Semiclassical Description of Wavepacket Revival

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Informação Quântica

Laboratoire de Mathématiques et Physique Théorique, Université de Tours, November 5th, 2009

Plan of the talk

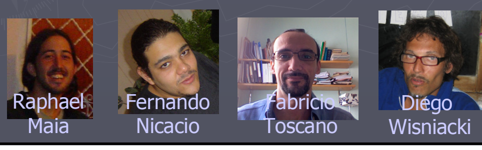
- Introduction
- Approximation #1
- Approximation #2
- Conclusions

Introduction

Related papers

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

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



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

Wigner function

vector in Hilbert space

$$|\psi\rangle \rightarrow W(q,p)$$

real function in phase space; displays classical features

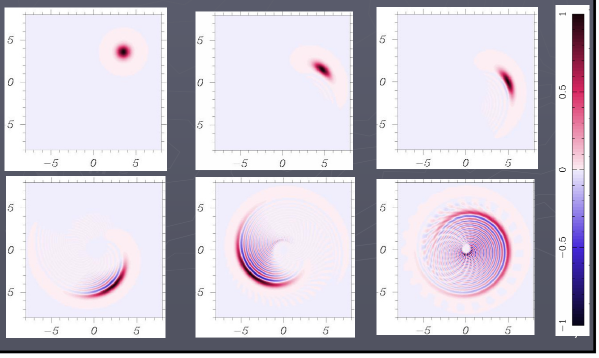
$$W(q,p) = \frac{1}{\pi\hbar}\int dy\, \psi^*(q+y)\,\psi(q-y)\, e^{2ipy/\hbar}$$

Wigner transform

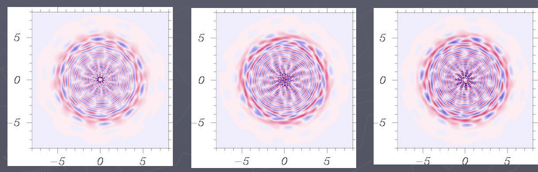
$$W(q,p) = \frac{1}{\pi\hbar}\langle\psi|\hat{R}_{(q,p)}|\psi\rangle$$

average of reflection operator

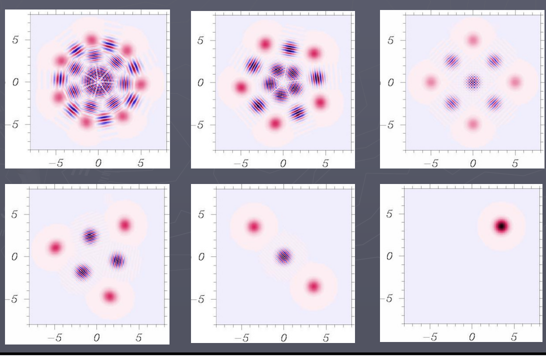
Initial stage – Snapshots – Wigner



Delocalization

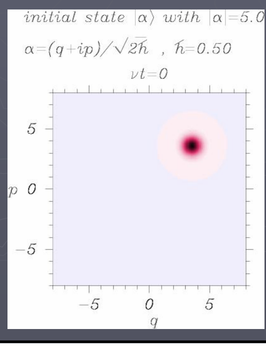


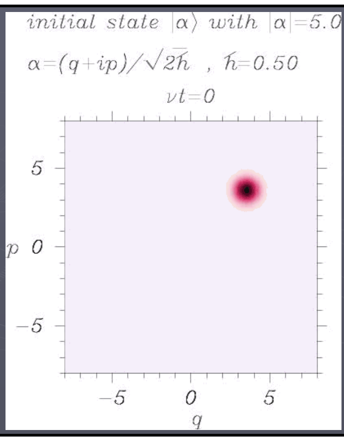
Fractional revivals



Revivals: The Film

by F. Toscano





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

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

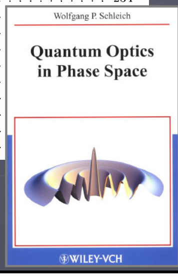
$$\hat{U}'_{m,k} = e^{-2\pi i\frac{m}{k}\hat{n}^2}$$

project onto HO basis

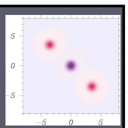
$$= \sum_{m=1}^{k} c_m e^{-2\pi i\frac{m}{k}\hat{n}}$$

sum of rotations !

