Overview:
Dynamics with Quantum Trajectories

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The 'conventional' computational methods: expand wave function in basis set and/or discretize on large Eulerian grids. These are excellent methods IF $N < \text{small number}$. The big drawback: rapid (approaching exponential) growth in computational effort with $N$.

Quantum trajectories lead to a computational framework for SOLVING the TDSE which is qualitatively different from the conventional approaches.

**General Goals in Quantum Dynamics**

1. Solve the time-dependent Schrödinger equation
2. Analyze and interpret the solution

1. Solve

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(x_1, \ldots, x_N, t) \right\} \Psi(x_1, \ldots, x_N, t) = i\hbar \frac{\partial \Psi(x_1, \ldots, x_N, t)}{\partial t}$$

Solve for the complex-valued wave function $\Psi(x_1, \ldots, x_N, t > 0)$

Multi-dimensional and/or Multi-particle system

Quantum trajectories lead to a computational framework for SOLVING the TDSE which is qualitatively different from the conventional approaches.

2. Analyze and Interpret

Quantum trajectories provide a conceptual model which leads to 'classical-like' insights into 'how' quantum processes occur. The resulting 'pictures' may lead to new algorithms for solving complicated physical problems. This has already started to occur!
A. **ANALYTIC...** (Traditional view) The QTs are run using an analytic or a pre-computed wave function, obtained by first solving the TDSE. Primary use: analysis, insight, and interpretation

B. **SYNTHETIC...** The QTs and the wave function are generated simultaneously, ON THE FLY. The QTs are used to SOLVE the TDSE. The Quantum Trajectory Method (1999) was the first viable synthetic approach. The various methods are now significantly better.

**Types of Synthetic QTs...**

A. **Exact** QTs generated by propagating an (large) ensemble of correlated ‘fluid elements’, using the exact equations of motion

B. **Approximate** QTs propagated one-at-a-time (DPM), using approx. equations of motion

**Synthetic QTs may be...**

A. **Traditional Bohmian..** Lagrangian trajectories which move at the flow velocity of the probability fluid

B. **Post-Bohmian..** Non-Lagrangian (ALE) trajectories.. Can be adaptive.. or non-adaptive... these trajectories form Designer Grids

**And these can be run in...**

A. **Real-space**, including Bohm and ALE type QTs running in real-valued phase space

B. **Complex-space**: trajectories running in complex-valued phase space

**Example:** synthetic-approximate-Lagrangian-complex
The analytical approach to quantum trajectories

1. (The traditional viewpoint) Given a pre-computed wave function, compute the velocity from the action function, then compute the trajectory.

\[ \psi(x,t) = R(x,t) e^{iS(x,t)/\hbar} \rightarrow v(x,t) = \frac{1}{m} \frac{\partial S(x,t)}{\partial x} \rightarrow x(t + \Delta t) = x(t) + v(x,t) \cdot \Delta t \]

Note: S determines the trajectories!

Through the phase derivative, the wave function acts as a ‘pilot wave’, guiding the ‘particle’.

Note: for a multi-particle system, these trajectories (and the wave function are running in abstract configuration space, not physical (x,y,z) space. Can we find quantum trajectories in the ‘reduced’ physical space?

2. A new viewpoint: Given a sequence of (experimental or computed) slices of the density for a series of time steps, compute the quantum trajectories. This is the density sampling method, DSM.

\[ \{\rho(x,t_j) = R(x,t_j)^2\}_{j=1}^M \rightarrow x_1(t), x_2(t), x_3(t), ... x_N(t) \]

M density slices \hspace{1cm} N quantum trajectories

Note: R determines the trajectories!
The two slit diffraction experiment

- Density sampling method
- Exact Bohm trajectories

From these ‘experimental’ Bohm trajectories, kinematic quantities can be determined (velocity, acceleration)
Examples of the analytic approach to quantum trajectories

- **Sanz and Miret-Artes**
  - Atom-surface scattering
  - Formation of vortices
  - Collision of Gaussian wave packets (complex space)
  - Interference effects in collision of wave packets (Bohmian real space approach)
- **Sanz and Miret-Artes**
  - Quantum carpets / Talbot effect
- **Sanz and Borondo**
  - Bohmian view on decoherence
- **C. D. Yang**
  - Stationary states / complex space: chaos, electron spin, square barrier tunneling
  - Hydrogenic atoms
- **Bowman**
  - Kicked rotator, harmonic oscillator classical limit of Bohmian mech.
- **Na and Wyatt**
  - Analysis of scattering resonances
- **Chou and Wyatt**
  - Stationary state scattering: Eckart barrier
  - Analysis of streamlines and vortices in complex space
- **Chattaraj**
  - Transition to chaos
  - Henon-Heiles + external field
Routes to synthetic quantum trajectories...

