Quantum Trajectories in Phase Space

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Workshop on Quantum Trajectories
Center for Nonlinear Studies, Los Alamos National Laboratory
Los Alamos, NM, July 27-30, 2008

Classical and Quantum Time Evolution

Classical

Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial q}$$

Quantum

Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Quantum dynamics

Schrödinger Representation

$$\Psi$$

Quantum dynamics

Quantum dynamics in the Wigner representation

Wigner Function

$$\rho_W$$

Quantum dynamics in the Wigner representation

Apologies to Professor Bohm!

Quantum and Classical Liouville Equation

The quantum Liouville equation:

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{\mathcal{H}}, \hat{\rho}]$$

The classical Liouville equation:

$$\frac{\partial \rho}{\partial t} = \{H, \rho\}$$

where the Poisson bracket is

$$\{H, \rho\} = \frac{\partial H}{\partial q}\frac{\partial \rho}{\partial p} - \frac{\partial \rho}{\partial q}\frac{\partial H}{\partial p}$$

These are connected by the Correspondence Principle:

$$[\hat{H}, \hat{\rho}] \rightarrow i\hbar\{\hat{H}, \hat{\rho}\} + \mathcal{O}(\hbar^3)$$

The Wigner Function

A phase space representation of a quantum density operator $\hat{\rho}$:

$$\rho_W(q,p,t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} < q - \tfrac{y}{2} | \hat{\rho}(t) | q + \tfrac{y}{2} > e^{ipy/\hbar}\, dy$$

For a pure state with wave function $\psi(q,t)$ this becomes

$$\rho_W(q,p,t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \psi^*(q + \tfrac{y}{2}, t)\psi(q - \tfrac{y}{2}, t) e^{ipy/\hbar}\, dy$$

Wigner Function Equation of Motion

The quantum Liouville equation again:

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = [\hat{\mathcal{H}}, \hat{\rho}]$$

After some algebra, the Wigner transform the Liouville equation can be written as

$$\frac{\partial\rho_W}{\partial t} = -\frac{p}{m}\frac{\partial\rho_W}{\partial q} + \int_{-\infty}^{\infty} J(q, p-\xi)\rho_W(q,\xi,t)d\xi$$

where

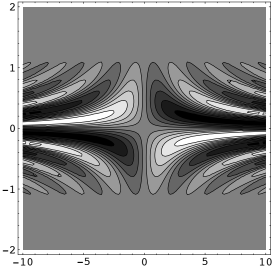
$$J(q,\eta) = \frac{i}{2\pi\hbar^2}\int_{-\infty}^{\infty}\left[V(q+\tfrac{y}{2}) - V(q-\tfrac{y}{2})\right]e^{-i\eta y/\hbar}\,dy$$

Expression for the Kernel $J(q, \eta)$

The kernel can be evaluated to give

$$J(q, \eta) = \frac{4}{\hbar^2} \mathrm{Im} \left(\hat{V}(2\eta/\hbar) e^{-2i\eta q/\hbar} \right)$$

The result for a Gaussian barrier:



Wigner Function Equation of Motion

For a $V(q)$ with a power series expansion $J(q,p)$ becomes

$$J(q,p) = -V'(q)\,\delta'(p) + \frac{\hbar^2}{24} V'''(q)\,\delta'''(p) + \cdots$$

The Wigner function equation of motion is then

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + V'(q)\frac{\partial \rho_W}{\partial p} - \frac{\hbar^2}{24} V'''(q)\frac{\partial^3 \rho_W}{\partial p^3} + \cdots$$

The n^{th} term:

$$\frac{(-1)^n \hbar^{2n}}{2^{2n}(2n+1)!}\,\frac{d^{2n+1}V(q)}{dq^{2n+1}}\,\frac{\partial^{2n+1}\rho_W(q,p)}{\partial p^{2n+1}}$$

Classical Liouville Equation

Classical Continuity in Phase Space

The classical Liouville equation

$$\frac{\partial \rho}{\partial t} = \{H, \rho\}$$

is a continuity equation for incompressible flow in phase space:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0$$

