CECAM-FR-MOSER Discussion Meeting

Practical problems with dynamical nuclear quantum effects through semi-classical methods

Paris, June 26-28, 2017

Organizers:
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The atomic nuclei are quantum particles, but their dynamics is generally treated classically since their mass is relatively large. However, the thermal wavelength of light nuclei such as the proton is not negligible with respect to inter-atomic distances. Quantum effects can be, to a certain point, obtained through several semi-classical methods; the limits thereof are however rapidly reached : to what extent are they problematic? Experimentalists observe nuclear quantum effects in vibrational spectra and/or quasi-elastic neutron scattering: how do we have access to comparable information? Moreover, there exist several semi-classical or approximate methods, which rely on distinct approximations. Therefore, the question arises about their reliability – which could be checked against more rigorous methods in test cases – and their ability to probe specific observables.

Promising attempts at combining different approaches to describe nuclear quantum effects are being undertaken in several instances, in a variety of directions and purposes. A non exhaustive list includes path-integral based methods, Langevin-based dynamics, the Wigner formulation of quantum mechanics, Bohmian dynamics, quantum propagators and initial-value representations. The aim of this meeting is to gather people who are working on those methods (but others are equally welcome) to further pursue analysis of the advantages and shortcomings of each specific technique. The field is sufficiently mature to achieve a critical view of the available approaches, which employ to a different extent mathematical tools and algorithmic intuitions; we hope that a closer insight into each specific method will consolidate effective approaches and facilitate identifying new routes for improvements. Given the developing landscape of initiatives in this field, we intend to contribute by triggering focused discussions on selected topics of specific interest to applications in solid state problems and, importantly, that can act as gateways for more general discussions. The discussion will include examining benchmark systems gauged for these topics to be later included in an open repository.

The approach of this meeting would be to initiate working groups, possibly with the long term goal to sustain these discussions beyond the duration of the meeting. In practice, we propose to focus on the following topics, which are relevant in many research areas and often accessible through experiments:
1. Including nuclear quantum effects in vibrational spectra of solids
2. Zero-point energy leakage and measure conservation
3. Quantum simulations and experimental issues
4. Proton tunneling and quantum dynamics

Each session will be organized on the basis of a combination of three kinds of contributions: (i) general and pedagogical overviews on the state-of-the-art of the main approaches; (ii) technical insights into the mathematics and algorithms; (iii) informal discussions, led by an active chair, with a relevant allotted time. This discussion meeting could also serve as the seed of regular meetings (every two years) that could better coordinate the scientific activity on quantum dynamics around the French nodes of CECAM and contribute to similar activities within the European community.

CECAM discussion meeting "Practical problems with dynamical nuclear quantum effects through semi-classical methods" , June 26-28, 2017

The meeting will be held in the Jussieu campus, Tower 22, 1st floor, corridor 22-23, room 107

Monday afternoon		***Nuclear quantum effects and vibrational spectra***
	13:30 – 14:00	WELCOME COFFEE
F. Finocchi	14:00 – 14:15	Introductory remarks
D. Manolopoulos	14:15 – 15:15	Keynote: Ring-Polymer Molecular Dynamics
D. Lauvergnat	15:15 – 15:45	Quantum Dynamics with sparse-grids: Hénon-Heiles potential and H_2 clathrates
M. Ceotto	15:45 – 16:15	Semiclassical "Divide-and-Conquer" method for spectroscopic calculations of high-dimensional molecular systems
	16:15 – 16:45	TEA TIME
M. Rossi	16:45 - 17:15	Colored Noise Thermostats for Path Integral Approximations to Dynamical Observables
M. Calandra	17:15 – 17:45	Stochastic self-consistent harmonic approximation: theory and examples
R. Vuilleumier	17:45 – 18:30	DISCUSSION "Vibrational spectra"
	18:45 – 19:45	COCKTAIL at Jussieu campus
Tuesday morning		***Zero-point energy leakage and measure conservation***
S. Bonella	09:00 – 10:00	Keynote: (Wigner) Sampling of quantum initial conditions and classical trajectories
S. Huppert	10:00 – 10:30	Langevin-based simulations and zero-point energy leakage
	10:30 – 11:00	COFFEE BREAK
L. Kantorovich	11:00 – 11:30	Generalized Langevin Equation : from classical to quantum
M. Casula	11:30 – 12:00	Combining Quantum Monte Carlo with Path Integral Langevin Dynamics
Ph. Depondt	12:00 – 12:45	DISCUSSION "Stochastic approaches to NQE"
	13:00 – 14:00	Lunch at "L'Ardoise" restaurant
Tuesday afternoon		***Quantum simulations and experimental issues***
J. Teixeira	14:15 – 15:15	Keynote: Observation of quantum effects in liquid water and glasses
M. Benoit	15:15 – 15:45	Isotope fractionation of dissolved ionic species via path-integral molecular dynamics
F. Calvo	15:30 – 16:00	NQE in clusters via path-integral and quantum baths: successes and failures
	16:15 – 16:45	TEA TIME
F. Dulieu	16:45 – 17:15	Diffusion of O atoms on cold amorphous surfaces: evidence of tunneling ?
G. Geneste	17:15 – 17:45	Proton-conducting oxides: quantum effects
F. Finocchi	17:45 – 18:30	DISCUSSION "Simulations vs experimental issues"
	19:30 -	SOCIAL DINNER at "La Voie Lactée" restaurant
Wednesday morning		***Proton Tunneling and Quantum Dynamics***
S. Althorpe	09:00 – 10:00	Keynote: Quantum reaction rates via instanton theory and ring-polymer molecular dynamics
S. Ivanov	10:00 – 10:30	Semi-classical Propagation: Hilbert Space versus Wigner Representation
	10:30 – 11:00	COFFEE BREAK
S. Habershon	11:00 – 11:30	Accelerating quantum dynamics simulations using machine-learning
I. Tavernelli	11:30 – 12:00	Bohmian quantum dynamics: from model systems to molecular simulations
M. Ceotto	12:00 – 12:45	DISCUSSION "Tunneling and delocalization"
S. Bonella	12:45 – 13:15	Concluding remarks