

CCP6 2008 Workshop

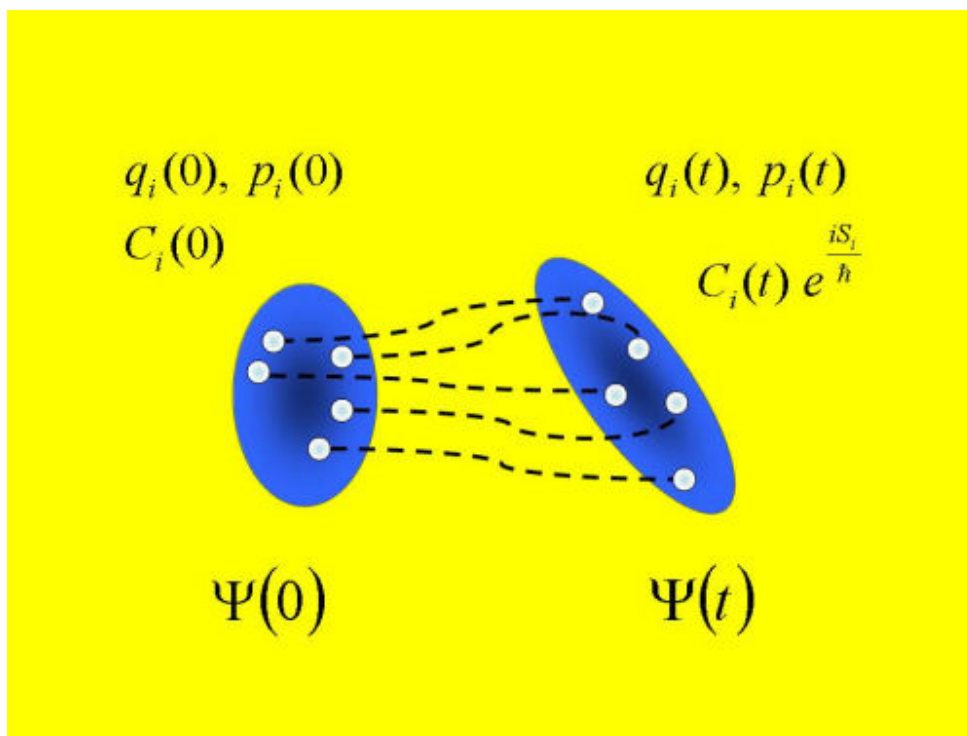
Multidimensional Quantum Mechanics with Trajectories

School of Chemistry, University of Leeds, 1st-3rd September

CCP6 (UK Collaborative Computational Project 6) is pleased to announce details of its 2008 meeting. The focus of this meeting is computational methods of quantum mechanics which in various ways rely on trajectories such as:

- Semiclassical approximations in quantum mechanics
- Exact quantum techniques based on basis sets or grids guided by classical trajectories
- Exact and approximate quantum techniques which rely on various forms of "nonclassical" trajectories

A common aspiration of all those approaches is to develop a quantum analog of classical molecular dynamics capable of simulating quantum effects in systems with many degrees of freedom. Many achievements in this direction have been reported in the last decade. By bringing together people developing different methods we hope for synergy between approaches and groups. According with CCP6 tradition a collection of short articles by the speakers will be published upon the completion of the meeting.



<http://www.chem.leeds.ac.uk/CCP608/>

Monday, 1st September 2008

Numerical and analytical methods based on semiclassical approximation

9:30 – 9-50	CCL ¹		Registration
9-50 – 10-00	1.53		Welcome and introduction
10-00 - 10-40	1.53	Kenneth Kay	Higher-Order Semiclassical Initial Value Approximations for the Propagator
10- 40 – 11-20	1.53	Michele Ceotto	First-principles Semiclassical Molecular Dynamics
11-20 – 11 -40			Coffee
11-40 – 12 -20	1.53	Frank Grossmann	Non-Markovian Dissipative Semiclassical Dynamics
12 -20 -13- 00	1.53	David Coker	Iterative linearized approach to condensed phase nonadiabatic dynamics
13-00 -14 -00	CCL		Lunch and posters CCP6 members meeting
14-00 - 14-40	1.53	Scott Habershon and David Manolopoulos	Theory and Applications of the Ring Polymer Molecular Dynamics Model
14-40 - 15-20	1.53	Jonathan Connor	New theoretical methods for understanding chemical reactions in the energy- and time-domains
15-20 - 16 -00	1.53	Vladimir Osherov and Vladimir Ushakov	Two-dimensional nonadiabatic scattering. Exact quantum solutions.
16-00 - 16-20			Coffee
16-20 - 17-00	1.53	Eli Pollack	The semiclassical route to real time quantum dynamics
17-00 - 17 -40	1.53	Florian Mintert and Eric Heller	Simulation of open quantum systems

¹ Registration, Lunch, and Posters will be in the Chaston Chapman Library School of Chemistry. Talks will be presented in the Room 1.53 .