The classical continuity equation:

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{j} = \{H, \rho\}$$

where

$$\vec{\nabla} = \begin{pmatrix} \partial/\partial q \\ \partial/\partial p \end{pmatrix} \qquad \vec{j} = \begin{pmatrix} \partial H/\partial p \\ -\partial H/\partial q \end{pmatrix} \rho \qquad \partial \dot{q}/\partial q + \partial \dot{p}/\partial p = 0$$

The current $\vec{j}$ is then the density times the phase space velocity field

$$\vec{v} = \vec{j}/\rho = \begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} \partial H/\partial p \\ -\partial H/\partial q \end{pmatrix}$$

Recovering Hamilton's equations!

Solving the Classical Liouville Equation Using Trajectories

Represent the continuous function $\rho(q, p, t)$ in phase space by a discrete sampling with N trajectories.

$$\rho(q, p, t) = \frac{1}{N} \sum_{j=1}^{N} \delta(q - q_j(t)) \delta(p - p_j(t))$$

where $q_j(t)$ and $p_j(t)$ is the phase space location of the j^{th} trajectory at time t.

Each member of the ensemble then evolves (independently) under Hamilton's equations.

Quantum Liouville Equation in the Wigner Representation

The Wigner function obeys the phase space equation

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + V'(q)\frac{\partial \rho_W}{\partial p} - \frac{\hbar^2}{24}V'''(q)\frac{\partial^3 \rho_W}{\partial p^3} + \cdots$$

Cast as a continuity equation (even though ρ_W can be negative!):

$$\frac{\partial \rho_W}{\partial t} + \vec{\nabla}\cdot\vec{j}_W = 0$$

which defines a *quantum current* $\vec{j}_W$:

$$\vec{\nabla}\cdot\vec{j}_W = \frac{\partial}{\partial q}\left(\frac{p}{m}\rho_W\right) + \frac{\partial}{\partial p}\left(-V'(q)\rho_W + \frac{\hbar^2}{24}V'''(q)\frac{\partial^2 \rho_W}{\partial p^2} + \cdots\right)$$

Quantum Trajectories

The quantum current then defines a vector field in phase space:

$$\vec{v} = \vec{j}_W / \rho_W$$

These give a generalization of Hamilton's equations:

$$\dot{q} = v_q = \frac{p}{m}$$

$$\dot{p} = v_p = -V'(q) + \frac{\hbar^2}{24} V'''(q) \frac{1}{\rho_W} \frac{\partial^2 \rho_W}{\partial p^2} + \cdots$$

A ρ_W–dependent Bohmesque "quantum force".

Energy Conservation

The quantum trajectories *do not* conserve energy individually.

$$\frac{dH}{dt} = \dot{q}\frac{\partial H}{\partial q} + \dot{p}\frac{\partial H}{\partial p} = \frac{p}{m}\left(\frac{\hbar^2}{24}V'''(q)\frac{1}{\rho}\frac{\partial^2 \rho}{\partial p^2} + \cdots\right)$$

Energy is conserved at the ensemble level.

$$\left\langle \frac{dH}{dt} \right\rangle = \int\int \rho \frac{dH}{dt} dqdp = \int\int \frac{p}{m}\left(\frac{\hbar^2}{24}V'''(q)\frac{\partial^2 \rho}{\partial p^2} + \cdots\right) dqdp = 0$$

This non-conservation of individual trajectory energy allows quantum effects to be modeled.