**Non-Stationary states**

**TDSE traditional approach**
- space fixed (x,t) Eulerian coords.
- introduce large grids/basis sets
- unfavorable scaling (exp.)

**Quantum Hydrodynamic Equations (Bohmian mechanics)**
- Equations of motion for QTs in Lagrangian frame
- Quantum effects brought in by quantum potential Q
- Trajectories x(t), p(t)

**Quantum Trajectories**
1. Real space route: Amplitude/phase $\rightarrow$ continuity, QHJE
   - Madelung, Bohm,…
2. Complex space route: exp. form $\rightarrow$ complex QHJE
   - Tannor, Wyatt,…
3. Phase space/Wigner function/moments
   - Takabayasi, Burghardt, Hughes,…
4. Analytic complex trajectories
   - John, Yang, Chu and Wyatt, Sanz and Miret-Artes

**Post-Bohmian (Non-Lagrangian) frame**
- Designer grids, paths x(t)
- Solve moving path transform of quantum hydrodynamic equations
- Wyatt, Hughes, Kendrick,…

**Stationary states**
1. Floydian trajectories and QSHJE
2. Quantum equivalence principle and QSHJE
   - Faraggi and Matone
3. Bipolar counter-propagating wave method
   - Poirier,… (recently extended to non-stat. states)
4. Analytic complex trajectories
   - John, Yang, Chu and Wyatt, Sanz and Miret-Artes
Uni-polar amplitude-phase ansatz for wave function (Madelung 1926):

\[ \Psi(x, t) = R(x, t) e^{iS(x, t)/\hbar} = e^{C(x, t) + iS(x, t)/\hbar} \]

Later, we will introduce a BIPOLAR form for the total wave function (B. Poirier, E. Floyd, A. Faraggi and E. Matone)

R (amplitude) and S (action function) are real-valued... and single-valued.

Substitute into the TDSE. Then separate into two equations (real and imag. parts).

1. \[ \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \frac{1}{m} \nabla S) \]
   - Eulerian frame
   - Trajectories coming soon!

2. \[ \frac{\partial S}{\partial t} = -\frac{1}{2m} \nabla S \cdot \nabla S - V(x, t) - Q_B(x, t) \]

Flow velocity \[ \nu(x) = j(x, t) / \rho(x, t) = \frac{1}{m} \nabla S \]

\[ \rho(x, t) = R(x, t)^2 \] probability density

The Bohm quantum potential is given by \[ Q_B(x, t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \]

The NODE PROBLEM...

(This potential first appeared in eq. 3 in Madelung’s 1926 paper.

The quantum force was explicitly identified in Kennard’s 1928 paper.)
So far...

\[ \frac{\partial \rho}{\partial t} = -\mathbf{r} \cdot \nabla (\rho \mathbf{v}) \]

\[ -\frac{\partial S}{\partial t} = \frac{1}{2} m v^2 + V + Q \]

Coupled system of PDEs in the Eulerian frame

Viewpoints for solving hydrodynamic equations...

**Eulerian Frame**

Coordinate system fixed in space: Monitor watches the fluid go by

**Lagrangian Frame**

Monitor moves along with the fluid velocity ‘go with the flow’

**Intermediate Frame…ALE**

Monitor moves along at ‘arbitrary’ velocity

* Developed at Los Alamos for CFD in early ’70s

Path  \( \mathbf{r}(t) \)  

Trajectory  \( \dot{\mathbf{r}}(t) \)

\[ \mathbf{R} = 0 \]

Use fixed in space time deriv.

\[ \frac{\partial f}{\partial t} \]

Use the ‘moving’ time deriv.

