

Master thesis proposal

INSP/SU, Campus P. et M. Curie (Jussieu)
Director: Geoffroy Prevot

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

Keywords: Potential energy exploration, nuclear quantum effect, partition function, machine learning, Bayesian method, nested sampling

Scientific description: 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.

Very recently, the formation of a few atoms' 2D clusters of noble gas confined in a graphene sandwich has been observed ([Längle et al., Nature Materials, 2024](#)). However, theoretical predictions of the stable configurations of these benchmark systems do not completely agree with the measurements. Moreover, for large clusters, a liquid-solid phase transition is also observed at a temperature that depends on the number and type of atoms.

The proposed thesis work will consist of exploring the energy landscape of such systems and including the quantum effects of the nuclei by varying the mass of the atomic gas (from helium to xenon). The computed solid-liquid and/or solid-solid phase transition temperatures, and stable configuration will be compared to the observed ones.

The inclusion of the nuclear quantum effects is obtained using Feynman's path integral approach. The chosen exploration method is the nested sampling, a Bayesian machine learning method that has several advantages with respect to other sampling techniques. In particular, the partition function and all thermodynamic properties can be extracted in a single exploration. This advantage is lost when the potential explicitly depends on the temperature, like when quantum effects of light nuclei are included. To solve this issue, we recently developed a new method ([Maillard et al., J. Chem. Phys. 163, 184109 \(2025\), arXiv:2509.02361](#)) that requires, as a trade-off, the introduction of new hyperparameters for sampling. A method to fine-tune the hyperparameters, which vary from case to case, will be investigated. Moreover, the development of the code on GPU will be welcome. (At present it is parallelized for multi-core CPUs only.).

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

Industrial partnership: N

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Internship location: INSP, Sorbonne Université, 4 place Jussieu, 75005 Paris

Possibility for a Doctoral thesis: Yes (to be financed via the doctoral school)