Semiclassical Propagation of Wavepackets

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Plan of the talk

- Introduction
- WKB for wavepackets (heuristic)
- WKB (rigorous)
- Semiclassical propagation of Wigner functions
- Perspectives

Introduction

Gaussian wavepackets in semiclassical regimes

Quantum-to-classical transition

Environment induced decoherence
Zurek, Paz, Habib, Bhattacharya,..., Davidovich
ARR Carvalho

Continuous quantum measurements
Sundaram, Jacobs, ...

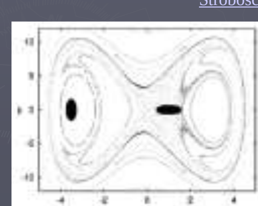
One example from EID

Monteoliva-Paz
PRL00, PRE01

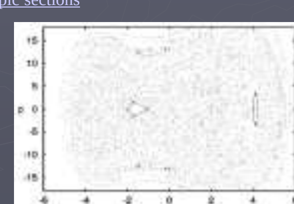
Duffing oscillator

$$H_0(x,p,t)=\frac{p^2}{2m}-bx^2+\frac{x^4}{64a}+\varepsilon x\cos(\omega t)$$ + diffusive reservoir

Stroboscopic sections



mixed



mostly chaotic

Decoherence rate for wavepackets

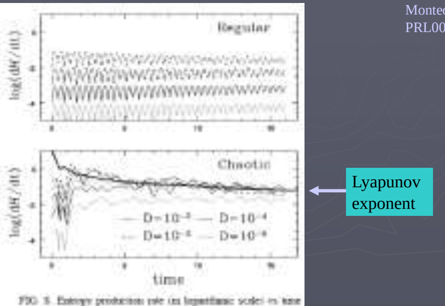


FIG. 5. Entropy production rate (in logarithmic scale) vs time (in units of the driving period). The bold curve is the (time dependent) Lyapunov exponent. The linear dependence of the rate on D

Monteoliva-Paz
PRL00, PRE01

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Zurek-Paz explanation

a rate which depends on the diffusion constant D. However, for chaotic states the rate should become independent of D and should be fixed by the Lyapunov exponent. The origin of this D-independent phase can be understood using a simple minded argument (presented first in [3] and later discussed in a more elaborate way in [7]): Chaotic dynamics tends to contract the Wigner function along some directions in phase space competing against diffusion. These two effects may balance each other giving rise to a critical width below which Wigner function cannot contract. This local width should be approximately $\sigma_c^2 = 2D/\lambda$ (being λ the local Lyapunov exponent). Once this critical size has been reached, the contraction stops along the stable direction (the expansion continues along the unstable one, driven by the system's dynamics). When this condition is achieved, entropy grows linearly in time at a D-independent rate fixed by the Lyapunov exponents (see below).

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Wavefunction structure – Closed system

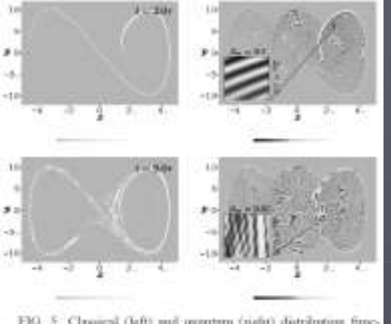

FIG. 5. Classical (left) and quantum (right) distribution functions for four different times. Already, for early times, interference

Monteoliva-Paz
PRE01

Wigner functions

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Diffusive reservoir

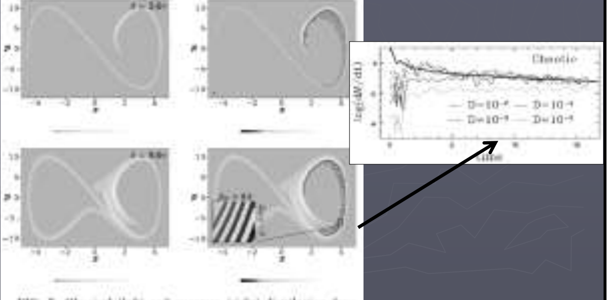

FIG. 7. Classical (left) and quantum (right) distribution functions for the same initial condition as in Fig. 5, at $t = 2\tau$ and $t = 9\tau$, when the system is opened to the action of the environment ($D = 0.01$).