\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + \mathbf{R} \cdot \nabla \]

**Path**  \( \mathbf{r}(t) \)  

**Trajectory**  \( \dot{\mathbf{r}}(t) \)
Equations of motion in the moving (ALE) frame

EOM for quantum trajectories

\[ \frac{dC}{dt} = (\frac{\mathbf{r}}{v}) \cdot \nabla C - \frac{1}{2} \frac{\mathbf{r}}{m} \cdot \nabla v \]
\[ \frac{\mathbf{r}}{v} = \frac{1}{m} \nabla S \]

Continuity
\[ R = e^C \]

Slip velocity
\[ v = \frac{\mathbf{r}}{v} \]

New non-Lagrangian dynamical terms when \[ v \neq \frac{\mathbf{r}}{v} \]

Action
\[ \frac{dS}{dt} = (\frac{\mathbf{r}}{v}) \cdot (m \dot{v}) + \frac{1}{2} m \dot{v} \cdot \nabla v - (V + Q) \]

quantum Lagrangian

Trajectory for each ‘pseudo-particle’ or grid point is specified by \[ \frac{1}{r}(t) \]

In the ALE frame, an algorithm is used to specify the trajectory.
It might be specified ‘in advance’, or adaptively ‘on the fly’.

Also note: spatial 1-st and 2-nd derivatives are needed; this is the ‘DERIVATIVE PROBLEM’
Applications of real-space / Bohmian / ALE methodologies

Mixed quantum-classical dynamics
Burghardt, Parlant, Hughes 2005-

Dynamics of rare gas clusters
Bittner, Maddox, Derrickson, 2003, 2007

Quantum trajectory approach to decoherence
Na and Wyatt

Hybrid QT / fixed grid method
moving boundary truncation method
O+H2, O+HD reactions
Pettey and Wyatt, 2008

Adaptive grids and ALE
Hughes, Wyatt 2002-2003

Reaction dynamics and non-adiabatic transitions
Garaschuk and Rassolov
approximate quantum force 2004
O+H2 reaction 2006
Na+FH reaction 2008

Barrier Transmission / 2D
ALE / adaptive method
Kendrick ALE 2003

Scattering resonances
Kendrick, Bittner, Derrickson 2005

N-dim model for reactive scattering
Kendrick 2004

Reactive scattering: multi-mode
up to 200 oscillators coupled to reaction coordinate
Babyuk, Wyatt 2006
Complex-valued trajectories have been used for decades in semiclassical approaches to barrier tunneling. For example:

- Stine and Marcus (1972)
- Miller and George (1972-1973)
- Heller, Huber, and Littlejohn GGWP (1987)
- Boiron and Lombardi (1998)
- de Aguiar and co-workers

Studies based upon the analytical approach to complex valued quantum trajectories....

The wave function is known in advance of the trajectory propagation. These exact quantum trajectories are the generated from this wave function. Why do this? Analysis, insight, interpretation

- Moncy John, 2002: harmonic oscillator, potential step
- C.-D. Yang, 2005-present: H atom eigen-trajectories, harmonic oscillator
- rectangular barrier tunneling, double slit diffraction, electron spin
- Chou and Wyatt, 2006-present: potential steps (soft and hard), barriers (Eckart and Gaussian), reflection-less potential,
- Wyatt and Rowland, 2008: time-dependent scattering from Gaussian and Eckart barriers
- Sanz and Miret-Artes, 2008: collision of two Gaussian wave packets
Quantum trajectories in complex space

Use QTs to solve the complex-valued quantum Hamilton-Jacobi equation for the complex action function, \( S(z,t) \). These QTs propagate in complex phase space, with complex coordinates and momenta.

The quantum potential in this equation is NOT the same as the Bohm quantum potential. Comparison of these potentials for barrier scattering: Rowland and Wyatt, CPL, published on-line.

Synthetic approach using approximate quantum trajectories

Develop equations of motion for approximate individual quantum trajectories using the derivative propagation method (DPM). Method originally developed for real-valued Bohm type QTs:


The idea: Develop an infinite hierarchy of coupled DEs for \( S \) and its spatial derivatives evaluated along the trajectory.

To make progress, truncate the infinite coupled system at some order. The highest spatial derivative retained has order \( n \).