Entangled Trajectory Molecular Dynamics

For the j^{th} trajectory:

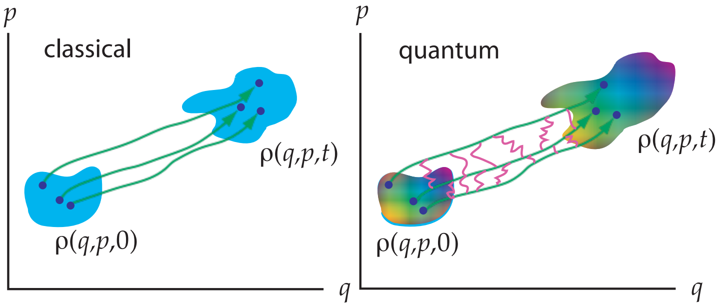
$$\dot{p}_j = -V'(q_j) + \frac{\hbar^2}{24} V'''(q_j) \frac{1}{\rho_W(q_1, q_2, \ldots, p_N)} \frac{\partial^2 \rho_W(q_1, q_2, \ldots, p_N)}{\partial p^2} + \cdots$$

The equations of motion depend not only on the Hamiltonian $H(q, p)$ at each point in phase space, but on the *entire state* ρ_W. This, in turn, depends on the *entire ensemble*.

The members of the ensemble are thus *entangled* with each other. The *statistical independence* of ensemble members in classical mechanics is thus *lost* for quantum trajectories!

Trajectories in Phase Space

Classical and Quantum Trajectories



A Caveat

The Wigner function $\rho_W(q, p, t)$ is real, but can become negative. Can its evolution be represented by an ensemble of trajectories evolving under these equations of motion?

Numerical Methodology: Local Gaussian Ansatz

An approximate *local Gaussian ansatz* for the Wigner function.

$$\rho(q,p) = Ae^{-\beta_q(q-q_k)^2-\beta_p(p-p_k)^2+\gamma(q-q_k)(p-p_k)+\alpha_q(q-q_k)+\alpha_p(p-p_k)}$$

around the point k.

Assumption: ρ is *on average* positive and smooth (formalize later).

The parameters α_q, α_p, β_q, β_p, and γ are determined locally for each member of the ensemble from the moments of the whole ensemble. Then,

$$\frac{1}{\rho}\frac{\partial^2\rho}{\partial p^2} = \alpha_p^2 - 2\beta_p \qquad \frac{1}{\rho}\frac{\partial^4\rho}{\partial p^4} = \alpha_p^4 - 12\alpha_p^2\beta_p + 12\beta_p^2$$

etc.

The Trick: Modified Moments

The generator of modified moments is

$$\tilde{I} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\beta_q \xi^2 - \beta_p \eta^2 + \gamma \xi \eta + \alpha_q \xi + \alpha_p \eta} \, \phi_{h_q, h_p}(\xi, \eta) \, d\xi \, d\eta,$$

where this includes a *local Gaussian window function* ϕ:

$$\phi_{h_q, h_p}(\xi, \eta) = \exp\left(-h_q \xi^2 - h_p \eta^2\right)$$

The *modified* m^{th}, n^{th} moment of ξ, η is then

$$\langle \xi^{\tilde{m}} \eta^n \rangle \equiv \frac{\langle \xi^m \eta^n \phi \rangle}{\langle \phi \rangle} = \frac{\int \int \xi^m \eta^n \phi(\xi, \eta) \rho(\xi, \eta) d\xi d\eta}{\int \int \phi(\xi, \eta) \rho(\xi, \eta) d\xi d\eta}$$

Modified Moments

For ρ a local Gaussian, these moments are generated by derivatives of $\tilde{I}$:

$$\langle \xi^m \tilde{\eta}^n \rangle = \frac{1}{\tilde{I}} \frac{\partial^{(m+n)}}{\partial \alpha_q^m \partial \alpha_p^n} \tilde{I}$$

Generalized variances and correlation:

$$\tilde{\sigma}_\xi^2 = \langle \tilde{\xi^2} \rangle - \langle \tilde{\xi} \rangle^2 \qquad \tilde{\sigma}_\eta^2 = \langle \tilde{\eta^2} \rangle - \langle \tilde{\eta} \rangle^2 \qquad \tilde{\sigma}_{\xi\eta}^2 = \langle \tilde{\xi\eta} \rangle - \langle \tilde{\xi} \rangle \langle \tilde{\eta} \rangle$$