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

B. Yurke
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
and
D. Stoler
AT&T Bell Laboratories, Whippany, New Jersey 07981

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.

Applications – Example

IOP PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS
J. Phys. B: At. Mol. Opt. Phys. **41** (2008) 074018 (7pp) doi:10.1088/0953-4075/41/7/074018

Selective control of molecular rotation

Sharly Fleischer, I Sh Averbukh and Yehiam Prior
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Online at stacks.iop.org/JPhysB/41/074018

Abstract
We demonstrate selective control over rotational motion of small, linear molecules. By means of sequential excitation of the rotational motion by ultrashort pulses, we first prepare transiently aligned molecules with periodically revived angular distribution. Upon further, properly timed excitation, the rotational energy can be increased or decreased, depending on the exact timing of the second pulse. We show how this approach can be applied for selective rotational control of a single component in a molecular mixture. We discuss this selectivity in

New Journal of Physics
The open-access journal for physics

Revivals of quantum wave packets in graphene

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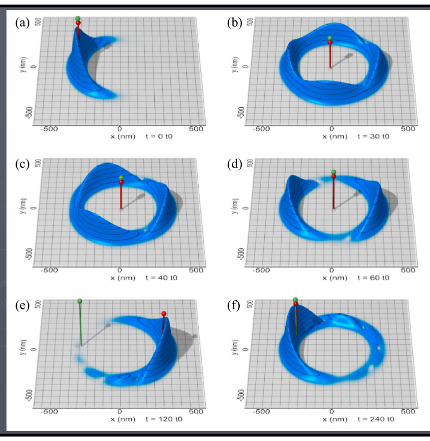
Abstract. We investigate the propagation of wave packets on graphene in a perpendicular magnetic field and the appearance of collapses and revivals in the time evolution of an initially localized wave packet. The wave-packet evolution in graphene differs drastically from the one in an electron gas and 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.



Question

Is it possible to describe wavepacket revivals in the quartic oscillator using primitive semiclassical theories?

- (real) time-dependent WKB → numerical
- Van Vleck propagation → analytical

Context (Quantum Chaos)

Long-time validity of semiclassical dynamics for integrable/chaotic systems

Conjecture:

$$t_{\text{break}} \approx \begin{cases} \hbar^{-1} & \text{integrable} \\ \hbar^{-\mu}, \log\hbar\,? & \text{chaotic} \end{cases} \qquad \left(\hbar \to \frac{\hbar}{S}\right)$$

Focus

- Wavefunction

$$\psi(q,t) = \langle q | \underbrace{\overbrace{e^{-iHt/\hbar}}^{\text{Van Vleck}} | \alpha_0 \rangle}_{\text{WKB}}$$

- Autocorrelation function

$$C(t) = \langle \alpha_0 | e^{-iHt/\hbar} | \alpha_0 \rangle$$

First Part

Semiclassical propagator

Van Vleck-Gutzwiller SC propagator

M. Mallalieu, C. R. Stroud Jr. (1994)
M. S. Barnes, M. Nauenberg, M. Nockleby, S. Tomsovic (1994)
Z. Wang, E. J. Heller (2009)

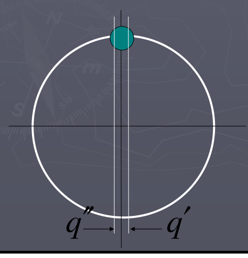
$$K(q'',q',t) \approx \frac{e^{-i\pi/4}}{\sqrt{2\pi\hbar}} \sum_k A_k e^{iS_k(q'',q',t)/\hbar - i\mu_k\pi/2}$$

k : trajectories joining q' with q'' in time t
S : Lagrangian action
μ : Maslov index
A : ...