‘Regional non-locality’ is built in because some of the spatial derivatives of \( S \) are retained.
Bohmian Mechanics with Complex Action:
A New Trajectory-Based Formulation of Quantum Mechanics

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In recent years there has been a resurgence of interest in Bohmian mechanics as a numerical tool because of its local dynamics, which suggest the possibility of significant computational advantages for the simulation of large quantum systems. However, closer inspection of the Bohmian formulation reveals that the nonlocality of quantum mechanics has not disappeared — it has simply been swept under the rug into the quantum force. In this paper we present a new formulation of Bohmian mechanics in which the quantum action, $S$, is taken to be complex. This leads to a single equation for complex $S$, and ultimately complex $x$ and $p$ but there is a reward for this complexification — a significantly higher degree of localization. The quantum force in the new approach vanishes for Gaussian wavepacket dynamics, and its effect on barrier tunneling processes is orders of magnitude lower than that of the classical force. We demonstrate tunneling probabilities that are in virtually perfect agreement with the exact quantum mechanics down to $10^{-7}$ calculated from strictly localized quantum trajectories that do not communicate with their neighbors. The new formulation may have significant implications for fundamental quantum mechanics, ranging from the interpretation of nonlocality to measures of quantum complexity.


Also..
Interference effects in reflected wave packet, 2007-8
Equations of motion for complex-valued QTs

Ansatz: exponential form for the time-dependent wave function
\[ \psi(x, t) = e^{iS(x,t)/\hbar} \]

S is the complex-valued quantum action function.

Substitute into the time-dependent Schrödinger equation to obtain…

\[ -\frac{\partial S}{\partial t} = \frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 + V + \frac{\hbar}{2mi} \frac{\partial^2 S}{\partial x^2} \]

This is the quantum Hamilton-Jacobi equation in the Eulerian frame.

Define

The complex-valued quantum potential, which explicitly brings in quantum effects

\[ Q_C = \frac{\hbar}{2mi} \frac{\partial^2 S}{\partial x^2} \]

\( Q_C \) is NOT the same as the Bohm quantum potential \( Q_B \).

Example: Gaussian wave packet

Usually neglected in semiclassical approaches

Origin of complex-valued dynamics

complex action \( S \) \( \rightarrow \) complex momentum \( p \) \( \rightarrow \) complex coordinate \( z \)

\[ S(z,t) \quad p(z,t) = \frac{\partial S(z,t)}{\partial z} \quad \frac{dz}{dt} = \frac{p(z,t)}{m} \]
How to approximately solve the QHJE using individual trajectories

The quantum HJ equation

\[-\frac{\partial S}{\partial t} = \frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 + \frac{\hbar}{2mi} \frac{\partial^2 S}{\partial x^2} + V\]

Notation for derivs.

\[-\frac{\partial S_0}{\partial t} = \frac{1}{2m} S_1^2 + \frac{\hbar}{2mi} S_2 + V\]

\[S_1 = \frac{\partial S}{\partial x}, \quad S_2 = \frac{\partial^2 S}{\partial x^2}, \ldots\]

Now, start the DPM…(1) take the spatial derivatives

Take the x-derivative

\[-\frac{\partial S_1}{\partial t} = \frac{1}{2m} 2S_1S_2 + \frac{\hbar}{2mi} S_3 + V_1\]

Another x-derivative

\[-\frac{\partial S_2}{\partial t} = \frac{1}{2m} 2(S_1S_3 + S_2^2) + \frac{\hbar}{2mi} S_4 + V_2\]

Keep going, do it n times

\[\frac{\partial S_n}{\partial t} = F(S_1, \ldots S_n, S_{n+1}, S_{n+2})\]

n nonlinear 1-st order DEs for derivatives

Down-coupling to lower terms

Up coupling to ‘higher terms’

Next, convert to the moving frame
(2) Convert these equations of motion to the moving frame

\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x}, \quad v = \frac{dx}{dt} \]

The ‘observer’ moves at ‘arbitrary’ velocity \( v \)

Special case: Lagrangian dynamics \( v_L = \frac{1}{m} S_1 \)

This gives \( \frac{dS_n}{dt} = F(S_1, \ldots, S_n, S_{n+1}, S_{n+2}) + v S_{n+1} \) \( n=0,1,2,\ldots \)

These are the equations of motion in the ALE frame (Los Alamos, early 1970s)

However, we still have an infinite coupled hierarchy of equations. What to do?