The *original* Gaussian parameters can then be reconstructed:

$$\alpha_p = \frac{\tilde{\sigma_\xi}^2 \langle \tilde{\eta} \rangle - \tilde{\sigma_{\xi\eta}}^2 \langle \tilde{\xi} \rangle}{\tilde{\sigma_\xi}^2 \tilde{\sigma_\eta}^2 - \tilde{\sigma_{\xi\eta}}^4} \qquad \beta_p = \frac{\tilde{\sigma_\xi}^2}{2(\tilde{\sigma_\xi}^2 \tilde{\sigma_\eta}^2 - \tilde{\sigma_{\xi\eta}}^4)} - h_p$$

etc.

Modified Moments from Ensemble

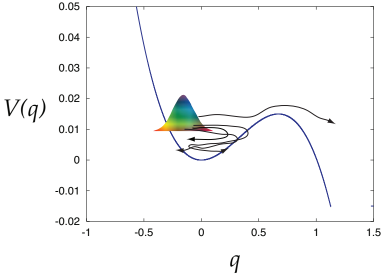
The required modified moments can be calculated easily from the evolving ensemble:

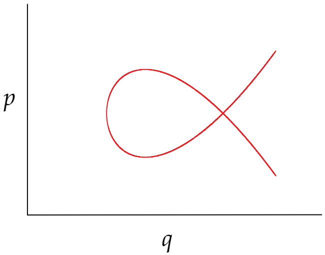
$$\langle \tilde{\xi^m \eta^n} \rangle_k = \frac{\sum_{j=1}^{N} (q_j - q_k)^m (p_j - p_k)^n \phi(q_j - q_k, p_j - p_k)}{\sum_{j=1}^{N} \phi(q_j - q_k, p_j - p_k)}$$

- This employs *local* data when determining the local Gaussian fit.
- Distinct parts of the ensemble will be represented by different Gaussian functions, in general.
- The method is stable–no NaNs.
- In practice, the local window function ϕ is taken to be a minimum uncertainty Gaussian. An implicit Husimi representation (see below).

Tunneling Through a Barrier

Tunneling in a Cubic Potential





ETMD for Cubic Potential

$$V(q) = \frac{1}{2} m \omega_o^2 q^2 - \frac{1}{3} b q^3$$

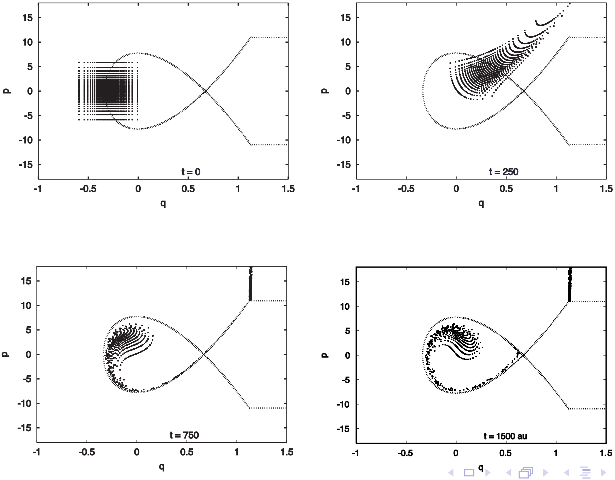
The quantum force on the j^{th} member of the ensemble:

$$\dot{p}_j = -V'(q_j) - \frac{\hbar^2 b}{12} \frac{\partial^2 \rho / \partial p^2 (q_j, p_j)}{\rho(q_j, p_j)}$$

