WORKSHOP ON

QUANTUM TRAJECTORIES

Los Alamos, New Mexico
July 27-30, 2008

Conference Proceedings

WORKSHOP ON QUANTUM TRAJECTORIES

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Conference Schedule

Sunday, July 27
Welcome Reception
7:00PM - 9:00 PM

Monday, July 28
Opening
8:40AM - 8:50AM

Session I: Fundamentals
8:50AM - 12:10PM

Session II: Quantum Trajectory Approaches I
3:00PM - 6:00PM

Poster Session
8:00PM - 10:00PM

Tuesday, July 29
Session III: Bipolar Approaches
8:30AM – 12:10PM

Session IV: Complex Approaches
3:00PM – 5:20PM

Banquet
6:00PM - 10:00PM

Wednesday, July 30
Session V: Statistical/Phase Space Approaches
8:30AM – 11:30AM

Working Lunch
11:30AM – 12:20PM

Session VI: Quantum Trajectory Approaches II
12:20PM – 2:20PM

Tour to Bandelier
3:00PM - 6:00PM

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Conference material created by: Adam Shipman, Ellie Vigil, Kelle Ramsey, and Charlotte Carter
of the Center for Nonlinear Studies at Los Alamos National Laboratory.

MONDAY, JULY 28, 2008

Session I: Fundamentals

Chair: Bill Poirier (Texas Tech University, Lubbock)

8:40-8:50 AM **Brian Kendrick** (Los Alamos National Laboratory)
Welcome and Introductory Comments

8:50-9:10 AM **Robert E. Wyatt** (University of Texas, Austin)
Overview: Dynamics with Quantum Trajectories

9:10-9:50 AM **Sheldon Goldstein** (Rutgers University)
Can the Velocity in Bohmian Mechanics be Measured?

9:50-10:10 AM **Coffee Break**

10:10-10:50 AM **Gary Bowman** (Northern Arizona University)
Are Decoherent Trajectories Coherent?

10:50-11:30 AM **Eli Pollak** (Weizmann Institute, Israel)
The Semiclassical Route to Quantum Dynamics in Real Time

11:30-12:10 PM **Vitaly A. Rassolov** (University of South Carolina)
Computational Complexity of Non-relativistic Quantum Mechanics: Implications for the Quantum Potential

12:10-3:00 PM **Lunch Break (On Your Own)**

Session II: Quantum Trajectory Approaches I

Chair: Alon Faraggi (University of Liverpool, UK)

3:00-3:40 PM **Salvador Miret-Artés** (CSIC, Spain)
Trajectory Formulation of Quantum Mechanics: Topology and Singularities

3:40-4:20 PM **Angel S. Sanz** (CSIC, Spain)
Superposition and Nonlocality in Bohmian Mechanics

4:20-4:40 PM **Coffee Break**

4:40-5:20 PM **Sophya Garashchuk** (University of South Carolina)
Stable Long-Time Semiclassical Description of Zero-point Energy in High-dimensional Molecular Systems

5:20-6:00 PM **Dirk A. Deckert** (Mathematisches Institut der Universitat Munchen)
Quantum Dynamics with Bohmian Trajectories

6:00-8:00 PM **Dinner Break (On Your Own)**

8:00-10:00 PM **Poster Session**

Overview: Dynamics with Quantum Trajectories

Robert E. Wyatt
Department of Chemistry and Biochemistry
The University of Texas at Austin

An overview will be presented of the two approaches to quantum trajectories. In the first of these, the *analytic* approach, quantum trajectories are propagated using pre-computed information, usually the time-dependent wave function. This approach is used primarily for analysis, interpretation, and insight. The second (and newer) approach is the *synthetic* one, which does not use pre-computed information. Rather, this approach is used to directly solve the time-dependent Schrodinger equation. Quantum information, including the wave function, is computed on-the-fly along one or more evolving trajectories. Within this approach are several types of quantum trajectory, including those propagating in either real or complex phase space. Traditional Bohmian trajectories form an example of those running in real valued space. The equations of motion for the real space and complex space approaches will be reviewed, and recent applications of both approaches will be mentioned. Finally, a number of recent studies and research trends in the field of quantum trajectories will be mentioned.

Can the Velocity in Bohmian Mechanics be Measured?

Sheldon Goldstein
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Abstract

Howard Wiseman has proposed the use of "weak measurements" for the determination of the velocity of a quantum particle at a given position, and has shown that according to quantum mechanics the result of such a procedure is the Bohmian velocity of the particle. Although Bohmian mechanics is empirically equivalent to variants based on velocity formulas different from the Bohmian one, and although it has been proven that the velocity in Bohmian mechanics is not measurable, we argue for the somewhat paradoxical conclusion that Wiseman's weak measurement procedure indeed constitutes a genuine measurement of velocity in Bohmian mechanics. We reconcile the apparent contradictions and elaborate on some of the different senses of measurement at play here.

Are Decoherent Trajectories Coherent

Gary Bowman
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Abstract

Decoherence has taken on great importance in both applied and fundamental physics. But the physical meaning of decoherence - like that of quantum mechanics itself - can be elusive. I will introduce the decoherence mechanism in its simplest form, and discuss its implications for the measurement problem in standard quantum mechanics. I'll then turn to the interpretation of decoherence in the context of Bohmian mechanics, my main goal being to frame (coherently, I hope!) some interesting questions.

The semiclassical route to quantum dynamics in real time

Eli Pollak
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Abstract:

One of the central challenges facing theoretical Chemistry and Physics is the computation of quantum dynamics in complex systems. Due to the oscillatory nature of quantum mechanical properties, this problem has remained elusive even with present state of the art powerful computational facilities. The need for a general methodology cannot be overstated, since the ability of computing quantum dynamics in real time would impact our understanding of diverse topics, such as spectroscopy, molecular reaction dynamics, solid state physics, ab-initio quantum chemistry, quantum computation, Bose-Einstein condensates to name a few.