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Goal

Theory for "quantum filaments":

1) $\psi(q,t) \qquad D = 0$

2) $W(q,p,t) \qquad D \neq 0$

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Theories

- Complex TDWKB
  (Heller, ..., de Aguiar)
- Variety of methods in chemical physics
  (Miller, Heller, Herman-Kluk, Kay, Grossmann, Pollack, Shalashilin, ...)
- Real TDWKB ?

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TDWKB theory

TDWKB

$$H(\hat{p},q,t)\,\varphi(q,t) = -i\hbar\frac{\partial}{\partial t}\varphi(q,t)$$

WKB
Van Vleck, PNAS28
Dirac's book
Maslov, 60's-70's
Berry-Balazs, JPA79
Littlejohn, JSP92

Initial wavefunction

$$\varphi(q,t=0) \cong A_0(q)\,e^{iS_0(q)/\hbar}$$

WKB form
$A(q)$, $S(q)$ real
vary slowly

At a later (short) time …

$$\varphi(q,t) \cong A_t(q)\,e^{iS_t(q)/\hbar}$$

primitive WKB

Problem: find $A_t(q)$, $S_t(q)$

Solution

Littlejohn, JSP92

$$H\left(\frac{\partial S}{\partial q}, q, t\right) + \frac{\partial}{\partial t}S(q,t) = 0$$

Hamilton-Jacobi

$$\rho(q,t) = |A(q,t)|^2$$

$$\frac{\partial}{\partial t}\rho(q,t) + \frac{\partial}{\partial q}\left[\rho(q,t)\,\mathrm{v}(q,t)\right] = 0$$

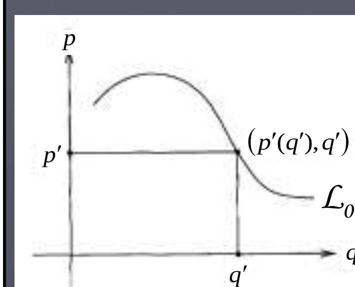
$$\mathrm{v}(q,t) \equiv \frac{\partial}{\partial p}H(p,q,t)\Big|_{p=\frac{\partial S}{\partial q}}$$

transport equation

Geometrical Interpretation

$$\varphi(q,t=0) \cong A_0(q)\,e^{iS_0(q)/\hbar}$$

Initial wavefunction

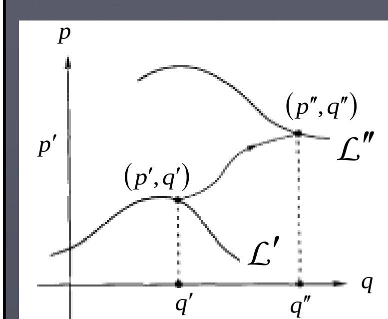


$$p = p_0(q) = \frac{\partial S_0(q)}{\partial q}$$

Lagrangian manifold

$$S_0(q) = \int_{\dots}^{q} p\,dq$$

Solving the Hamilton-Jacobi equation



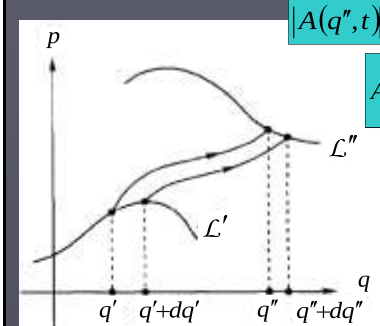
$$S(q'',t'') = \int_{\dots}^{q''} p\,dq$$

new phase

Continuity equation

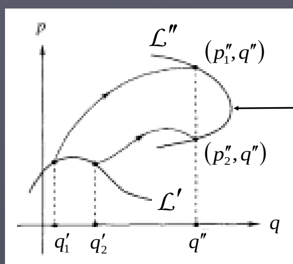
$$|A(q'',t)|^2\,dq'' = |A(q',t)|^2\,dq'$$

$$A(q'',t) = A(q',t)\left|\frac{dq'}{dq''}\right|^{1/2}$$



new amplitude

Caustics



$$A(q'',t) = A(q',t)\left|\frac{dq'}{dq''}\right|^{1/2}$$

multiple branch WKB

$$\varphi(q'',t'') \cong \sum_b A_b(q'',t'')\, e^{iS_b(q'',t'')/\hbar - i\kappa_b \pi/2}$$

