Generalized Gaussian wave packet dynamics: integrable and chaotic systems

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Today's Thread of Logic

1) Gaussian wave packet dynamics
   a) Linearized wave packet dynamics (Heller, 1975-7)
   b) Method of steepest descents - GGWPD (Huber, Heller, Littlejohn, 1988)
      - Saddle points – classical trajectories with complex (q,p)
      - Equivalence to complex, time-dependent WBK
      - Implementation challenges
   c) Off-center real trajectory sums
      - Chaotic - heteroclinic orbits (Tomsovic, Heller, 1991-3)
      - Integrable - shearing orbits (Barnes, Nockleby, Tomsovic, Nauenberg, 1994)
2) Off-center real trajectories $\Longrightarrow$ complex saddle points
   a) Geometry
   b) Newton-Raphson equations
3) Illustration using a simple dynamical system
   a) Kicked rotor
   b) Chaotic regime
   c) Near-integrable regime

Linearized wave packet dynamics

For wave packets

$$\phi_\alpha(\vec{x}) = \left(\frac{2^D \mathrm{Det}(\mathbf{b}_\alpha)}{\pi^D}\right)^{\frac{1}{4}} \mathrm{e}^{-(\vec{x}-\vec{q}_\alpha)^T\cdot\mathbf{b}_\alpha\cdot(\vec{x}-\vec{q}_\alpha)+\frac{i}{\hbar}\vec{p}_\alpha\cdot(\vec{x}-\vec{q}_\alpha)}$$

two typical dynamical quantities of interest are the time propagation of $\phi_\alpha(\vec{x})$ and its overlap with a final state

$$\mathcal{C}_{\beta\alpha}(t) = \int \mathrm{d}\vec{x}\; \phi^*_\beta(\vec{x}) U_{\hat{H}}(t,0)\phi_\alpha(\vec{x})$$

Linearizing the dynamics about the wave packet center generates an approximation depending exclusively on classical mechanical information.

The center of the wave packet, $(\vec{q}_\alpha, \vec{p}_\alpha)$, is the initial condition for the classical trajectory used in the approximation.

Linearized wave packet dynamics (cont.)

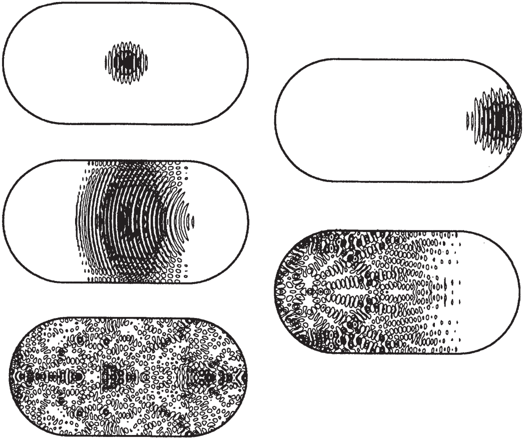
Advantageous properties

- Only requires a single classical trajectory whose initial conditions are known, i.e. no root search. Can propagate, and calculate stabilities and Maslov index.
- Analytical dynamical expressions require only evaluating Gaussian integrals.
- Can be implemented in any number of degrees of freedom. Can be quite accurate.

Limitations

- Effectively, can only work up to an Ehrenfest time scale.
- No way to improve the approximation without introducing many complications.

Wave packet propagation example



Ehrenfest time ends in upper right frame

Method of steepest descents

The ultimate semiclassical approximation

- Exponential arguments are complex functions, thus roots are generally expected to be saddle points.
- Saddle points are classical trajectories with complex initial conditions $(\vec{\mathcal{Q}}_0, \vec{\mathcal{P}}_0)$.
- Essential ambiguity of wave packet center:

$$2\sum_{k=1}^{D} [\mathbf{b}_\alpha]_{jk} \left(\vec{\mathcal{Q}}_\alpha\right)_k + \frac{i}{\hbar}\left(\vec{\mathcal{P}}_\alpha\right)_j = 2\sum_{k=1}^{D} [\mathbf{b}_\alpha]_{jk} \left(\vec{q}_\alpha\right)_k + \frac{i}{\hbar}\left(\vec{p}_\alpha\right)_j$$

  equal to Lagrangian manifold condition $\vec{\mathcal{P}}_0(\vec{\mathcal{Q}}_0) = \nabla \mathcal{S}_0(\vec{\mathcal{Q}}_0)$.
- This approximation called generalized Gaussian wave packet dynamics (GGWPD) turns out to be equivalent to a complexified time-dependent WBK.