In this talk I will discuss the semiclassical initial value representation approach, comparing it to the classical Wigner dynamics approximation. Using a novel time dependent perturbation theory, I will show that the semiclassical approximation to the exact quantum propagator may be considered to be the zero-th order term in a time dependent perturbation theory expansion of the exact propagator. This leads to profound new insight into quantum dynamics. Exact quantum dynamics may be obtained purely from classical paths. Deep tunneling is effected through coherent classical paths. New and efficient approximate semiclassical propagators may be used to improve convergence properties.

Examples of applications will include vibrational relaxation and the general semiclassical theory for dissipative systems. A first example of ab-initio semiclassical dynamics will be presented for the absorption spectrum of formaldehyde.

Computational complexity of non-relativistic quantum mechanics: Implications for the Quantum Potential

Vitaly A. Rassolov and Sophya Garashchuk
Department of Chemistry and Biochemistry
University of South Carolina

Abstract

Different branches of quantum chemistry encounter exponential complexity of the underlying exact wavefunctions. The suggested solutions are specific to each subdivision. On the other hand, recent developments in quantum computing theory prove that a general ground state search problem with two-body Hamiltonians cannot be solved in polynomial time. We suggest that a quantum chemical problem of the ground state energy search is also non-polynomial in time with respect to the system size. If so, we show that complexity of the Quantum Potential is inevitable, and no easy fix is possible in the context of exact quantum trajectory propagation.

Trajectory Formulation of Quantum Mechanics: Topology and Singularities

A. S. Sanz and S. Miret-Artés

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From the very beginning, Quantum Mechanics has revealed as a very successful and powerful theory to describe nature. However, its standard formalisms or pictures (Shrödinger, Heisenberg and Interaction) are very often unable to provide a satisfactory, intuitive insight into the underlying dynamics of physical processes. This situation is even worse if one takes into account that there must be some kind of correspondence between the predictions of Quantum and Classical Mechanics in the appropiate limit. The trajectory formulation initiated basically by Madelung and Bohm, in our opinion, provides a new and very attractive theoretical framework where more and more applications are being developed very fast in the last years.

The main goal of this talk is to show recent investigations by the Madrid group focusing on some topological aspects of quantum trajectories as well as classical and quantal singularities. Examples going from single scattering of two Gaussian wavepackets to a collision of atoms by surfaces passing by time dependent DFT will serve us to expose all the new ideas and findings of our research [1-7].

References

[1] A. S. Sanz, F. Borondo and S. Miret-Artés, *Phys. Rev. B* **61**, 7743 (2000); *Europhys. Lett.* **55** 303 (2001).

[2] A. S. Sanz, F. Borondo and S. Miret-Artés, *J. Phys. : Condens. Matter* **14**, 6109 (2002).

[3] R. Guantes, A. S. Sanz, J. Margalef-Roig and S. Miret-Artés, *Surf. Sci. Rep.* **53**, 199 (2004).

[4] A. S. Sanz and S. Miret-Artés, *Phys. Rep.* **451**, 37 (2007).

[5] A. S. Sanz and S. Miret-Artés, *Chem. Phys. Lett.* **445** 350 (2007); **458** 239 (2008)

[6] A. S. Sanz, X. Giménez, J. M. Bofill and S. Miret-Artés, in *Theory of Chemical Reactivity* edited by P. Chattaraj, Taylor and Francis, (to be appeared).

[7] A. S. Sanz and S. Miret-Artés, *Trajectory Formulations of Quantum Mechanics* (to be appeared in the Springer series "Lecture Notes in Physics", 2009).

Superposition and nonlocality in Bohmian mechanics

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Abstract

As is well known, standard quantum mechanics can be recast into a trajectory-grounded theory of motion: Bohmian mechanics [1,2]. This one-to-one transformation confers (Bohmian) quantum trajectories a clear advantage over other trajectory formulations considered in the literature [3,4] to explain the quantum world, which are based on approximations or even in a direct application of classical mechanics. Bohmian mechanics allows us to treat quantum phenomena at the same level as in the standard version of quantum mechanics, because the rules of motion are quantum-mechanical. Thus, for instance, we can explain the formation of a diffraction pattern trajectory by trajectory (as happens in the corresponding real experiment) at the same time that the individual paths pursued by the particles can be monitored [5,6]. This is, precisely, the idea behind the rapidly increasing interest in Bohmian mechanics noted in the last 10 years. Apart from the conceptual-theoretical motivations [2], which can be traced back to de Broglie and Madelung (and later on to Bohm and Takabayashi), two important streams are nowadays the leading ones: computational [7] and interpretational [2,4].

The work that we present here can be considered within the interpretational line, although many of the ideas can be of much interest within the computational one. In particular, we are going to focus the discussion on two important properties of standard quantum mechanics because of their direct implications Bohmian mechanics: superposition and nonlocality. As will be shown, superposition is brings interesting physical situations when it is analyzed from a Bohmian perspective, which can be directly related with the two well-known cases in a two-slits experiment: (1) both slits open at the same time or (2) only one slit open at a time. On the other hand, nonlocality leads to behaviors which make the particle motion to depend on the whole ensemble considered (specified through the corresponding wave function or probability density). To illustrate these properties and make them more evident, we will analyze simple cases, such us the superposition of two wave packets under different regimes [8]. This analysis leads us immediately to interesting problems, such as the Talbot effect [9], the fractal quantum trajectories [10], or the decoherence in two-slits experiments [11], for instance. Moreover, we will provide a brief overview of the analogous situation for the electromagnetic field, which cannot be directly considered within the standard Bohmian framework (restricted to matter particles), but through an analogous theory derived from the Maxwell equations [12].