Applying TDWKB to Gaussian wavepackets

$$\varphi_0(q) \propto e^{-q^2/4\sigma^2} \equiv A_0(q)\; e^{iS_0(q)/\hbar}$$

$$\sigma \propto \sqrt{\hbar}$$

amplitude "not smooth"!

$$O(1) \;\; vs \;\; \hbar \frac{\partial^2 A(q)}{\partial q^2}$$

discarded term is large

End of Introduction

Proposition

1. In closed chaotic systems Gaussian wavepackets eventually evolve into WKB states:

$$\varphi(q'',t'') \cong \sum_b A_b(q'',t'')\, e^{iS_b(q'',t'')/\hbar - i\kappa_b \pi/2}$$

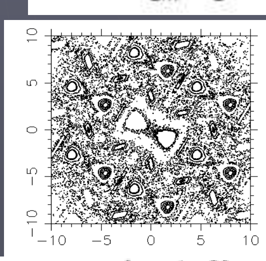
2. Construction (exact)

3. Even if TDWKB fails to propagate Gaussian wavepackets !

Kicked Harmonic Oscillator

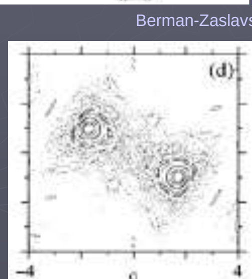
$$H(p,q,t) = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + K\cos(kq) \sum_{n=0}^{\infty} \delta(t - n\tau)$$

Berman-Zaslavsky

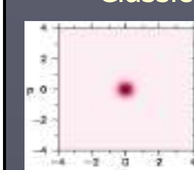


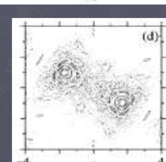
$m = \omega = k = 1,\; K = 2$

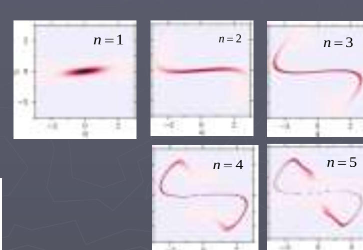
$\tau = T/6$



Classical Dynamics (Liouville)

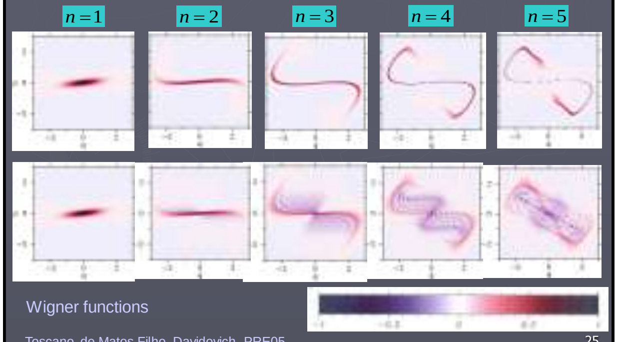






Toscano, de Matos Filho, Davidovich, PRE05

Classical vs. Quantum



Wigner functions

Toscano, de Matos Filho, Davidovich, PRE05

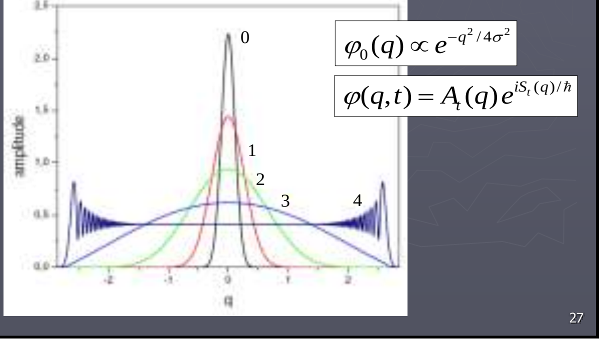
Observation

Chaotic dynamics stretches wavepackets (nonlinearly).