Method of steepest descents (cont.)

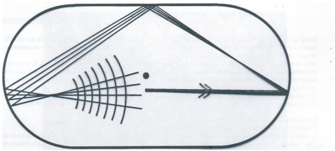
Challenges:

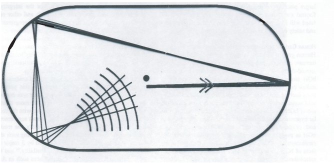
- Requires finding saddle points, which are intersections of two $2D$-dimensional infinite hyperplanes in $4D$-dimensional space. ($D =$ number of degrees of freedom)
- The geometry of complexified classical mechanics is rather complicated. For example, some trajectories lead to infinite momenta in finite times and generate Stokes phenomena.
- The number of saddle points must increase at least linearly with increasing time for integrable systems, and at least exponentially fast for chaotic systems.
- Implemented in a couple of works for a $D = 1$ Morse oscillator, that's it.

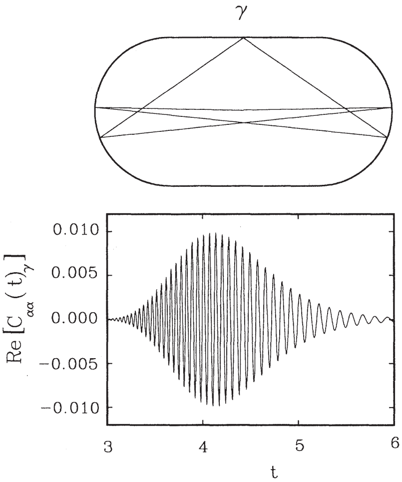
Off-center real trajectories: heteroclinic orbits

- Dynamics in chaotic (K-) systems is generally hyperbolic and there is a convergence zone extendable to infinity along the asymptotes.
- Identify the unstable manifold of the phase point $(\vec{q}_\alpha, \vec{p}_\alpha)$ and the stable manifold of $(\vec{q}_\beta, \vec{p}_\beta)$.
- If "$\hbar$" is small enough, all relevant classical transport follows the unstable manifold away from $(\vec{q}_\alpha, \vec{p}_\alpha)$ and the stable manifold toward $(\vec{q}_\beta, \vec{p}_\beta)$. The complete transport problem is solved as a sum over heteroclinic orbits found at the intersections of the two manifolds.
- Whether one thinks about it this way or not, using a stability analysis around a heteroclinic orbit constructs a saddle that is just a complicated Gaussian integral.

Heteroclinic chirp illustration







Off-center real trajectories: shearing orbits

- Dynamics in integrable systems generally involves shearing locally.
- All transport follows tori. To transport from the phase space region locally surrounding $(\vec{q}_\alpha, \vec{p}_\alpha)$ to the region surrounding $(\vec{q}_\beta, \vec{p}_\beta)$, one needs only to identify those tori that intersect both regions.
- Ideally in action-angle variables, construct the surfaces of constant angle variables with varying actions that intersect the points $(\vec{q}_\alpha, \vec{p}_\alpha)$ and $(\vec{q}_\beta, \vec{p}_\beta)$, respectively.
- Propagate the former and find the intersections with the latter; gives a complete solution to the classical transport problem as a sum over shearing orbits.

Geometrical considerations

A complex saddle point trajectory must satisfy the Lagrangian manifold conditions:

$$
\begin{aligned}
2\sum_{k=1}^{D}[\mathbf{b}_\alpha]_{jk}\left[\vec{\mathcal{Q}}_0-\vec{q}_\alpha\right]_k+\frac{i}{\hbar}\left[\vec{\mathcal{P}}_0-\vec{p}_\alpha\right]_j &= 0\\
2\sum_{k=1}^{D}[\mathbf{b}_\beta]^*_{jk}\left[\vec{\mathcal{Q}}_t-\vec{q}_\beta\right]_k-\frac{i}{\hbar}\left[\vec{\mathcal{P}}_t-\vec{p}_\beta\right]_j &= 0
\end{aligned}
$$

meaning that the initial condition is on the initial manifold and the propagated point is on the final manifold.