Tuesday, 2nd September 2008

Exact trajectory based methods: Bohmian Mechanics and Gaussian grids.

10-00 - 10-40	1.53	Bob Wyatt	Dynamics with Quantum Trajectories
10- 40 - 11-20	1.53	Keith Hughes	Quantum Hydrodynamics for Mixed States
11-20 - 11 -40			Coffee
11-40 -12 -20	1.53	David Tannor	Bohmian Mechanics with Complex Action: An Exact Formulation of Quantum Mechanics with Complex Trajectories
12 -20 -13- 00	1.53	Craig Martens	Quantum Trajectories in Phase Space
13-00 -14 -00	CCL		Lunch and posters
14-00 - 14-40	1.53	Todd Martinez	New Developments in Spawning for Nonadiabatic and Tunneling Phenomena
14-40 - 15-20	1.53	Graham Worth	Quantum dynamics using Gaussian Wavepackets: The vMCG method.
15-20 - 16 -00	1.53	Dmitrii Shalashilin	Coupled Coherent States and a family of related techniques derived from variational principle.
16-00 - 16-20			Coffee
16-20- 17-00	1.53	Irene Burghardt	The G-MCTDH method: correlated system-bath dynamics using Gaussian wavepackets
17-00 - 17-40	1.53	Rocco Martinazzo	Local Coherent-State Approximation to system-bath quantum dynamics

19-00	Devonshire Hall	Conference dinner
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Wednesday, 3rd September 2008

Path Integrals and RPMD.

10-00 - 10-40	1.53	Bill Poirier	Bipolar Quantum Trajectory Simulations: Trajectory surface hopping and path integral Monte Carlo
10- 40 -11-20	1.53	Jeremy Schiff	A path integral approach to BOMCA
11-20 - 11 -40			Coffee
11-40 –12 -20	1.53	Mark Child	Accurate Scaling Laws for Strongly Anharmonic Vibrational Matrix Elements
12 -20 -13- 00	1.53		Concluding remarks and final discussion
13-00 -14 -00	CCL		Lunch and end of the workshop

Posters:

1	Adam Kirrander	CCL	Quantum dynamics in optical fields
2	Stewart Reed	CCL	Quantum simulations of Inramolecular Vibrational energy Redistribution
3	Xiao Shan	CCL	Reactive Angular Scattering using Parameterized Scattering Matrix Elements
4	Ashley Totenhofer	CCL	Nearside-Farside and Complex Angular Momentum Methods for Understanding the Angular Scattering of Chemical Reactions
5	Aaron Virshup	CCL	Clustering and Markov-Like Models for Visualization and Analysis of Trajectory-Based Quantum Dynamics
6	Vadim Volokhov	CCL	Trajectories and caustic near exchange reaction barrier
7	Xiahou Chengkui	CCL	Local Angular Momentum Analysis of Reactive Angular Scattering

Directions: Accommodation will be at **Devonshire Hall**

Address: Devonshire Hall, Off Cumberland Road, Leeds, LS6 2EQ (e-mail: devonshireconferences@leeds.ac.uk)



Devonshire Hall is located within walking distance of the School of Chemistry and 10 to 15 minutes by taxi from Leeds train station and 30 minutes from Leeds Bradford Airport.

Look for the directions at: <http://www.universallyleeds.co.uk/devonshirehall.html>

Dinner will be served on Sunday the 31st of August at Devonshire Hall at 19:00. Devonshire Hall personnel will be there to meet you 24 hours a day but we advise you to let Mandy Clarkson (m.j.clarkson@leeds.ac.uk), Dmitri (d.shalashilin@leeds.ac.uk) and Marcelo (m.miranda@leeds.ac.uk) know the time of your arrival. Devonshire Hall is about 15 minutes walk from the **School of Chemistry**.



Devonshire hall



School of Chemistry

List of participants:

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Article for Workshop Booklet

We ask all speakers to prepare a short article for publication in the CCP6 booklet. Having the article during the workshop helps the discussion so please bring yours with you. You can download a template from the workshop website using the following link.

<http://www.chem.leeds.ac.uk/CCP608/abstract.htm>

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