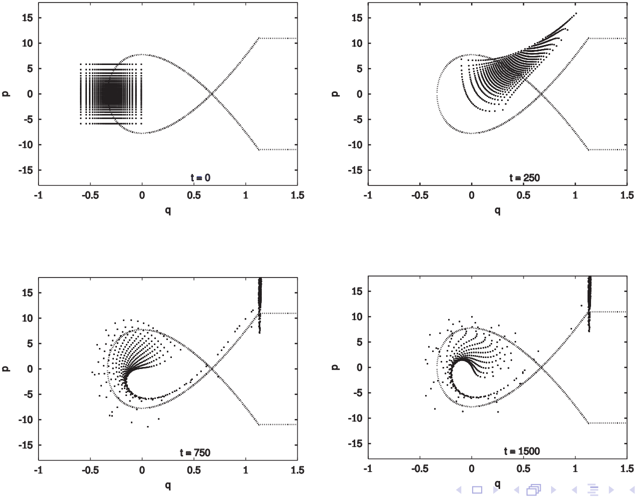
$$\dot{p}_j = -V'(q_j) - \frac{\hbar^2 b}{12} (\alpha_{p,j}^2 - 2\beta_{p,j})$$

$$\alpha_p = \frac{\tilde{\sigma_\xi}^2 \langle \tilde{\eta} \rangle - \tilde{\sigma_{\xi\eta}}^2 \langle \tilde{\xi} \rangle}{\tilde{\sigma_\xi}^2 \tilde{\sigma_\eta}^2 - \tilde{\sigma_{\xi\eta}}^4} \qquad \beta_p = \frac{\tilde{\sigma_\xi}^2}{2(\tilde{\sigma_\xi}^2 \tilde{\sigma_\eta}^2 - \tilde{\sigma_{\xi\eta}}^4)} - h_p$$

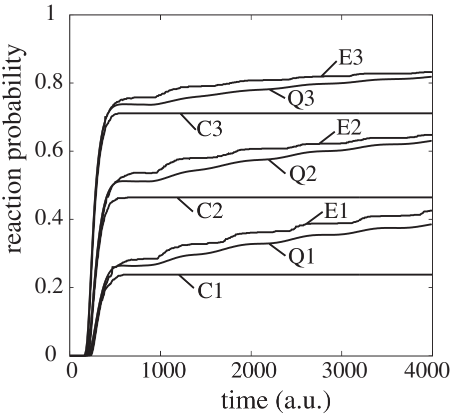
Classical Ensemble in Phase Space



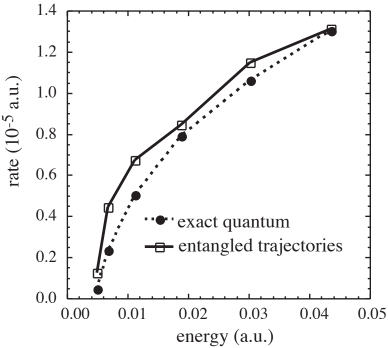
Entangled Ensemble in Phase Space



Reaction Probability vs. Time: Classical and Entangled

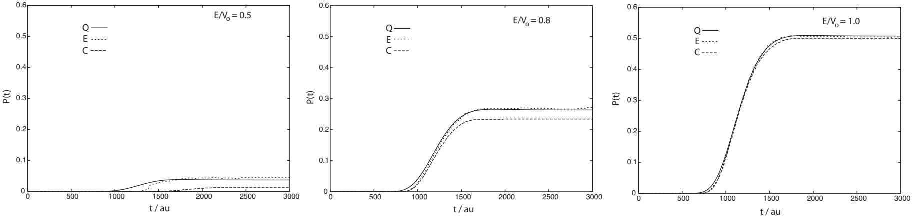


Tunneling Rate vs. Mean Energy



Eckhart Barrier

The method also captures the quantum corrections to tunneling through the Eckhart barrier.