References

[1] D. Bohm, *Phys. Rev.* **85**, 166, 184 (1952).
[2] P. R. Holland, *The Quantum Theory of Motion* (Cambridge University Press, 1993).
[3] A.S. Sanz and S. Miret-Artés, in *Quantum Dynamics of Complex Molecular Systems*, ed. by D. Micha and I. Burghardt, Springer Series in Chemical Physics, **83** (Springer, 2006), p. 343-368.
[4] A.S. Sanz and S. Miret-Artés, *Trajectory Formulations of Quantum Mechanics* (to appear in Springer Series "Lecture Notes in Physics", 2009).
[5] A.S. Sanz, F. Borondo and S. Miret-Artés, *Phys. Rev. B* **61**, 7743 (2000).
[6] A.S. Sanz, F. Borondo and S. Miret-Artés, J. Phys.: *Condens. Matter* **14**, 6109 (2002).
[7] R.E. Wyatt, *Quantum Dynamics with Trajectories* (Springer, 2006).
[8] A.S. Sanz and S. Miret-Artés, *J. Phys. A* (submitted, 2008); quant-ph:0806.2105.
[9] A.S. Sanz and S. Miret-Artés, *J. Chem. Phys.* **126**, 234106 (2007).
[10] A.S. Sanz, *J. Phys. A* **38**, 6037 (2005).
[11] A.S. Sanz and F. Borondo, *Eur. Phys. J. D* **44**, 319 (2007).
[12] M. Davidovic, A.S. Sanz, D. Arsenovic, M. Bozic and S. Miret-Artés, *Europhys. Lett.* (submitted, 2008); quant-ph:0805.3330.

Stable long-time semiclassical description of zero-point energy in high-dimensional molecular systems

Sophya Garashchuk and Vitaly A. Rassolov

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Abstract

Semiclassical implementation of the quantum trajectory formalism [J. Chem. Phys. **120**, 1181 (2004)] is further developed to give stable long-time description of zero-point energy in anharmonic systems of high dimensionality. The method is based on a numerically cheap linearized quantum force approach; stabilizing terms compensating for the linearization errors are added into the time evolution equations for the classical and nonclassical components of the momentum operator. The wavefunction normalization and energy are rigorously conserved. Numerical tests are performed for model systems of up to 40 degrees of freedom.

Quantum Dynamics with Bohmian Trajectories

D.-A. Deckert*, D. Dürr†, P. Pickl‡

Abstract

We describe some advantages and disadvantages of the use of Bohmian trajectory-grids for numerical simulations of quantum dynamics. In particular we stress the following:

- In the hydrodynamic formulation of Bohmian Mechanics it is the quantum potential term that ensures the crucial non-crossing property of Bohmian mechanics. The quantum potential has to be paid careful attention to in numerical simulations. Failure to do so either causes instabilities or leads to false simulations.
- Fitting algorithms with smoothing behavior, especially the least square fitting algorithm, are inappropriate for the computation of the quantum potential because they will generically produce trajectory crossings.
- Because of equivariance $|\psi|^2$ distributed Bohmian grids will remain $|\psi|^2$ distributed for all times, which can be advantageous for long-time asymptotics as well as real-time error-detection.

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MONDAY, JULY 28, 2008

Poster Session

1) **Gennady Berman** (Los Alamos National Laboratory)
   Quantum Trajectories in "Action-angle" Representation

2) **Tim Coffey, Robert E. Wyatt, and Wm. C. Schieve** (University of Texas, Austin)
   Monte Carlo Generation of Bohmian Trajectories

3) **Chia-Chun Chou and Robert E. Wyatt** (University of Texas, Austin)
   Quantum Vortices and Streamlines Within the Complex Quantum Hamilton-Jacobi Formalism

4) **Julianne Kuck David and Robert E. Wyatt** (University of Texas, Austin)
   Cluster DPM: Introduction and Comparison of Methods

5) **Dirk A. Deckert, D. Dürr, and P. Pickl** (Mathematisches Institut der Universitat Munchen)
   Quantum Dynamics with Bohmian Trajectories

6) **Toufik Djama, and Bill Poirier** (Texas Tech University, Lubbock)
   The Analytic Solutions of the General Eckart and Morse Potentials Using the Bipolar Counter-propagating Wave Decompositions

7) **Brian K. Kendrick** (Los Alamos National Laboratory)
   Quantum Wavepacket Dynamics with Trajectories: Computational Issues

8) **Jeremy Maddox and Bill Poirier** (Texas Tech University, Lubbock)
   Quantum Trajectory simulations: Trajectory Surface Hopping and Path Integral Monte Carlo

9) **Kisam Park and Bill Poirier** (Texas Tech University, Lubbock)
   Quantum Trajectory Calculations for Bipolar Wavepacket Dynamics in One Dimension

10) **Keith H. Hughes, Steven M. Parry, Gerard Parlant, and Irene Burghardt** (University of Wales Bangor, UK)
    Mixed Quantum-classical Dynamics from Coupled Hydrodynamic and Phase Space Representations

Quantum trajectories in "action-angle" representation

Gennady Berman, T-13, LANL

As a rule, the process of evolution of a quantum system in the Wigner representation is described in the "coordinate-momentum" variables. However, in the classical limit there are some advantages to describe the dynamics of the nonlinear system in the "action-angle" variables ensuring the separation of the motion into the fast (phase) and slow (e.g. diffusion in action). Therefore in the quantum analysis of such systems in Wigner representation it is useful to generalize it for the case of "action-angle" variables. We demonstrate this approach using a simple example of a quantum kicked rotator. We show that the quantum dynamics is reduced to a classical discrete map with a quasi-random force. In the quasi-classical region of parameters the influence of the quasi-random force is small, and the dynamics of observables can be described by the discrete trajectories.