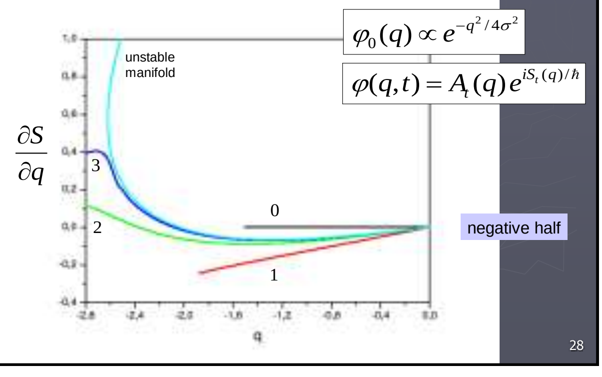
After a certain time (log $\hbar$) a wavepacket becomes a smooth primitive WKB state.

From then on it can be propagated with TDWKB.

Amplitude: exact propagation

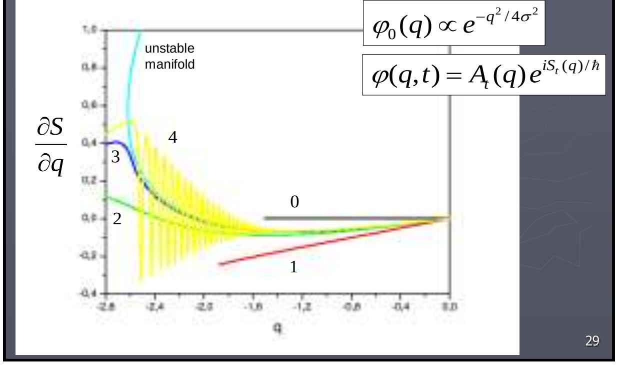


Phase: exact propagation



negative half

Phase: exact propagation



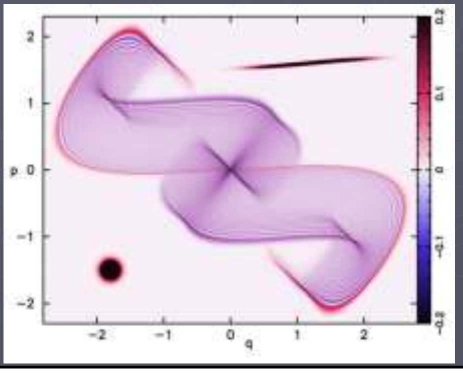
Recipe

Propagate during a short time either
- > numerically,
- > using the linear dynamics (if satisfactory),
- > complex TDWKB,
- > etc

Resume propagation with (real) TDWKB

Wigner function

$\pi\hbar W(p,q)$



Semiclassical (TDWKB) Wigner function

$$\varphi(q'',t'') \cong \sum_b A_b(q'',t'')\, e^{iS_b(q'',t'')/\hbar - i\kappa_b\pi/2}$$

$$W(p,q) = \frac{1}{\pi\hbar}\int d\xi\, \varphi^*(q-\xi/2)\,\varphi(q+\xi/2)\, e^{-ip\xi/\hbar}$$