This won't be true for any of the real off-center trajectories, but can use stability matrix:

$$
\begin{pmatrix}\delta\vec{\mathcal{P}}_t\\ \delta\vec{\mathcal{Q}}_t\end{pmatrix}=\begin{pmatrix}\mathbf{M}_{11} & \mathbf{M}_{12}\\ \mathbf{M}_{21} & \mathbf{M}_{22}\end{pmatrix}\begin{pmatrix}\delta\vec{\mathcal{P}}_0\\ \delta\vec{\mathcal{Q}}_0\end{pmatrix}
$$

Newton-Raphson Scheme

This generates the Newton-Raphson Scheme (after some algebra):

$$
\begin{aligned}
-\left[\vec{\mathcal{C}}_0\right]_j &= 2\sum_{k=1}^{D}[\mathbf{b}_\alpha]_{jk}\left[\delta\vec{\mathcal{Q}}_0\right]_k + \frac{i}{\hbar}\left[\delta\vec{\mathcal{P}}_0\right]_j \\
-\left[\vec{\mathcal{C}}_t\right]_j &= 2\sum_{k=1}^{D}[\mathbf{b}_\beta]^*_{jk}\left[\mathbf{M_{21}}\delta\vec{\mathcal{P}}_0 + \mathbf{M_{22}}\delta\vec{\mathcal{Q}}_0\right]_k + \\
&\quad \frac{i}{\hbar}\left[\mathbf{M_{11}}\delta\vec{\mathcal{P}}_0 + \mathbf{M_{12}}\delta\vec{\mathcal{Q}}_0\right]_j
\end{aligned}
$$

These equations are used iteratively. The first time through, they give a complex deviation to the off-center real trajectory in either the shearing or heteroclinic trajectory sums.

The Kicked Rotor

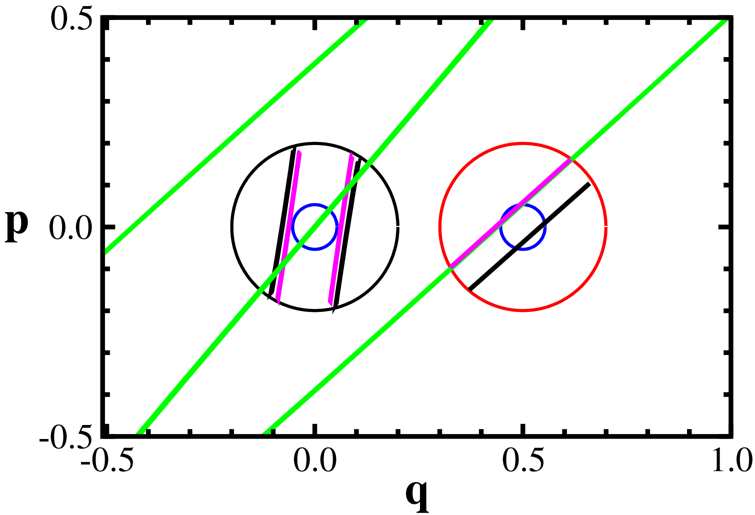
The classical Hamiltonian and mapping equations:

$$\begin{aligned} H &= \frac{p^2}{2} - \frac{K}{4\pi^2} \cos\left(2\pi q\right) \sum_{n=-\infty}^{\infty} \delta\left(t-n\right) \\ p_{i+1} &= p_i - \frac{K}{2\pi} \sin 2\pi q_i \qquad \text{mod } 1 \\ q_{i+1} &= q_i + p_{i+1} \qquad \text{mod } 1 \end{aligned}$$

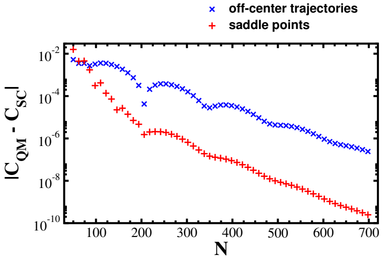
The quantum unitary propagator is:

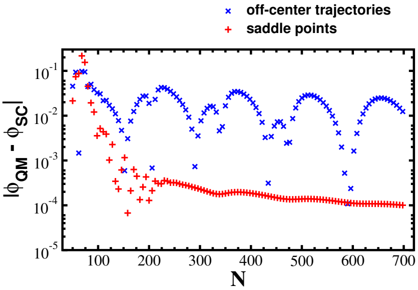
$$U_{nn'} = \frac{1}{N} \exp\left(\frac{iNK}{2\pi} \cos\left(\frac{2\pi(n'+\alpha)}{N}\right)\right) \times \sum_{m=0}^{N-1} \exp\left(-\pi i \frac{(m+\beta)^2}{N} + \frac{2\pi i (m+\beta)(n-n')}{N}\right)$$

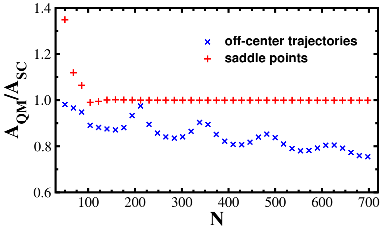
Chaotic Regime



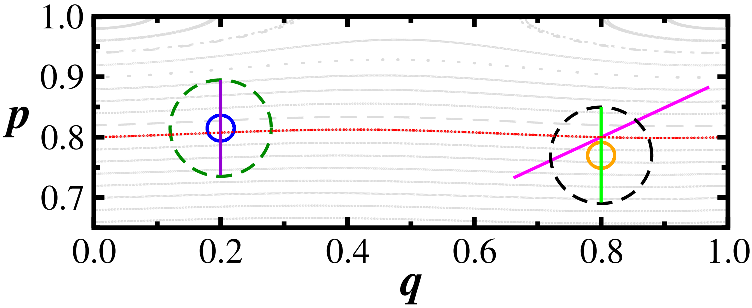
Chaotic Regime (cont.)



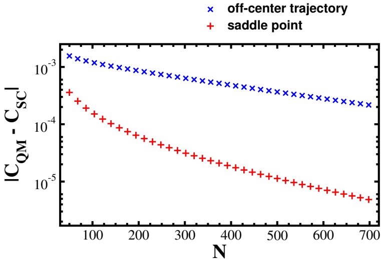


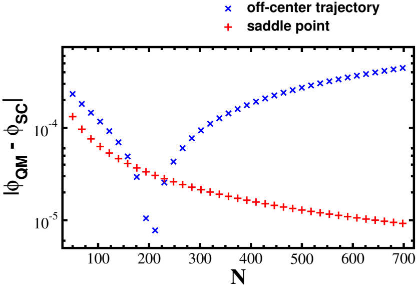


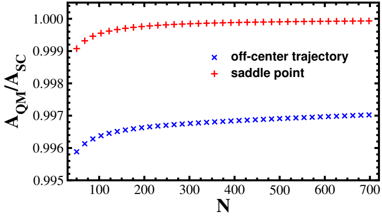
Near-integrable Regime



Near-integrable Regime (cont.)







Conclusions

- GGWPD, the ultimate semiclassical approximation, has never been carried out for anything but a 1D Morse oscillator. Don't forget: the hyperplane Lagrangian manifolds extend to infinity and complex trajectories that run off to infinite momenta in finite times create Stokes surfaces.
- Classical transport for integrable and chaotic systems can be fully solved with shearing trajectory and heteroclinic trajectory sums, respectively.
- Each transport pathway (term in the sum) can be uniquely associated with a complex saddle point trajectory. A Newton-Raphson scheme converges rapidly to it. Thus real off-center trajectories can be used to find all saddle points associated with allowed processes.

Conclusions (cont.)

- Instead of searching the intersection points of two 2D surfaces embedded in a 4D space, GGWPD can be reduced to the intersection points of two D-1 surfaces embedded in a 2D-2 dimensional space followed by a Newton-Raphson scheme.
- Cutting off strongly Gaussian damped contributions is straightforward using the real off-center trajectories and so is avoiding Stokes phenomena.
- Improving implementation of GGWPD reduces to improving implementation of real off-center trajectory methods.
- It would be very interesting to develop an extension that finds saddle points for non-allowed processes.