Overview:
Dynamics with Quantum Trajectories

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General Goals in Quantum Dynamics

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

1. Solve

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

Multi-dimensional and/or Multi-particle system

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

The 'conventional' computational methods: expand wave function in basis set and/or discretize on large Eulerian grids. These are excellent methods IF N < 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.

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!

Taxonomy of quantum trajectories

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.

$$\psi(x,t) = R(x,t)e^{iS(x,t)/\mathrm{h}} \longrightarrow v(x,t) = \frac{1}{m}\frac{\partial S(x,t)}{\partial x} \longrightarrow x(t+\Delta t) = x(t) + v(x,t)\cdot\Delta t$$

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.

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

M density slices N quantum trajectories

Note: R determines the trajectories!

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Monte Carlo Generation of Bohmian Trajectories

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Abstract. We report on a Monte Carlo method that generates one-dimensional trajectories for Bohm's formulation of quantum mechanics that doesn't involve differentiation or integration of any equations of motion. At each time, $t = n\delta t$ ($n = 1, 2, 3 \ldots$), N particle positions are randomly sampled from the quantum probability density. Trajectories are built from the sorted N sampled positions at each time. These trajectories become the exact Bohm solutions in the limits $N \to \infty$ and $\delta t \to 0$. Higher dimensional problems can be solved by this method for separable wave functions. Several examples are given, including the two-slit experiment.

The Density Sampling Method

Tim Coffey

The wave function is NOT used as input.

Phase information is NOT (directly) involved.

NO derivatives or integrals are evaluated.

There are no equations of motion!

Method is based upon random sampling of an input density.

Is there any physics?

The two slit diffraction experiment

+ Density sampling method
- Exact Bohm trajectories

From these 'experimental' Bohm trajectories, kinematic quantities can be determined (velocity, acceleration)

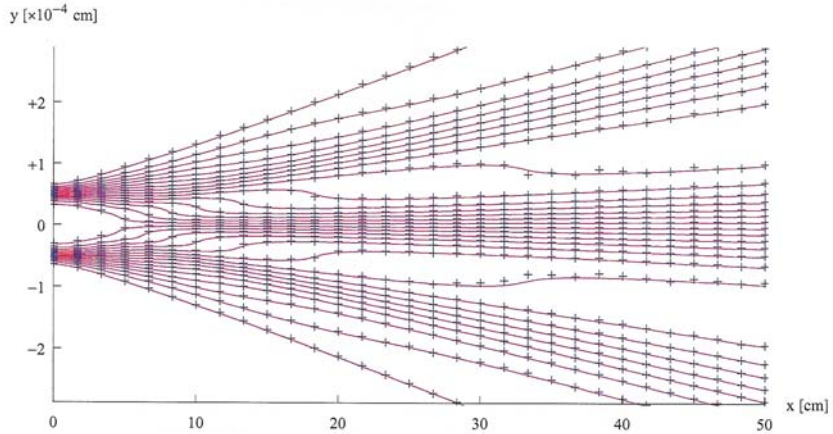

Figure 5. (color online). Two-Slit Experiment as described in §5.1.2 of P.R. Holland, *The Quantum Theory of Motion: An Account of the de Broglie-Bohm Causal Interpretation of Quantum Mechanics*, (Cambridge University Press, New York, 1993). The density sampled trajectories (+) are plotted superposed on the Bohmian trajectories (solid). The initial positions are assumed Gaussian in the slits (left side of figure), and the ensemble of trajectories makes the familiar bands of bright and dark on the screen (right side of the figure).

Examples of the analytic approach to quantum trajectories

Sanz and Miret-Artes
Atom-surface scattering
Formation of vortices

Sanz and Miret-Artes
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
Bohmian approach to quantum fractals

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..

Stationary states

Non-Stationary states

TDSE traditional approach

space fixed (x,t) Eulerian coords.
introduce large grids/basis sets
unfavorable scaling (exp.)

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

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

Quantum Trajectories

1. Real space route: Amplitude/phase→continuity, QHJE
   Madelung, Bohm,…
2. Complex space route: exp. form → complex QHJE
   Tannor, Wyatt,..
3. Phase space/Wigner function/moments
   Takabayasi, Burghardt, Hughes…

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)

The real-space route to quantum trajectories: Bohmian and post-Bohmian

Uni-polar amplitude-phase ansatz for wave function (Madelung 1926):

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

Advantages? Disadvantages? of this form for the wave function

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 $v(x) = j(x,t)/\rho(x,t) = \frac{1}{m}\nabla S$ 'guidance condition'

$\rho(x,t) = R(x,t)^2$ 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…

It can be dealt with!

(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.. $\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot (\rho \vec{v})$ $-\frac{\partial S}{\partial t} = \frac{1}{2} m v^2 + V + Q$ Coupled system of PDEs in the Eulerian frame

Viewpoints for solving hydrodynamic equations…

Path $\vec{r}(t)$ Trajectory $\vec{r}(t)$

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

Intermediate Frame…ALE*
Monitor moves along at 'arbitrary' velocity

Lagrangian Frame
Monitor moves along with the fluid velocity 'go with the flow'

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

$\vec{\dot{r}} = 0$ $\vec{\dot{r}}$ *arbitrary* $\vec{\dot{r}} = \frac{1}{m} \vec{\nabla} S$

Use fixed in space time deriv. $\frac{\partial f}{\partial t}$

Use the 'moving' time deriv. $\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{\dot{r}} \cdot \vec{\nabla}$

