Internships offered in M2
2017-2018

Responsibles for internship

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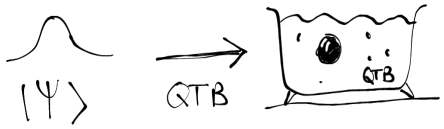
Internship topic: Modelling the quantum behaviour of nuclei in condensed matter

Many materials display intriguing properties caused by the quantum delocalization of atomic nuclei. Nonetheless, nuclei are usually considered as classical particles in numerical simulations. This is not always valid, especially for light nuclei such as hydrogen; many systems display strong isotope effects that can be measured experimentally but cannot be understood within classical statistical mechanics. Nuclear quantum effects remain a challenge for simulations; specifically, dynamical properties such as vibrational spectra that are essential to compare to experiments but for which no fully reliable and numerically efficient method exists.

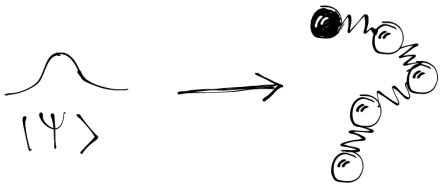
The theory group at INSP works on two complementary approaches for modelling nuclear quantum effects (NQE):

- The Quantum Thermal Bath (QTB), in which the quantum indeterminacy is mimicked via a Langevin equation with a suitable random force (the "bath"). This method has been and is currently used in our group to model NQE in complex condensed-matter systems (for instance, ice and hydrates under very high pressure [1,2]). It provides a semi-classical approximation to the quantum behavior of the nuclei with a limited numerical overcost with respect to classical simulations, but it proves insufficient in some cases. For this reason, we are developing a refined version of the QTB method with the aim of eliminating some of its most embarrassing drawbacks, such as the *zero-point energy leakage* [3].



In the Quantum Thermal Bath, a classical particle is immersed in a frequency-dependent bath that enforces the quantum Bose-Einstein distribution rather than the classical Boltzmann statistics.

- The most widespread methods for simulating NQEs are based on Feynman path-integrals that provide accurate results (at the price of a significant numerical overcost with respect to classical or QTB simulations) for *static* properties, such as atomic distributions, but none of the techniques imagined to model *dynamical* properties is fully satisfying. In collaboration with S. Bonella at EPF-Lausanne, we are implementing a method that applies path-integrals for sampling the Wigner function of the system under study [4,5], which provides a quantum analogue of the statistical probability distribution in classical mechanics. Thus, we expect to obtain an adequate description for the quantum dynamics of the nuclei.



In the Feynman path-integral formalism, a quantum particle is represented as a classical polymer made of P beads with temperature-dependent springs.

During the internship, the student will participate in the development of new methods and their testing on systems of increasing complexity. A taste for simulations and scientific computation is of course recommended, and both quantum and statistical physics will be essential ingredients of the internship work.

[1] Y. Bronstein et al. *Quantum-driven phase transition in ice described via an efficient Langevin approach* Phys.Rev. **B** 89, 214101 (2014).
[2] Y. Bronstein, Ph.D thesis (2016).
[3] F. Brieuc et al *Zero-point energy leakage in Quantum Thermal Bath simulations*, J.Chem.Theory Comp. **12**, 5688 (2016).
[4] J. Beutier et al *Computing thermal Wigner densities with the phase integration method*, J.Chem. Phys. **141**, 084102 (2014).
[5] J. Beutier, Ph.D thesis (2017).

Techniques involved: Path-integral molecular dynamics, quantum calculations on model systems, ab initio (DFT) molecular dynamics (option).
Paid internship: Yes
Can this internship be continued for a PhD? yes
If yes, type of PhD funding envisaged is: École doctorale