Husimi Distribution: Positive Phase Space Distribution

The Husimi Distribution

The Husimi distribution is a locally-smoothed Wigner function:

$$\rho_H(q,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \rho_W(q',p') e^{-\frac{(q-q')^2}{2\sigma_q^2}} e^{-\frac{(p-p')^2}{2\sigma_p^2}} dq' dp'$$

where the smoothing is over a minimum uncertainty phase space Gaussian,

$$\sigma_q \sigma_p = \frac{\hbar}{2}$$

Operator Formulation of Husimi Distribution

The smoothing can be represented using *smoothing operators* $\hat{Q}$ and $\hat{P}$

$$\hat{Q} = e^{\frac{1}{2}\sigma_q^2 \frac{\partial^2}{\partial q^2}} \qquad \hat{P} = e^{\frac{1}{2}\sigma_p^2 \frac{\partial^2}{\partial p^2}}$$

The Husimi can then be written as a smoothed Wigner function as:

$$\rho_H(q,p) = \hat{Q}\hat{P}\rho_W(q,p)$$

This is related to the interesting identity:

$$e^{-a(x-x')^2} = e^{\frac{1}{4a}\frac{\partial^2}{\partial x^2}}\ \delta(x-x')$$

Smoothing and Unsmoothing

We can consider the inverse *unsmoothing* operators $\hat{Q}^{-2}$ and $\hat{P}^{-1}$:

$$\hat{Q}^{-1} = e^{-\frac{1}{2}\sigma_q^2 \frac{\partial^2}{\partial q^2}} \qquad \hat{P}^{-1} = e^{-\frac{1}{2}\sigma_p^2 \frac{\partial^2}{\partial p^2}}$$

so that the Wigner function can be written (at least formally) as an "unsmoothed" Husimi:

$$\rho_W(q,p) = \hat{Q}^{-1}\hat{P}^{-1}\rho_H(q,p)$$

(Unsmoothing is risky in practice, of course!)

Equation of Motion for the Husimi Distribution

We can then derive an equation of motion for the Husimi distribution.

$$\frac{\partial \rho_H}{\partial t} = -\frac{1}{m}\hat{P}p\hat{P}^{-1}\frac{\partial \rho_H}{\partial q} + \int_{-\infty}^{\infty} \hat{Q}J(q,\eta)\hat{Q}^{-1}\rho_H(q,p+\eta,t)\,d\xi$$

Note that there are no approximations; the Husimi representation provides and *exact* description of quantum dynamics.

Powers of the coordinates and momenta become differential operators:

$$\hat{Q}q\hat{Q}^{-1} = q + \sigma_q^2\,\frac{\partial}{\partial q} \qquad \hat{P}p\hat{P}^{-1} = p + \sigma_p^2\,\frac{\partial}{\partial p}$$

$$\hat{Q}q^2\hat{Q}^{-1} = q^2 + \sigma_q^2 + 2\sigma_q^2 q\frac{\partial}{\partial q} + \sigma_q^4\frac{\partial^2}{\partial q^2}$$

etc.

Equation of Motion for the Husimi Distribution

Wigner function equation of motion:

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + (m\omega_o^2 q - bq^2)\frac{\partial \rho_W}{\partial p} + \frac{\hbar^2 b}{12}\frac{\partial^3 \rho_W}{\partial p^3}$$

Husimi equation of motion:

$$\frac{\partial \rho_H}{\partial t} = -\frac{1}{m}\hat{P}p\hat{P}^{-1}\frac{\partial \rho_H}{\partial q} + (m\omega_o^2\hat{Q}q\hat{Q}^{-1} - b\hat{Q}q^2\hat{Q}^{-1})\frac{\partial \rho_H}{\partial p} + \frac{\hbar^2 b}{12}\frac{\partial^3 \rho_H}{\partial p^3}$$

where

$$\hat{Q}q\hat{Q}^{-1} = q + \sigma_q^2\frac{\partial}{\partial q} \qquad \hat{P}p\hat{P}^{-1} = p + \sigma_p^2\frac{\partial}{\partial p}$$

$$\hat{Q}q^2\hat{Q}^{-1} = q^2 + \sigma_q^2 + 2\sigma_q^2 q\frac{\partial}{\partial q} + \sigma_q^4\frac{\partial^2}{\partial q^2}$$

Continuity in the Husimi Representation

We again invoke continuity, now rigorous for a positive probability distribution.