Monte Carlo Generation of Bohmian Trajectories

Timothy M. Coffey and Wm. C. Schieve

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Robert E. Wyatt

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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 $N \rightarrow \infty$ and $\delta t \rightarrow 0$. Higher dimensional problems can be solved by this method for separable wave functions. Several examples are given, including the two-slit experiment.

Quantum Vortices and Streamlines within the Complex Quantum Hamilton-Jacobi Formalism

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Quantum vortices and streamlines are investigated in the framework of the quantum Hamilton-Jacobi formalism. A quantum vortex forms around a node in the wave function in the complex space, and the quantized circulation integral originates from the discontinuity in the real part of the complex action. The local structure of the quantum momentum function and the Pólya vector field near a stagnation point or a pole are analyzed. Although the quantum momentum field displays *hyperbolic flow* around a node, the corresponding Pólya vector field displays *circular flow*. Streamlines near a stagnation point of the quantum momentum function may spiral into or from it, or they become circles centered on this point. Additionally, streamlines near a pole display East-West and North-South opening hyperbolic structure. On the other hand, streamlines near a stagnation point of the Pólya vector field for the quantum momentum function display general hyperbolic structure, and streamlines near a pole become circles enclosing the pole.

Cluster DPM: Introduction and Comparison of Methods

Julianne Kuck David, Robert E. Wyatt
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Abstract

The standard derivative propagation method (DPM) has been extended from the single-trajectory form, in which hard truncation is used to obtain a closed system of equations of motion for the derivatives of the action, to a new multiple-trajectory form. This "cluster derivative propagation method" (CDPM) allows for soft truncation, where spatial derivatives of S higher than the one at which the DPM hierarchy is truncated are approximated through curve fitting of the derivatives of the action of several simultaneously launched trajectories. A comparison of results using different fitting methods, including least-squares and finite difference, with varying orders of the fitting function, as well as different orders of DPM (including the "DPM-like" propagation of the Quantum Hamilton Jacobi equation alone), are given.

Quantum Dynamics with Bohmian Trajectories

D.-A. Deckert*, D. Dürr†, P. Pickl‡

Abstract

We describe some advantages and disadvantages of the use of Bohmian trajectory-grids for numerical simulations of quantum dynamics. In particular we stress the following:

- In the hydrodynamic formulation of Bohmian Mechanics it is the quantum potential term that ensures the crucial non-crossing property of Bohmian mechanics. The quantum potential has to be paid careful attention to in numerical simulations. Failure to do so either causes instabilities or leads to false simulations.
- Fitting algorithms with smoothing behavior, especially the least square fitting algorithm, are inappropriate for the computation of the quantum potential because they will generically produce trajectory crossings.
- Because of equivariance $|\psi|^2$ distributed Bohmian grids will remain $|\psi|^2$ distributed for all times, which can be advantageous for long-time asymptotics as well as real-time error-detection.

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The Analytical solutions of the general Eckart and Morse potentials using the Bipolar counter-propagating wave decompositions.

Toufik Djama and Bill Poirier

Department of Chemistry and Biochemistry,

Texas Tech University, Box 41061, Lubbock, Texas 79409-1061.

Abstract

We obtain analytical solutions for bipolar counter-propagating wave decompositions for standard potentials, specifically, the Morse oscillator and the general Eckart barrier systems. The latter includes the familiar symmetric Eckart barrier, the barrierless uphill ramp, and a more general form with both barriers and asymmetry. These analytical solutions provide important insight into the effectiveness of the bipolar approach for a wide range of model reaction profiles, particularly vis-a-vis limiting behavior. Finally, the bipolar analytic solutions are extended into the complex plane; ramifications for complex Bohmian mechanics are discussed.

Quantum wavepacket dynamics with trajectories: computational issues

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Abstract

A time-dependent quantum wave packet method is presented which is based on solving the hydrodynamic equations of motion associated with the de Broglie-Bohm formulation of quantum mechanics. The hydrodynamic equations are solved using a meshless method based upon a moving least squares approach. An Arbitrary Lagrangian-Eulerian (ALE) frame of reference and a regridding algorithm which adds and deletes computational points are used to maintain a uniform and nearly constant interparticle spacing. Averaged fields are used to maintain unitary time evolution and the numerical instabilities associated with the formation of nodes in the reflected portion of the wave packet are avoided by adding artificial viscosity to the equations of motion. For systems with many degrees of freedom, a vibrational decoupling scheme can be used for which the computational cost scales linearly with respect to the dimensionality of the problem. The computational issues associated with this methodology will be discussed in the context of several applications: (1) tunneling through an Eckart barrier; (2) a one-dimensional model chemical reaction that is known to exhibit a quantum resonance; and (3) an N-dimensional model chemical reaction.

Quantum trajectory simulations: Trajectory surface hopping and path integral Monte Carlo

Jeremy B. Maddox and Bill Poirier
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Abstract

We report on the development of several new quantum trajectory algorithms for calculating transmission and reflection probabilities relevant to problems involving quantum scattering. Our approach is based upon the counter-propagating wave methodology (CPWM) which has been previously used to determine stationary state wavefunctions in terms of counter-propagating (bipolar) wavefunction components and a set of well-behaved, though interdependent, trajectories. The new methods are designed to accomplish this same task using completely independent trajectories thereby rendering the calculation amenable to massively parallel computational strategies. This is accomplished by appealing to a novel path integral approach to the CPWM and stochastic numerical algorithms. Accuracy and convergence benchmark studies of several one-dimensional potential barriers are presented and the viability of these methods towards multi-dimensional scattering problems is addressed.