Feynman Path Integral → Stationary Phase

Correlation function: Trajectories

$$C(t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq''dq'\, \psi_0^*(q'')\,\psi_0(q')\,\underset{\text{semiclassical}}{\underset{\uparrow}{K}}(q'',q',t)$$

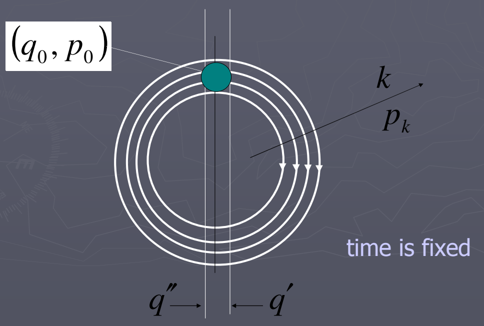


$$\psi_0(q) = (\pi\hbar)^{-1/4} e^{-q^2/2\hbar} e^{ip_0 q/\hbar}.$$

Relevant trajectories are almost periodic

$$q', q'' \approx \sqrt{\hbar}$$

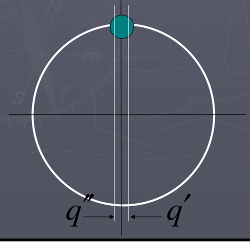
Trajectories (qualitative)



Wave function: Trajectories

$$\psi(q'') = \int_{-\infty}^{\infty} dq' \quad \psi_0(q')\, \underset{\text{semiclassical}}{K(q'', q', t)}$$

$$\psi_0(q) = (\pi\hbar)^{-1/4} e^{-q^2/2\hbar} e^{ip_0 q/\hbar}\,.$$



$q' \approx \sqrt{\hbar}$

$q'' \approx \sqrt{\hbar}$ ⟸ Our choice

Relevant trajectories are almost periodic or "half-periodic"

Ingredients

$$K(q'', q', t) \approx \frac{e^{-i\pi/4}}{\sqrt{2\pi\hbar}} \sum_k A_k e^{iS_k(q'', q', t)/\hbar - i\mu_k \pi/2}$$

$$S_k(q'', q', t) = \int_0^t (p\dot{q} - H)\,dt\,,$$

$$\begin{aligned} q(t) &= \sqrt{2I}\sin[\beta + \omega(I)t]\,, \\ p(t) &= \sqrt{2I}\cos[\beta + \omega(I)t]\,, \end{aligned}$$

classical perturbation theory around (half) periodic trajectories (hbar) ➔ $q', q'' \approx \sqrt{\hbar}$

$$\begin{aligned} S_k &\approx \frac{\pi^2 k^2}{\gamma t} + \sqrt{\frac{2\pi k}{\gamma t}}\,(q'' - q') + \frac{(q'' - q')^2}{8k\pi}\,, \\ A_k &\approx A_k^{(0)} = \frac{1}{\sqrt{4 I_k \gamma t}}\,. \end{aligned}$$

periodic trajectories

Analytical expressions

classical perturbation theory around periodic trajectories

$$C(t) \approx \frac{e^{-i\pi/4}}{\sqrt{2\pi}} \sum_{k=1}^{\infty} e^{i\pi^2 k^2/\gamma\hbar t} e^{-ik\pi} \frac{e^{-(p_k - p_0)^2/a_k \hbar}}{\sqrt{k\, a_k}}$$