(3) Truncation of the infinite hierarchy

Hard truncation: Set the ‘next two’ higher spatial derivs. to zero \( S_{n+1} = 0, \quad S_{n+2} = 0 \)

This leads to the ‘usual’ DPM (derivative propagation method)

Soft truncation: Put in approximations for \( S_{n+1}, \quad S_{n+2} \)

For example, run a small cluster and compute \( S_{n+1}, \quad S_{n+2} \) from \( S_n \)

This leads to CDPM (cluster derivative propagation method); David and Wyatt

In either case, we have a closed system of equations:
(\( n+1 \) coupled DEs for the functions \( S_0, S_1, \ldots, S_n \))
Example: Truncate system at $n = 2$

Equations of motion in the Eulerian frame

Now have 4 equations in the ALE frame

$$\frac{dS_0}{dt} = -\frac{1}{2m} S_1^2 - \left(\frac{h}{2mi}\right) S_2 + V + \nu S_1$$  

$$\frac{dS_1}{dt} = -\frac{1}{m} S_1 S_2 - V_1 + \nu S_2$$  

$$\frac{dS_2}{dt} = -\frac{1}{m} S_2^2 - V_2$$

In the Lagrangian frame

$$\frac{dz}{dt} = \frac{p}{m} = S_1 / m$$

The result: complex classical trajectories launched with quantum initial conditions and carrying approximate quantum phase

This is CVDPM(2)
Quantum Trajectories in Complex Space:
Current work, Developments, Problems, and Questions

Why go complex?
What are the advantages?
Feasibility beyond a few degrees of freedom?
Does it overcome difficulties of running real valued QTs?

Use of low-order approximate quantum trajectories to predict oscillatory structure and nodes: superimpose amplitudes carried by several trajectories
Tannor and co-workers

Density, flux, and continuity equation in complex space

The isochrone problem: find launch points for quantum trajectories
Can circumvent, but this doesn’t solve the problem

Beyond single approximate quantum trajectories:
Soft truncation of DPM, David-Wyatt 2008

More developments on the next 3 overheads
The bipolar counter propagating wave method
Bill Poirier (with G. Parlant, C. Trahan, …)

Original motivation: reconcile profound differences between semiclassical and Bohmian mechanics

Decomposition of the wave function \( \psi = \psi_+ + \psi_- = R_+ e^{iS_+} + R_- e^{iS_-} \)

Each component is smooth, slowly varying in space, and node and interference free, even when the total wave function is wildly oscillatory and loaded with nodes.

Bipolar trajectories, running on two Langangian manifolds, are ‘classical like’ and well behaved.

There are 6 papers in the BP-BP series:

1. Stationary bound states, 2004
2. Stationary scattering states for discontinuous potentials, 2006
3. Stationary scattering states for continuous potentials, 2006
5. 1D wave packet dynamics, 2008

1D stationary states

fixed grid, no trajectories
This approach is based upon an equivalence postulate (similar in content to the equivalence principle of general relativity) rather than on the traditional Copenhagen axioms and interpretation of quantum mechanics.

The EP states: all one particle systems can be connected by coordinate (point) transformations.

The EP implies the QSHJE. This quantum version of the Hamilton–Jacobi equation differs from the classical one by the presence of the quantum potential (a self energy, somewhat like a rest energy). The QSHJE implies the Schrödinger equation with normalization of the wave function, and thus quantization of energy, due to continuity conditions of the quantum potential. The theory, a work in progress, includes a trajectory description of quantum mechanics.

Questions…
Extensions to multi-particle and/or multi-dimensional systems?
Non-stationary systems?
Does the EP ‘imply’ the time dependent Schrodinger equation?
Some Additional Research Areas Involving Quantum Trajectories

- Mixed quantum-classical dynamics
  Bittner, Burghardt, Hughes..

- Bohmian mechanics for the density matrix
  Bittner, Burghardt, Durr, Goldstein,

- Connection of Bohmian mechanics to WKB and semiclassical mechanics
  Goldfarb, Schiff, Tannor
  Sanz, Miret-Artes

- Chaotic dynamics and transition to chaos
  Durr, Goldstein; Wu, Sprung
  Falsaperla, Fonte; Chattaraj

- Quantum trajectories for the Wigner function
  Rowland and Wyatt

- Applications to systems with high dimensionality

- Approximations to the quantum potential
  Garaschuk and Rassolov

New opportunities for you in Bohmian mechanics
Use your expertise in Bohmian mechanics to make $$$ !


Dynamics of price trajectories (of stocks, options, etc) in price phase space
The information wave function evolves according to the financial Schrödinger equation
The quantum force becomes the ‘information force’

Bohmian brain mechanics: de Broglie Pilot-wave theory in cognitive psychology

A. Khrennikov, Classical and quantum mechanics of ideas on decision trees, Biosystems, 56, 95 (2000).

A. Khrennikov, Quantum psychological model of the stock market, 2003

Now for.....

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