

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

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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. Quantum simulations and experimental issues
3. Zero-point energy leakage and measure conservation
4. Proton tunneling

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, 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.