Quantum Trajectory Calculations for Bipolar Wavepacket Dynamics in One Dimension

Kisam Park and Bill Poirier
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Abstract

A numerical method for the quantum trajectory calculations in one dimension is developed, based on the bipolar wavepacket time-evolution equation presented in a previous article [J. Chem. Phys. 128, 164115 (2008)]. The preliminary fixed grid quantum trajectory calculations which employ the Crank-Nicholson method show that the symmetric and antisymmetric linear combinations of counter-propagating wavepackets can provide useful initial conditions for moving grid (synthetic) quantum trajectory calculations. In the moving grid calculations, the equations of motion for the C-amplitudes and the actions of the bipolar wavepackets are derived in the arbitrary Lagrangian-Eulerian frame, where the spatial derivatives are determined by various least squares methods. The quantum trajectories are propagated by using the 4th-order Runge-Kutta method. The resultant wavepacket can be reconstructed by summing all component bipolar wavepackets, which individually exhibit only a minor interference pattern. The moving grid and the fixed grid calculation results for the symmetric Eckart barrier scattering in one dimension show good agreement.

Mixed quantum-classical dynamics from coupled hydrodynamic and phase space representations

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(Dated: July 9, 2008)

Abstract

The hybrid quantum-classical approach of [Burghardt, Parlant, *J. Chem. Phys.* **120**, 3055 (2004)], referred to here as the quantum-classical moment (QCM) approach, is demonstrated for the dynamics of various quantum systems coupled to a classical harmonic coordinate. The approach combines the quantum hydrodynamic and classical Liouvillian representations by the construction of a particular type of moments (i.e., partial hydrodynamic moments) whose evolution is determined by a hierarchy of coupled equations. For pure states, which are at the center of the present study, this hierarchy terminates at the first order. In the Lagrangian picture, deterministic trajectories result whose dynamics is Hamiltonian in the classical subspace while the projection onto the quantum subspace evolves under a generalized hydrodynamic force. Importantly, this force also depends upon the classical (Q, P) variables. The method is exact if the classical subspace is harmonic, as is the case for the systems studied here.

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TUESDAY, JULY 29, 2008

Session III: Bipolar Approaches

Chair: Bob Wyatt (University of Texas at Austin)

8:30-9:10 AM	**Marco Matone** (University of Padova, Italy) *Time and the Quantum Hamilton Jacobi Equation*
9:10-9:50 AM	**Ned Floyd** *EPR-Bohr and Quantum Trajectories*
9:50-10:10 AM	**Coffee Break**
10:10-10:50 AM	**Aion Faraggi** (University of Liverpool, UK) *Duality and Equivalence and the Quest for Unification*
10:50-11:30 AM	**Bill Poirier** (Texas Tech University, Lubbock) *Bipolar Quantum Wavepacket Dynamics for Multidimensional Systems*
11:30-12:10 PM	**Gérard Parlant** (LSDMS, France) *Bipolar Quantum Trajectory Dynamics*
12:10-3:00 PM	**Lunch Break (On Your Own)**

Session IV: Complex Approaches

Chair: Marco Matone (University of Padova, Italy)

3:00-3:40 PM	**David Tannor** (Weizmann Institute, Israel) *Bohmian Mechanics with Complex Action: An Exact Formulation of Quantum Mechanics with Complex Trajectories*
3:40-4:20 PM	**Robert E. Wyatt** (University of Texas, Austin) *Quantum Dynamics with Un-real Trajectories*
4:20-4:40 PM	**Coffee Break**
4:40-5:20 PM	**Jeremy Schiff** (Bar-Ilan University, Israel) *A Path Integral Approach to BOMCA*
5:20-6:00 PM	**Break**
6:00-10:00 PM	**Banquet** (Gabriel's, guests pay for drinks, transportation leaves hotel at 6:00 PM, photo op stop, transportation leaves Gabriel's at 9:00 PM)

Time and the quantum Hamilton Jacobi equation

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Abstract

After introducing the main steps leading to the QHJE from the Equivalence Postulate we review how this implies energy quantization without appeling to any probabilistic interpretation of the wave function. We then show that in such a context time cannot be defined as a continuous local parameter. This also implies a sort of energy time uncertainty relation which may lead to a deeper understanding of why the Copenaghen interpretation works. We also discuss some key properties of the quantum potential, including its role of intrinsic energy as implied by the EP.

EPR-Bohr and Quantum Trajectories

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Abstract

Quantum trajectories are used to investigate the EPR-Bohr paradox in a modern sense by examining entanglement and nonlocality. We synthesize a single "EPR-molecule" from the two scattered particles of the EPR experiment. Herein, we explicitly investigate the behavior of the EPR-molecule rather than the behaviors of the two scattered particles to gain insight into the EPR-Bohr paradox. We develop the EPR-molecule's wave function in polar form and its reduced action, both of which manifest entanglement. We next apply Jacobi's theorem to the reduced action to generate the equation of motion for the EPR-molecule to produce its quantum trajectory. The resultant quantum trajectory manifests entanglement and has retrograde segments interspersed between segments of forward motion in the quantum trajectory. This alternating of forward and retrograde segments generates nonlocality. Analysis of the equation of motion renders an additional component manifesting entanglement while also rendering a classical behavior of the two scattered particles. The behavior of the entanglement component and its relationship to nonlocality is discussed.