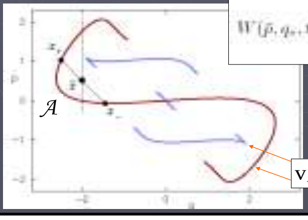
stationary phase

Semiclassical Wigner function

$$W(\bar p,\bar q,t) = \frac{2\sqrt{2}}{\sqrt{\pi\hbar}} A_0(q_+)A_0(q_-)\frac{\cos(\mathcal{A}/\hbar - \pi/4)}{\sqrt{|v_+ \wedge v_-|}}.$$

one chord

$\bar x = (\bar p, \bar q)$

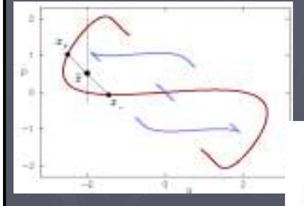


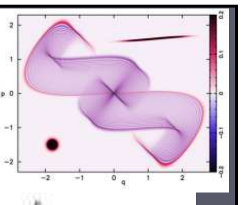
$$W(\bar p, q_*, t) \approx \frac{2A_*^2(q_*)}{(\hbar^2 p_*'')^{1/3}}\mathrm{Ai}\left[-\frac{2(\bar p - p_*)}{(\hbar^2 p_*'')^{1/3}}\right]$$

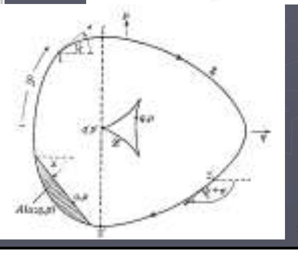
close to the manifold

$v_+ \wedge v_- = 0$

Caustics



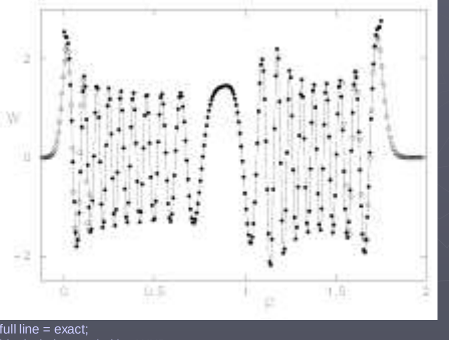




Berry 77

Quantum vs. WKB – Wigner section

Quantum vs. WKB – Wigner section



full line = exact;
black circles = primitive WKB
open circles = Airy transitional approximation

Example II

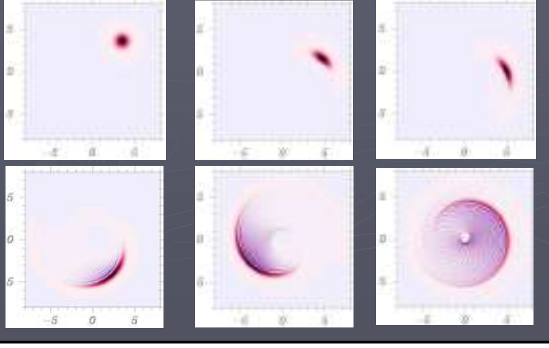
Wavepacket dynamics in the quartic oscillator

Evolution of a coherent state with a Kerr-type Hamiltonian:

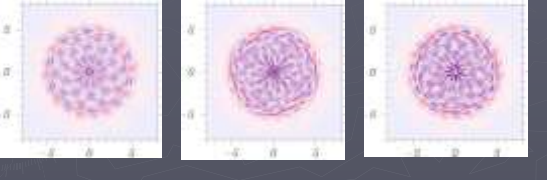
$$\hat{H} = \gamma\hbar^2 \left(\hat{a}^\dagger \hat{a} + \frac{1}{2}\right)^2 \equiv \gamma\hbar^2 \left(\hat{n} + \frac{1}{2}\right)^2$$

- One degree of freedom mechanical oscillator, or
- Single mode of radiation field

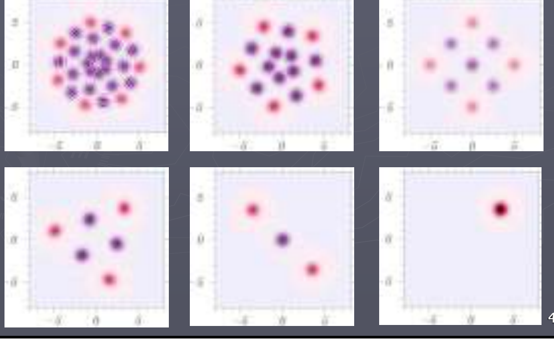
Initial stage – Snapshots – Wigner



Delocalization

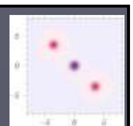


Fractional revivals



Theory and experiments

Cat state generation



Volume 57, Number 1 PHYSICAL REVIEW LETTERS 7 July 1986

Generating Quantum Mechanical Superpositions of Macroscopically Distinguishable States via Amplitude Dispersion

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and
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It is pointed out here that a coherent state propagating through an amplitude dispersive medium will, under suitable conditions, evolve into a quantum superposition of two coherent states 180 degrees out of phase with each other.

