INTERNSHIP PROPOSAL

(One page maximum)

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Internship location: Campus Jussieu

Thesis possibility after internship: YES
Funding: YES If YES, which type of funding: ED PIF

Machine learning-assisted study of nuclear quantum effects in 2D noble gas clusters

Summary: The proposed thesis is centred on the implementation of the nested sampling method for exploring complex potential energy landscapes of condensed matter systems that include nuclear quantum effects. More particularly, to study noble gas clusters confined in two dimensions.
The *nested sampling algorithm* is a machine learning method issued from Bayesian statistics, used here to explore complex scalar functions. Unlike other methods such as simulated tempering and Wang-Landau sampling, nested sampling is able to provide the partition function of the system, and thus all the thermodynamic properties, from a single exploration, even in the presence of first-order transitions. This is achieved by using an evolving set of sampling points that allow the density of states evaluation during the potential exploration. However, this advantage is lost when the potential explicitly depends on the temperature, like in mean-field potentials, or when quantum effects of light nuclei are considered. To solve this issue, we recently developed a new method (Maillard et al., arXiv:2509.02361) that requires, as a trade-off, the introduction of new hyperparameters for sampling, which have to be adjusted on a case-by-case basis.
The proposed thesis work will mainly consist of 1) developing an automatic procedure to fine-tune the hyperparameters for exploring temperature-dependent potentials and 2) the theoretical determination of these hyperparameters from first principles (if possible). Lennard-Jones clusters in 2D will be considered as a benchmark test system. Such systems have recently been experimentally realised using noble gas atoms confined in a graphene sandwich (Längle et al., Nat. Mater., 2024). In particular, such 2D clusters show a liquid-solid phase transition at a temperature that depends on the number and type of atoms. The experimental results will be compared to the predicted ones. In particular, by exploring the dependence on the atomic mass, the contribution of nuclear quantum effects will be studied.

Techniques/methods in use:
The work will be centred on the use of the already existing code Nested_fit (https://github.com/martinit18/nested_fit) that will be further developed and driven by Python scripts. The nuclear quantum effects are evaluated using the Feynman path integral formalism.

Applicant skills:
Python coding (eventually also modern Fortran coding), basic knowledge of statistics and condensed matter. The knowledge of machine learning methods is welcome.

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO
Quantum Physics: YES Theoretical Physics: YES