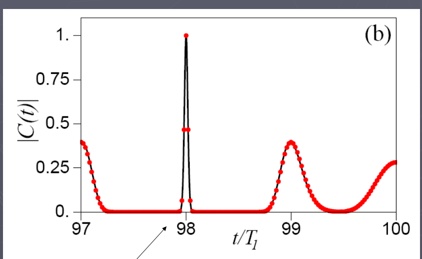
$$\psi(q,t) \approx \cdots$$

$$q \approx \sqrt{\hbar}$$

$$a_k = 1 - \frac{i}{2k\pi}$$

$$p_k = \sqrt{2k\pi/\gamma t}$$

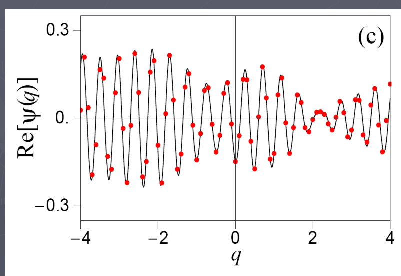
VVG: Numerical comparisons
I. Autocorrelation function

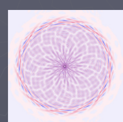


revival!

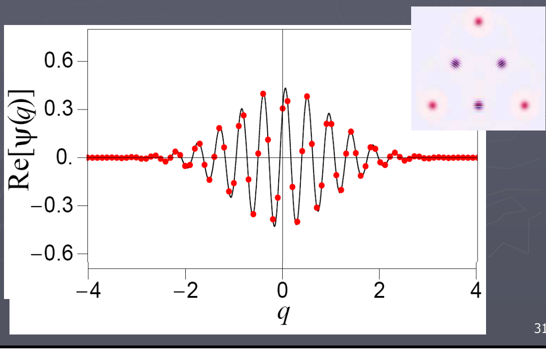
line: exact
dots: semiclassical

VVG: Numerical comparisons
II. Wavefunction





Numerical comparisons: Revival



Analytical comparisons

$$C(t) = e^{-|\alpha_0|^2} \sum_{n=0}^{\infty} \frac{|\alpha_0|^{2n}}{n!} e^{-i\gamma\hbar(n+1/2)^2 t}$$

quantum: plane waves

Poisson transformation!

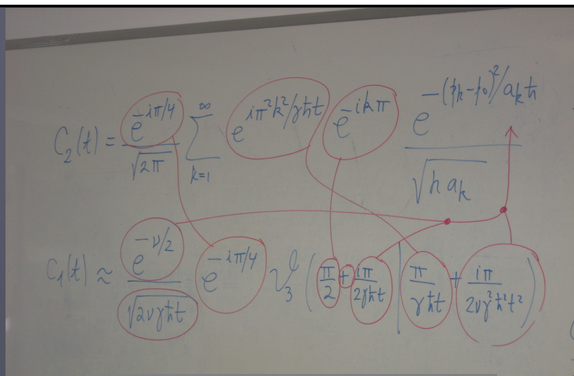
$$C(t) \approx \frac{e^{-i\pi/4}}{\sqrt{2\pi}} \sum_{k=1}^{\infty} e^{i\pi^2 k^2/\gamma\hbar t} e^{-ik\pi} \frac{e^{-(p_k-p_0)^2/a_k\hbar}}{\sqrt{k\, a_k}}$$

semiclassical: wavetrains
→Schleich's book, Ch. 9

$$a_k = 1 - \frac{i}{2k\pi} \qquad p_k = \sqrt{2k\pi/\gamma t}$$

Poisson Sum Formula

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} dx\, f(x)\, e^{-2\pi i k x}$$



long times + Poisson-to-Gaussian →
bounded error for arbitrary times

Second Part

Time-dependent WKB approach

Time dependent WKB theory

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

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

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

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

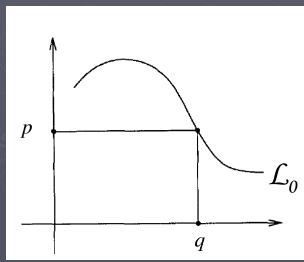
37

Geometrical interpretation

Littlejohn, JSP92

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

initial wavefunction



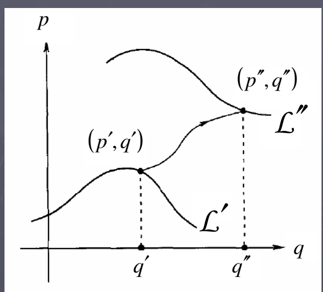
$$p=p_0(q)=\frac{\partial S_0(q)}{\partial q}$$