New Journal of Physics
The open-access journal for physics

Revivals of quantum wave packets in graphene

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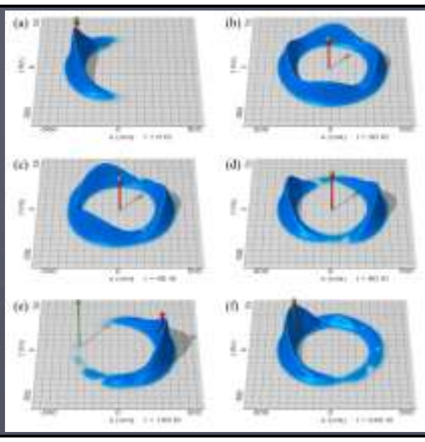
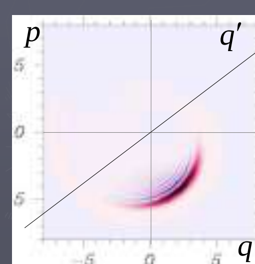
Abstract. We investigate the propagation of wave packets on graphene in a perpendicular magnetic field and the appearance of collapses and revivals in the time evolution of an initially localized wave packet. The wave-packet evolution in graphene differs drastically from the one in an electron gas and shows a rich revival structure similar to the dynamics of highly excited Rydberg states. We present a novel numerical wave-packet propagation scheme in order to solve the effective single-particle Dirac-Hamiltonian of graphene and show how the collapse and revival dynamics is affected by the presence of disorder. Our effective numerical method is of general interest for the solution of the Dirac equation in the presence of potentials and magnetic fields.



Extracting the manifold



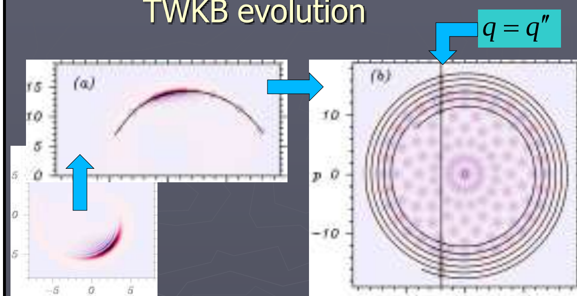
$\psi(q',t) = A(q')\, e^{iS(q')/\hbar}$

Primitive WKB form:
A(q′), S(q′) real,
slowly varying

$p'(q') = \frac{\partial S(q')}{\partial q'}$

support manifold

TWKB evolution



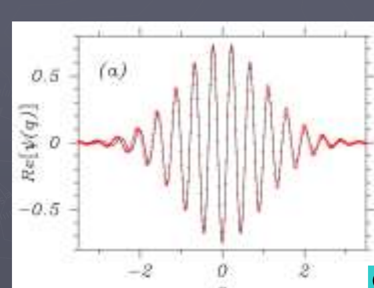
$q = q''$

$t = T_{rev}/16$

[illegible]

Comparison

$t = 4T_{rev}$



$(q_0, p_0) = (0, 1)$

$m, \gamma, \hbar = 1$

line: exact, dots: WKB

Decoherence

Decoherence

$$\dot W = \{H_0, W\}_{PB} + \sum_{n\geq 1} \frac{(-1)^n \hbar^{2n}}{2^{2n}(2n+1)!} \partial_x^{(2n+1)} V \partial_p^{(2n+1)} W$$
$$+ \cancel{2\gamma\partial_p(pW)} + D\partial_{pp}^2 W.$$

$$if \quad \dot W = D\partial_{pp} W$$

$$then \quad \hat\rho(t) = \int d\xi\, g(\xi; D, t)\, \hat T_\xi \hat\rho_0 \hat T_\xi^+ \qquad \xi \in R^2$$