$$\frac{\partial \rho_H}{\partial t} + \vec{\nabla} \cdot \vec{j}_H = 0$$

Then after a little algebra,

$$\vec{\nabla} \cdot \vec{j}_H = \frac{\partial}{\partial q} \left(\frac{p}{m} \rho_H \right)$$
$$+ \frac{\partial}{\partial p} \left(-V'(q)\rho_H + \frac{\hbar b}{2m\omega_o} \rho_H + \frac{\hbar b q}{m\omega_o} \frac{\partial \rho_H}{\partial q} + \frac{\hbar^2 b}{4m^2\omega_o^2} \frac{\partial^2 \rho_H}{\partial q^2} - \frac{\hbar^2 b}{12} \frac{\partial^2 \rho_H}{\partial p^2} \right)$$

Phase Space Vector Field in the Husimi Representation

The phase space vector field then becomes

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = -V'(q) + \frac{\hbar b}{2m\omega_o} + \frac{\hbar b q}{m\omega_o}\frac{1}{\rho_H}\frac{\partial \rho_H}{\partial q} + \frac{\hbar^2 b}{4m^2\omega_o^2}\frac{1}{\rho_H}\frac{\partial^2 \rho_H}{\partial q^2} - \frac{\hbar^2 b}{12}\frac{1}{\rho_H}\frac{\partial^2 \rho_H}{\partial p^2}$$

The quantum force now contains additional terms not present in the Wigner representation quantum force. This is related to the fact that classical propagation and smoothing *do not commute*.

These equations of motion can be propagated as before.

Free Particle in the Husimi Representation

Because of the smoothing, the free particle motion is nonclassical!

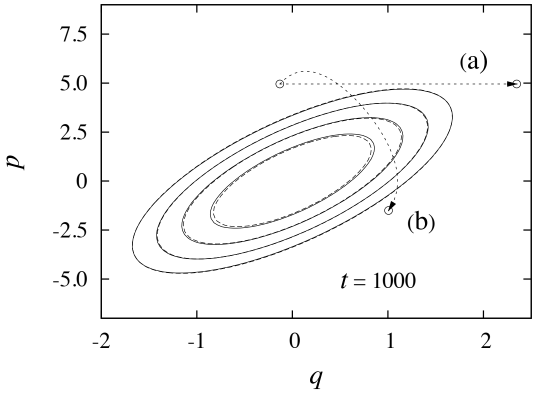
$$\frac{\partial \rho_H}{\partial t} = -\frac{1}{m} \hat{P} p \hat{P}^{-1} \frac{\partial \rho_H}{\partial q}$$

or

$$\frac{\partial \rho_H}{\partial t} = -\frac{1}{m} p \frac{\partial \rho_H}{\partial q} - \frac{\sigma_p^2}{m} \frac{\partial^2 \rho_H}{\partial q \partial p}$$

The extra terms due to noncommutativity of classical time evolution and smoothing.

Free Particle Propagation: Entangled vs. Exact



Solving the Integrodifferential Equation Directly

Methodology, Revisited

The Wigner equation of motion:

$$\frac{\partial \rho_W}{\partial t} = -\frac{p}{m}\frac{\partial \rho_W}{\partial q} + \int_{-\infty}^{\infty} J(q, p-\xi)\rho_W(q,\xi,t)d\xi$$

Write the divergence of the flux directly in this form:

$$\vec{\nabla} \cdot \vec{j}_W = \frac{\partial}{\partial q}\left(\frac{p}{m}\rho_W\right) - \int_{-\infty}^{\infty} J(q, \xi - p)\, \rho_W(q,\xi,t)\, d\xi$$