Lagrangian manifold

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

38

New phase

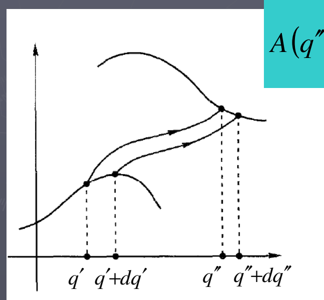


$$S(q'',t'')=\int_{\dots}^{q''}p\,dq$$

39

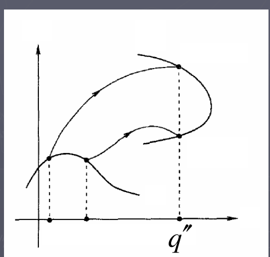
New amplitude

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



40

Multiple solutions

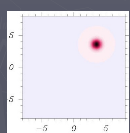


multiple branch WKB

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

41

t-WKB for wavepakets

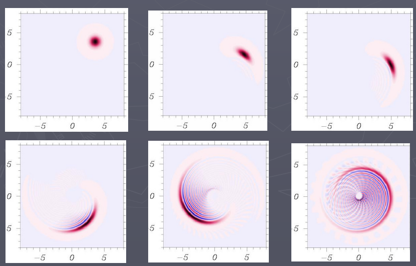


real WKB does not work:
no real manifold associated

42

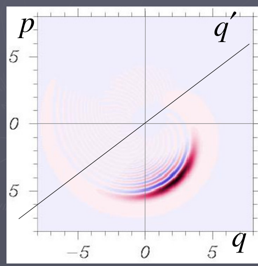
t-WKB for wavepackets: the trick

R. N. P. Maia, F. Nicacio, R. O. Vallejos, F. Toscano (2008)



a real WKB manifold grows !

Extracting the manifold



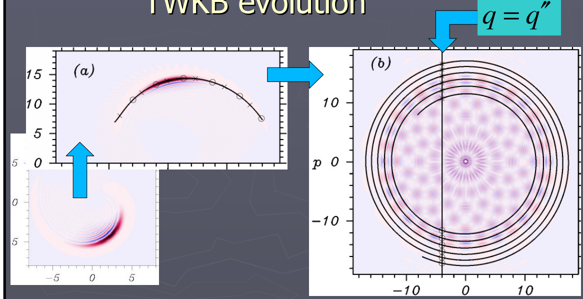
$$\psi(q',t_1) \cong A_1(q')\, e^{iS_1(q')/\hbar}$$

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

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

support manifold

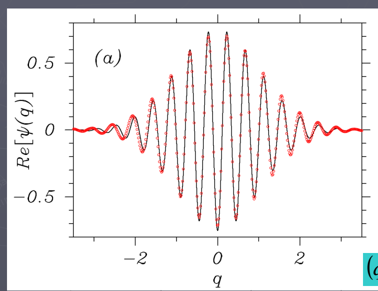
TWKB evolution



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

Comparison

$t = 4T_{\text{rev}}$



$(q_0, p_0) = (0, 14)$

$m, \gamma, \hbar = 1$

line: exact, dots: WKB

Final comments

New results
quartic oscillator – semiclassical

- Van Vleck works for infinite time
- Probably WKB also does;
  States are supported on spiraling classical manifolds —for all times

Perspectives

- Analyse integrable Hamiltonians like

$$\hat{H} = \hat{n}^3,\ f\left(\hat{n}\right), \ldots$$

- Morse & Coulomb potentials

- Wavepacket propagation in quantum open systems ! (Lindblad master equation)

Thanks !