Duality and equivalence and the quest for unification

Alon Faraggi
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Abstract

Phase space duality has been a corner stone in the equivalence postulate approach to quantum mechanics. I will discuss this approach and how its consistency necessitates the introduction of the bi-polar representation of the wave function. Existence of phase space duality and consistency of the equivalence postulate leads to the self dual states with a non-vanishing quantum self--energy. These observations lead to a novel perspective on foundational aspects of quantum mechanics and quantum field theories and on the search for unifying theory underlying all of the fundamental interactions.

Bipolar Quantum Wavepacket Dynamics for Multidimensional Systems

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Abstract

The semiclassical method is characterized by finite forces and smooth, well-behaved trajectories, but also by multivalued representational functions that are ill-behaved at caustics. In contrast, quantum trajectory methods---based on Bohmian mechanics (quantum hydrodynamics)---are characterized by divergent forces and erratic trajectories near nodes, but also well-behaved, single-valued representational functions. Multiple valued i.e. "multipolar" quantum trajectory methods, offer the best features of both, and in addition, satisfy the correspondence principle at the trajectory level. Recent developments vis-à-vis the application to multidimensional wavepacket dynamics will be emphasized, wherein a two-term or "bipolar" decomposition may be used, regardless of system dimensionality.

Bipolar Quantum Trajectory Dynamics

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Over the last decades, there has been a growing demand for simulation of large systems. Classical trajectory simulation (CTS) is the method of choice in this case, but its validity is difficult to assess. Quantum dynamical effects are suspected to be important, even in large systems. On the other hand, exact quantum calculations have been historically subject to the exponential scaling of computational effort with the system size, and are restricted in practice to small systems.

Less than ten years ago, the emergence of the Quantum Trajectory Method[1] raised the hope that it was possible to escape this dilemma. QTM runs trajectories in a formally exact quantum context, and at the same time provides the advantages of CTS (linear scaling, physical insight).

However, despite substantial progress[1], QTM still fails in the presence of interferences, an all too common occurence in real molecular systems. This is known as the "node problem". Moreover, an equally serious concern is that quantum trajectories do not ressemble their classical counterparts in the classical limit. In other words, QTM does not, in general, satisfy *classical correspondence*.

In a series of articles[2], Poirier has been exploring the use of an (exact) bipolar decomposition of the wavefunction, i.e. $\phi = \phi_+ + \phi_-$, into traveling waves, moving in opposite directions. Then, the total wavefunction interferences result from the superposition of the individual components $\phi_\pm$ which are, ideally, interference-free. Defining quantum trajectories for each wavefunction component separately ensures that these trajectories are well behaved and classical-like.

Recently, Poirier[3] extended his theoretical treatment, initially established for delocalized staionary wavefunctions, to localized time-dependent wavepackets. The resulting wavepacket components $\Psi_\pm$ are solutions to a 2-state time-dependent Schrödinger equation

$$i\hbar\frac{\partial \Psi_\pm}{\partial t} = \hat{H}\Psi_\pm \pm \frac{1}{2}\frac{\partial V}{\partial x}(\Psi_+ - \Psi_-) \qquad with \quad \Psi_\pm = \int^x \psi_\pm(x')dx'$$

which can be directly integrated over time by means of a standard fixed-grid method.

In this presentation, we explore the physical behaviour of the component wavepackets $\Psi_\pm$ and we check that they are well localized and interference-free, as expected. Moreover, we compute quantum trajectories associated with the component wavepackets $\Psi_\pm$ and we show that they are generally well behaved and classical-like. Interesting and unexpected behavior of these trajectories is also shown.

1. R. E. Wyatt, *Quantum dynamics with trajectories: Introduction to quantum hydrodynamics*. Springer, New York, 2005.

2. B. Poirier, *J. Chem. Phys.* **121**, 4501 (2004); C. Trahan and B. Poirier, *J. Chem. Phys.* **124**, 034115 (2006); C. Trahan and B. Poirier, *J. Chem. Phys.* **124**, 034116 (2006); B. Poirier and G. Parlant, *J. Phys. Chem.* A **111**, 10400 (2007); B. Poirier, *J. Theor. Comput. Chem.* **6**, 99 (2007).

3. B. Poirier, *J. Chem. Phys.* **128**, 164115 (2008).

Bohmian Mechanics with Complex Action: An Exact Formulation of Quantum Mechanics with Complex Trajectories

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Ever since the advent of Quantum Mechanics, there has been a quest for a trajectory based formulation of quantum theory that is exact. In the 1950's, David Bohm, building on earlier work of Madelung and de Broglie, developed an exact formulation of quantum mechanics in which trajectories evolve in the presence of the usual Newtonian force plus an additional quantum force. In recent years, there has been a resurgence of interest in Bohmian Mechanics (BM) as a numerical tool because of its apparently local dynamics, which could lead to 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 work, we present a new formulation of Bohmian mechanics in which the quantum action, S, is taken to be complex. This requires the propagation of complex trajectories, but with the reward of a significantly higher degree of localization. For example, using strictly localized trajectories (no communication with their neighbors) we obtain extremely accurate quantum mechanical tunneling probabilities down to 10^{-7}. We have recently extended the formulation to include interference effects, which has been one of the major obstacles in conventional Bohmian mechanics. Applications to one- and two-dimensional tunneling, thermal rate constants in one and two dimensions, and the calculation of eigenvalues will be provided. A variation on the method allows for the calculation of thermal rate constants and eigenvalues using just one or two zero-velocity trajectories. On the formal side, the approach is shown to be a rigorous extension of generalized Gaussian wavepacket methods to give exact quantum mechanics, and has intriguing implications for fundamental quantum mechanics.