Solving the Integrodifferential Equation Directly

The momentum component:

$$\frac{\partial}{\partial p} j_{W,p} = -\int_{-\infty}^{\infty} J(q, \xi - p)\, \rho_W(q, \xi, t)\, d\xi$$

or

$$j_{W,p} = -\int_{-\infty}^{\infty} \Theta(q, \xi - p)\, \rho_W(q, \xi, t)\, d\xi$$

where

$$\Theta(q, \xi - p) \equiv \int_{-\infty}^{p} J(q, \xi - z)\, dz$$

Solving the Integrodifferential Equation Directly

This can be written explicitly in terms of the potential $V(q)$:

$$\Theta(q, \xi - p) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \left[V(q + \tfrac{y}{2}) - V(q - \tfrac{y}{2}) \right] \frac{e^{-i(\xi - p)y/\hbar}}{y} \, dy$$

Then the quantum trajectory equations of motion become

$$\dot{q} = \frac{p}{m}$$

$$\dot{p} = -\frac{1}{\rho_W(q,p)} \int \Theta(q, p - \xi) \rho_W(q, \xi) \, d\xi$$

Numerical Approach

To proceed numerically, we write the Wigner function as a superposition of Gaussians:

$$\rho_W(q,p,t) = \frac{1}{N}\sum_{j=1}^{N} \phi(q - q_j(t), p - p_j(t))$$

where

$$\phi(q,p) = \frac{1}{2\pi\sigma_q\sigma_p}\exp\left(-\frac{q^2}{2\sigma_q^2} - \frac{p^2}{2\sigma_p^2}\right)$$

Numerical Approach

After some algebra, we find

$$\dot{p}(q,p) = -\frac{\sum_{j=1}^{N} \phi_q(q-q_j)\Lambda(q-q_j, p-p_j)}{\sum_{j=1}^{N} \phi_q(q-q_j)\phi_p(q-q_j)}$$

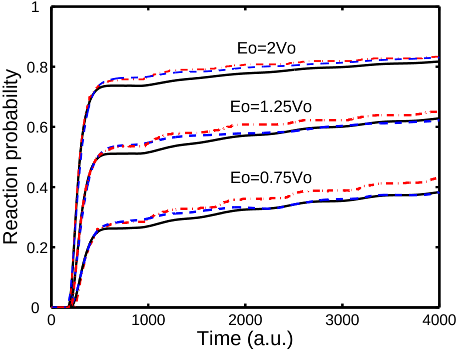
where

$$\Lambda(q-q_j, p-p_j) = \int \frac{V(q+z/2) - V(q-z/2)}{z} \exp\left[i\frac{(p-p_j)z}{\hbar} - \frac{\sigma_p^2 z^2}{2\hbar^2} \right] dz$$

This can be evaluated numerically for a given potential $V(q)$.

Reaction Probability vs. Time: Classical and Entangled

This method gives better long-time agreement for the cubic system:



(Black=exact, red=old method, blue=new method.)

Conclusions

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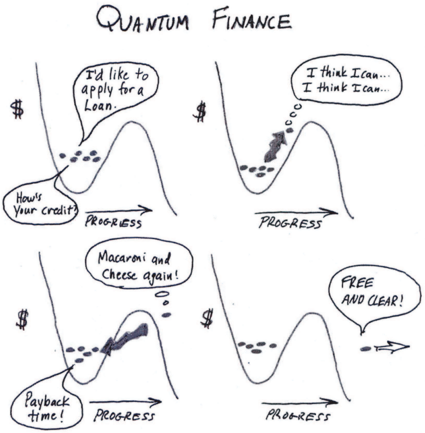
- It is possible to define quantum trajectories in a non-Bohmian phase space context.
- The phase space quantum trajectory formalism can give nearly quantitative results for manifestly quantum mechanical processes such as tunneling in model systems.
- The methodology gives an appealing picture of quantum processes. For instance, tunneling is accomplished by *borrowing*, not by *burrowing*.

Mortgage Crisis in Phase Space?



Acknowledgments

Thanks to:

★ Dr. Arnaldo Donoso (IVIC, Caracas, Venezuela)

Prof. Yujun Zheng (Shandong University)
Jacob Goldsmith
Patrick Hogan
Adam Van Wart

Supported by the
National Science Foundation