Gaussian channel

phase space translation (Glauber)

average over random translations

Continuous time

$$\dot W = \{H_0, W\}_{PB} + \sum_{n\geq 1} \frac{(-1)^n \hbar^{2n}}{2^{2n}(2n+1)!} \partial_x^{(2n+1)} V \partial_p^{(2n+1)} W$$
$$+ \cancel{2\gamma\partial_p(pW)} + D\partial_{pp}^2 W.$$

Use Lie-Trotter decomposition:

$$\dot W = \{H, W\}_{MB} + D\partial_{pp} W$$

$$W(t+dt) \approx e^{dt D \partial_{pp}}\, e^{dt\{H,\,\}_{MB}} W(t)$$

Stochastic unravelling

- Unitary dynamics – dt
- Random phase space translation – dt
- Iterate
- Repeat for another set of random translations
- Average over translations
  → ensemble of WKB states

Extensions

- Describe initial stretching within WKB
- Develop general semiclassical scheme for Lindblad equation

Correcting WKB

$$i\hbar \frac{\partial}{\partial t}\varphi(q,t) = -\frac{\hbar^2}{2}\Delta\varphi(q,t) + V\varphi(q,t)$$

$$\varphi(q,t) \cong A_t(q)\, e^{iS_t(q)/\hbar}$$

$$-\frac{\partial S}{\partial t}A + i\hbar\frac{\partial A}{\partial t} = \frac{1}{2}|\nabla S|^2 A + VA - i\hbar\nabla S\cdot\nabla A - \frac{i\hbar}{2}\Delta S\, A - \frac{\hbar^2}{2}\Delta A$$

$$\hbar^0: \quad -\frac{\partial S}{\partial t} = \frac{1}{2}|\nabla S|^2 + V \quad \Rightarrow S(q,t)$$

Transport equation for $A(q,t)$

$$i\frac{\partial A}{\partial t} = -i\nabla S\cdot\nabla A - \frac{i}{2}\Delta S\,A - \frac{\hbar}{2}\Delta A$$

$$= (H_0 + H_1)A$$

$\Rightarrow$ $A = T_0\,T_1 A_0$ $\qquad \dfrac{\partial T_1}{\partial t} = -i\,T_0 H_1 T_0^{+}\,T_1$

classical transport (T_0) — quantum dispersion (T_1) — curvilinear Laplacian ($T_0 H_1 T_0^{+}$)

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Transport equation

$$A = T_0\,T_1 A_0 \qquad \frac{\partial T_1}{\partial t} = \frac{i\hbar}{2}T_0\Delta\,T_0^{+}\,T_1$$

Comments:

$T_1 \equiv 1 \quad \Rightarrow \quad WKB$

$T_1 \to 1, \quad t \to \infty$

Idea: approximate T_1 by a Gaussian unitary !?

(Local linearization of the transport dynamics.
In 1D, Laplacian with time dependent factor.)

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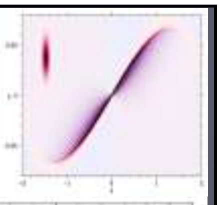
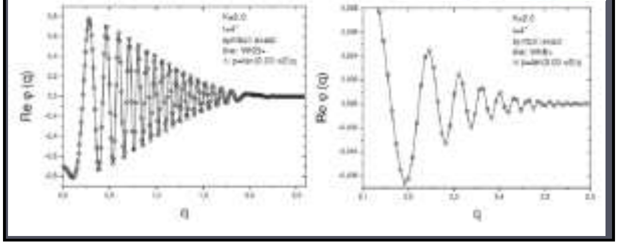
Numerical example (KHO)