Quantum Dynamics with Un-Real Trajectories

Robert E. Wyatt
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Quantum trajectories running in complex space provide a novel and useful approach to quantum dynamics. After mentioning some advantages and disadvantages of this approach, the use of approximate one-at-a-time quantum trajectories will be described. Equations of motion for these trajectories are derived by following the derivative propagation method (DPM). This approach will then be applied to barrier transmission on a two degree of freedom potential surface. An important issue concerns the location of isochrones, the surfaces defining the launch points such that trajectories all arrive on the real plane at the same time. Some problems with this approximate approach will be pointed out. Another propagation method involves small clusters of moving grid points. This method gives excellent results for oscillatory structure in the reflected wave packet and for the transmitted flux. Next, a computational approach to the direct propagation of wave packets is the complex plane will be described. This approach permits the computation of exact quantum trajectories for barrier scattering problems. Interesting features of the trajectory dynamics for the reflected wave packet will be illustrated, including the helical winding of trajectories around stagnation curves and hyperbolic flow around quasi-nodes.

A path integral approach to BOMCA

Jeremy Schiff
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Bar-Ilan University

Recently, the Tannor group has presented two different but related approaches to time-dependent quantum mechanics, both based on integration along trajectories in complex configuration space. The first of these approaches, complex WKB (CWKB), extends earlier work of Boiron and Lombardi. In this approach the trajectories are solutions of the (complex) classical equations of motion; the derivation of this scheme is based on an expansion in $\hbar$. The second approach, Bohmian mechanics with complex action (BOMCA), uses complex trajectories that are not classical; it is derived using a Taylor expansion of the logarithm of the wave function with respect to the spatial variables, and therefore may have convergence properties significantly different from those of CWKB. In both approaches, quantum interference arises by superposing the contributions from complex trajectories with different initial conditions that terminate at the same final (real) value of the position.

In this talk I will show that both CWKB and BOMCA can be derived from the path integral formulation of quantum mechanics. This has several advantages. 1) It provides an understanding of the origin and meaning of the different complex trajectories in the two methods. Whereas in CWKB we evaluate the path integral around a saddle point, corresponding to a solution of the classical equations of motion, in BOMCA we evaluate around a path which is close to, but not, a saddle point, chosen so the contribution to the integral takes a particular convenient form. 2) It provides a rigorous theoretical justification for the need to superpose the contributions of different complex trajectories, something that was absent in previous work. 3) By establishing a connection between path integrals, CWKB and BOMCA, it emerges that CWKB and BOMCA provide a great simplification over existing perturbative methods for evaluating higher order corrections in saddle-point integration of the path integral.

WEDNESDAY, JULY 30, 2008

Session V: Statistical/Phase Space Approaches

Chair: David Tannor (Weizmann Institute, Israel)

8:30-9:10 AM **Irene Burghardt** (ENS, France)
Real and Complex Quantum Trajectories for Mixed States

9:10-9:50 AM **Keith Hughes** (University of Wales Bangor, UK)
Moment Closure Scheme for Quantum Hydrodynamics

9:50-10:10 AM **Coffee Break**

10:10-10:50 AM **Craig Martens** (University California, Irvine)
Quantum Trajectories in Phase Space

10:50-11:30 AM **Eric Bittner** (University of Houston)
Variational Quantum Hydrodynamics at Finite Temperature

11:30-12:20 PM **Working Lunch (Lunch Provided)**

Session VI: Quantum Trajectory Approaches II

Chair: Salvador Miret-Artes (CSIC, Spain)

12:20-1:00 PM **Bradley Rowland** (University of Texas, Austin)
Barrier Scattering with Complex Trajectories

1:00-1:40 PM **Pratim Chattaraj** (IIT, India)
A Bohmian Analysis of the Possible Field Induced KAM-like Transitions in Anharmonic Oscillators

1:40-2:20 PM **Clemens Woywod** (University of Tromsø, Norway)
The Dynamics of Angular Degrees of Freedom: New Basis Set and Grid Representations of Hamiltonian Operators

2:20-3:00 PM **Break**

3:00-6:00 PM **Tour to Bandelier** (transportation leaves hotel at 3:00 PM, guided tour 4:00-5:00 PM, transportation leaves Bandelier at 5:30 PM)

Real and complex quantum trajectories for mixed states

Irene Burghardt

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This talk addresses the quantum hydrodynamic picture for mixed states, i.e., density matrices, which is usually formulated in terms of coupled equations for the momentum moments of the Wigner function [1]. We focus here on the possibility of an analogous formulation involving a complex-valued phase-space distribution, whose momentum moments yield a new type of hydrodynamic hierarchy. The associated hydrodynamic pressure and resulting quantum forces are characterized. For pure states, the complex quantum trajectory picture developed by John [2], Tannor and collaborators [3], Wyatt and collaborators [4] and others is recovered. The present framework further allows for the formulation of a quantum-classical theory involving complex quantum trajectories, analogously to our previous development of a hybrid hydrodynamic–Liouvillian representation [5].

[1] W. R. Frensley, *Rev. Mod. Phys.* **62**, 745 (1990), J. G. Muga, R. Sala, and R. F. Snider, *Phys. Scr.* **47**, 732 (1993), I. Burghardt and L. S. Cederbaum, *J. Chem. Phys.* **115**, 10303 (2001), I. Burghardt and K. B. Møller, *J. Chem. Phys.* **117**, 7409 (2002).

[2] M. John, *Found. Phys. Lett.* **15**, 329 (2002).