Equations of motion in the moving (ALE) frame

EOM for quantum trajectories

Continuity

$$R = e^{C}$$

$$\frac{dC}{dt} = (\dot{\vec{r}} - \vec{v}) \cdot \nabla C - \frac{1}{2} \nabla \cdot \vec{v}$$

$$\vec{v} = \frac{1}{m} \nabla S$$

New non-Lagrangian dynamical terms when $\dot{\vec{r}} \neq \vec{v}$

Slip velocity $\vec{w} = \dot{\vec{r}} - \vec{v}$

Action

$$\frac{dS}{dt} = (\dot{\vec{r}} - \vec{v}) \cdot (m\vec{v}) + \frac{1}{2} m\vec{v} \cdot \vec{v} - (V + Q)$$

quantum Lagrangian

Trajectory for each ‘pseudo-particle’ or grid point is specified by $\vec{r}(t)$

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-adiabiatic 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: classical, analytic quantum, and synthetic quantum

Complex-valued *classical* 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 GGWPD (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:

C. Trahan, K. Hughes, R. Wyatt, J. Chem. Phys. 118, 9911 (2003).

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.

The synthetic approach to approximate complex valued quantum trajectories

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 non-locality to measures of quantum complexity.

J. Chem. Phys. **125**, 231103 (2006)

J. Chem. Phys. 127, 197101(2007) comment by Sanz and Miret-Artes
J. Chem. Phys. 127, 197102(2007) reply to comment

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 $\psi(x,t) = e^{iS(x,t)/\mathrm{h}}$

S is the complex-valued quantum action function

Substitute into the time-dependent Schrodinger equation to obtain…

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V + \frac{\mathrm{h}}{2mi}\frac{\partial^2 S}{\partial x^2}$$

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

Define

$$Q_C = \frac{\mathrm{h}}{2mi}\frac{\partial^2 S}{\partial x^2}$$

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

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 → complex momentum p → complex coordinate z

$S(z,t)$ $\quad p(z,t) = \partial S(z,t)/\partial z$ $\quad dz/dt = p(z,t)/m$

How to approximately solve the QHJE using individual trajectories

The quantum HJ equation

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2+\frac{\mathrm{h}}{2mi}\frac{\partial^2 S}{\partial x^2}+V$$

$$-\frac{\partial S_0}{\partial t}=\frac{1}{2m}S_1^2+\frac{\mathrm{h}}{2mi}S_2+V$$

Notation for derivs.

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

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

Take the x-derivative

$$-\frac{\partial S_1}{\partial t}=\frac{1}{2m}2S_1S_2+\frac{\mathrm{h}}{2mi}S_3+V_1$$

Another x-derivative

$$-\frac{\partial S_2}{\partial t}=\frac{1}{2m}2(S_1S_3+S_2^2)+\frac{\mathrm{h}}{2mi}S_4+V_2$$

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 $\frac{dS_n}{dt} = F(S_1, \ldots S_n, S_{n+1}, S_{n+2}) + vS_{n+1}$ n=0,1,2,…

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

$$-\frac{\partial S_0}{\partial t} = \frac{1}{2m} S_1^2 + \frac{\mathrm{h}}{2mi} S_2 + V \qquad -\frac{\partial S_1}{\partial t} = \frac{1}{2m} 2S_1 S_2 + V_1 \qquad -\frac{\partial S_2}{\partial t} = \frac{1}{2m} 2S_2^2 + V_2$$

Equations of motion in the Eulerian frame

Now have 4 equations in the ALE frame

$$\frac{dS_0}{dt} = -\frac{1}{2m} S_1^2 - (\frac{\mathrm{h}}{2mi} S_2 + V) + vS_1$$

$$\frac{dS_1}{dt} = -\frac{1}{m} S_1 S_2 - V_1 + vS_2$$

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

Q_C is included

$$\frac{dz}{dt} = v$$

In the Lagrangian frame $\frac{dz}{dt} = p/m = S_1/m$

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

$$\frac{dS_1}{dt} = -V_1 \quad \text{or} \quad \frac{dp}{dt} = -V_1 = F_{classical}$$

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

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
Poirier 2008, Chou and Wyatt, 2008

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 $\psi = \underset{\longrightarrow}{\psi_+} + \underset{\longleftarrow}{\psi_-} = R_+ e^{iS_+} + R_- e^{iS_-}$

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
4. Multi-potential surface dynamics, 2007

1D stationary states

5. 1D wave packet dynamics, 2008
6. Multi-dimensional wave packet dynamics, 2008

fixed grid, no trajectories

The Equivalence Postulate and Quantum Mechanics

Alon Faraggi and Marco Matone, 1998-

Review: Int. J. Mod. Phys. 15, 1869 (2000)

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
Burghardt, Bittner, Hughes..

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

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

Quantum trajectories for the Wigner function
Rowland and Wyatt

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

Applications to systems with high dimensionality

Aproximations to the quantum potential
Garaschuk and Rassolov

Classical limit of Bohmian mechanics
Is there still confusion?
Bowman, Burghardt, …

New opportunities for you in Bohmian mechanics

Use your expertise in Bohmian mechanics to make $$$!!

O. Choustova, Application of Bohmian mechanics to dynamics of prices of shares,
Int. J. Theor. Phys. 47, 252 (2008)

O. Choustova, Bohmian mechanism for financial processes,
J. Mod. Optics 51, 1111 (2004)

E. Haven, Pilot wave theory and financial option pricing,
Int. J. Theor. Phys. 47, 252 (2008)

Dynamics of price trajectories (of stocks, options, etc) in price phase space
The information wave function evolves according to the financial Schrodinger 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

A. Khrennikov, Quantum-like brain: interference in minds
Biosystems, 84, 225 (2006).

Now for…..

Thanks to Brian, Bill, and all of the participants