr}(\hat{O} \hat{\rho}) = \sum_{yz} \langle y | \hat{O} | z \rangle \langle z | \hat{\rho} | y \rangle = \sum_z O(z) \langle z | \hat{\rho} | z \rangle = \sum_z O(z) f(z)$$

- **Semiclassical theory can certainly describe interference effects, but this requires going beyond the lowest order theory to perform “nonlocal operations”**

- JWKB eigenfunctions certainly display interference
- **Copenhagen macro/micro dividing line = size of the wavepackets!**



Why is it so hard to maintain quantum coherence?

Semiclassical theory provides an explanation

- **Answer:** Semiclassical phase is very large & plays an important role in coupled semiclassical-quantum systems

$$\delta S/h \gg 1$$

- **Statistical:** Many moving parts means that small perturbations to the action create order unity changes in the phase

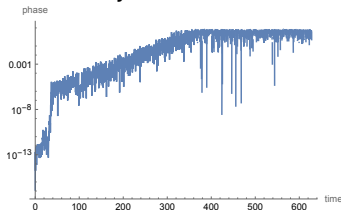
$$\delta S/h \sim \mathcal{O}(1)$$

- **Dynamical:** Chaotic trajectories generate exponential separation in the phase. If $\lambda =$ Lyapunov exponent, then

$$\delta S' \sim \delta S(\tau = 0) \exp(\lambda \tau)$$

- **Collisionless Damping:** decoherence likely controlled by collisionless processes

$|\delta S/h|$ for two chaotic trajectories



Conclusion: Semiclassical Theory of the Koopman-van Hove (KvH) Equation

- **The KvH equation arises from the first two orders of asymptotic JWKB theory**
 - Simply combines the infinitesimal Hamilton-Jacobi equation with the amplitude transport equation
 - **Natural Injection:** from configuration space into phase space linearizes KvH
 - **Natural Projection:** from phase space back to configuration space requires **semiclassical KvH equation**
- **Semiclassical phase space KvH has the same accuracy as configuration space JWKB**
 - Standard KvH is correct to 0th order but not 1st order: Bohr-Sommerfeld quantization
 - Semiclassical KvH is accurate through 1st order including the Maslov index & EBK quantization
 - Like JWKB, loses accuracy near turning points and caustics, etc.
- **Accurate coupling of quantum & semiclassical wavefunctions is now possible**
 - Semiclassical phase play an important role in the dynamics
 - Provides a physical explanation for decoherence

- **Mathematical aspects that require further investigation**

- Is there a symplectically invariant description for KvH? Is there a symplectically invariant asymptotic theory? Lopez& Dodin
- Better understanding of general solutions of the Hamilton-Jacobi equation for finite times
- Tunneling and resonance phenomena: Analytic continuation and complexification of phase space

- **Goal: Self-consistent coupling of quantum and semiclassical systems**

- Zeroth order theory developed by Bondar, Gay-Balmaz, Tronci PRSA 2019 requires first order corrections in order to achieve semiclassical accuracy
- Self-consistent theory accurate to first order developed by Littlejohn & Flynn in early 1990's
- Extended by Dodin, Ruiz, & Fu over last decade to include accurate spin-orbit coupling effects

- **Can phase space & configuration space inner products agree with each other?**
Sqrt delta function $\delta^{1/2}(z)$
- **Tunneling & Resonances:** Analytic continuation of phase space
- **Multicomponent wavefunctions = quantum-classical coupling:**
Mode Coupling, Spin-Orbit Coupling, Quantum measurement theory