[3] Y. Goldfarb, I. Degani, and D. J. Tannor, *J. Chem. Phys.* **125**, 4 (2006); Y. Goldfarb, D. J. Tannor, *J. Chem. Phys.* **127**, 161101 (2007).

[4] B. Rowland and R. E. Wyatt, *J. Phys. Chem. A* **111**, 10234 (2007); B. Rowland and R. E. Wyatt, *J. Chem. Phys.* **127**, 164104 (2007).

[5] I. Burghardt and G. Parlant, *J. Chem. Phys.* **120**, 3055 (2004); K. H. Hughes, S. M. Parry, G. Parlant, and I. Burghardt, *J. Phys. Chem. A* **111**, 10269 (2007).

Moment closure scheme for quantum hydrodynamics

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Abstract

Quantum Trajectories in Phase Space

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Abstract

We describe a method for simulating quantum processes using classical-like molecular dynamics in phase space. Our approach is based on solving the quantum Liouville equation using ensembles of classical trajectories. The nonlocality of quantum mechanics is incorporated in the trajectory representation as nonclassical interactions between the members of the ensemble, leading to an entanglement of their evolution. The statistical independence of the individual trajectories making up an ensemble in the classical limit is lost when quantum effects are included, and the entire state of the system must be propagated as a unified whole. We describe implementations of this approach in the Wigner and Husimi representations of quantum mechanics in phase space and apply the method to several model problems.

Variational Quantum Hydrodynamics at Finite Temperature

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Abstract

Small clusters of rare-gas atoms are ideal testing grounds for studying how quantum delocalization affects both the thermodynamics and structure of mesoscopic scale systems. In my talk I will discuss how we have been using "Bohm" inspired methods to minimize the free-energy functional for clusters of Ne atoms with up to 100 atoms. The chemical potential includes contributions from the quantum potential, Q, a mean-field interaction potential, and an entropic potential. One surprising result is that small clusters may have a negative heat-capacity at low temperatures due to the non-additive nature of the total free-energy.

Barrier Scattering with Complex Trajectories

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Abstract

Several recent studies have examined the role of quantum trajectories in both the real- and complex- planes for barrier scattering problems in which the wave function is not known in advance. Much recent work has been devoted to the application of complex-valued trajectory solutions of the complex quantum Hamilton-Jacobi equation. To this end, a comparison of real- and complex-valued trajectory solutions for one-dimensional Eckart and Gaussian barrier scattering (Lagrangian frame) will be presented. The difficulties of working with arbitrary Lagrangian-Eulerian trajectories in the complex plane will be examined. Details concerning a two-dimensional grid solution of the complex-valued Gaussian barrier scattering problem will be provided. To validate the grid solutions, we will introduce the use of numerical analytic continuation techniques (NAC). Both the complex grid and NAC methods provide invaluable insight into the behavior of complex quantum trajectories through examination of quantities such as the complex quantum momentum function. We will focus on the complex quantum potential as a mechanism to explain difficulties in running complex quantum trajectories. Finally, we conclude with results of current work, including the use of grid and NAC methods to generate 'exact' complex quantum trajectories and the use of clustered ALE trajectories to solve barrier scattering problems.

A Bohmian Analysis of the Possible Field Induced KAM-like Transitions in Anharmonic Oscillators

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Abstract

Classical anharmonic oscillators and their quantum variants are studied in the presence of external fields of different colors and of varying intensities. Classical Hamilton's equations of motion and time dependent density based quantum mechanics are made use of for this purpose. Temporal profiles of the distance between two Bohmian trajectories which were initially (at t=0) very close and the corresponding Kolmogorov-Sinai entropy as well as the autocorrelation function provide important insights into the associated transition from the regular to the chaotic behaviour. A cantorus like structure is obtained as the quantum equivalent of a classical torus.

References

1. P. K. Chattaraj and S. Sengupta, Phys. Lett. A, **181**, 225 (1993).
2. S. Sengupta and P. K. Chattaraj, Phys. Lett. A., **215**, 119 (1996).
3. P. K. Chattaraj, S. Sengupta and B. Maiti, Int. J. Quantum Chem., **100**, 254 (2004).
4. P. K. Chattaraj, S. Sengupta and S. Giri , J. Chem. Sci., **120**, 33 (2008).

The dynamics of angular degrees of freedom: new basis set and grid representations of Hamiltonian operators

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The Legendre functions $P_l(cosx)$ are the standard basis set for the construction of angular Hamiltonians and can be employed for variational as well as discrete representations. In Ref. [1] an alternative basis set, referred to as η basis has been presented that is related to Chebychev polynomials of the second kind. The $\eta_k(x)$ functions are, like the $P_l(cosx)$ functions, characterized by simple analytical expressions for matrix elements with the angular kinetic energy operator. In addition, the $\eta_k(x)$ functions can be considered an analogy to the so-called "Fourier" or "sinc" functions, a standard basis for the description of radial motion. The $\eta_k(x)$ and sinc functions have in common that they are related to equidistantly spaced quadrature grids, a convenient property for wave packet calculations with a discrete representation of the potential energy matrix.
The main disadvantage of the η basis is the fact that all $\eta_k(x)$ functions are vanishing at the interval borders. As a result, higher lying states in bound potential energy wells and rotational motion cannot be properly described by the η basis. This problem can be resolved by complementing the $\eta_k(x)$ functions appropriately.
We have investigated the performance of an extension of the η basis by adding orthogonalized linear combinations of $\eta_k(x)$ and $P_l(cosx)$ functions for different model problems. This extended basis set has been applied in both variational as well as discrete versions and can be shown to yield a very high accuracy, in many cases outperforming the Legendre method.

References

[1] C. Woywod, Chem. Phys. Lett. **281**, 168 (1997).

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