Towards a general semiclassical scheme for Lindblad equation

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WKB for mixed propagator

$$W(\beta',t) = \int d\alpha\, K(\beta',\alpha,t)\,\chi(\alpha)$$

Wigner function (W) — mixed propagator (K) — characteristic function (Gaussian) (χ)

$\Downarrow$

WKB theory in double phase-space !?
(Ozorio-Brodier)

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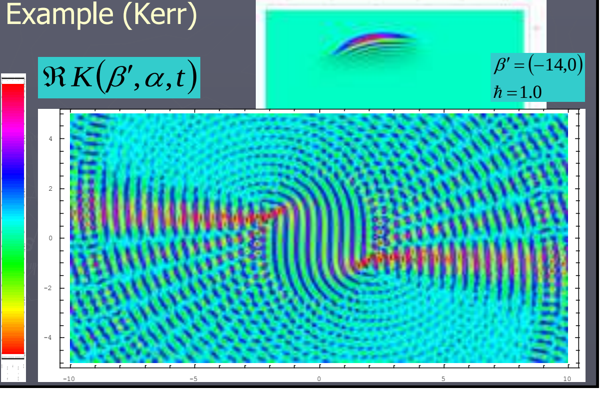
Unitary case – Example (Kerr)

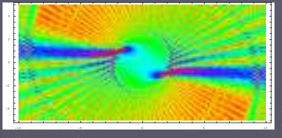
$\Re K(\beta',\alpha,t)$

$\beta' = (-14,0)$

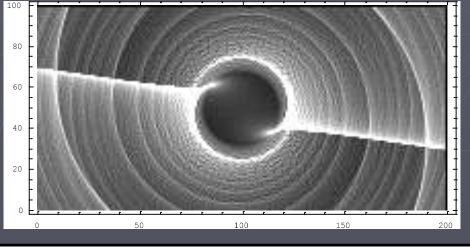
$\hbar = 1.0$



Caustics



quantum amplitude

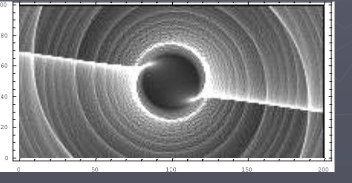


classical

Question

How does the caustic size scale with the relevant parameters?

$$r(t,\beta') >> \sqrt{\hbar} \quad ?$$



Conclusions

References

Semiclassical evolution of Gaussian wavepackets,
R. N. P. Maia, F. Nicacio, R. O. Vallejos, F. Toscano,
Phys. Rev. Lett. 100, 184102 (2008).

Semiclassical description of wavepacket revival,
F. Toscano, R. O. Vallejos, D. Wisniacki
Phys. Rev. E 80, 046218 (2009)

How do wavepackets spread?
R. Schubert, F. Toscano, R. O. Vallejos
preprint, J. Phys. A (2011)?

Semiclassical propagation of Wigner functions,
A. M. Ozorio de Almeida, O. Brodier, F. Toscano, R. O. Vallejos
2011?

Appendix

Explanation

$$\hat{H} = \gamma\hbar^2\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)^2 \equiv \gamma\hbar^2\left(\hat{n} + \frac{1}{2}\right)^2$$

$$\hat{U} = e^{-i\hat{H}\,t/\hbar} = e^{-i\gamma\hbar\left(\hat{n}+\frac{1}{2}\right)^2}$$

$$\hat{U} = \underbrace{e^{-i\gamma\hbar\hat{n}^2 t}}_{!}\;\underbrace{e^{-2i\gamma\hbar\hat{n}t}}_{HO}\;\underbrace{e^{-i\gamma\hbar t/4}}_{phase}$$

II

$$\hat{U}' = e^{-i\gamma\hbar\hat{n}^2 t}$$

revival times

$$\gamma\hbar t = 2\pi\frac{k}{m}$$

project onto HO basis

$$\hat{U}'_{m,k} = e^{-2\pi i\frac{m}{k}\hat{n}^2}$$

$$= \sum_{m=1}^{k} c_m\, e^{-2\pi i\frac{m}{k}\hat{n}}$$

sum of
rotations !