Laboratoire LAMBE

Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement
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Quantum Thermal Bath for Nuclear Quantum Effects calculations

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To take into account nuclear quantum effects on the dynamics of atoms, the path integral molecular dynamics (PIMD) method [1] used since 1980s is based on the formalism developed by R. Feynman. However, the huge computation time required for the PIMD reduces its range of applicability, in particular at low temperature and when using a first-principles description of the interatomic forces. Another drawback is the requirement of additional techniques to access time correlation functions (ring polymer MD or centroid MD).

We developed an alternative technique based on a quantum thermal bath (QTB) [2,3] which reduces the computation time by a factor of ~20. The QTB approach consists in a classical Langevin dynamics in which the white noise random force is replaced by a Gaussian random force having the power spectral density given by the quantum fluctuation-dissipation theorem. The method has yielded satisfactory results for weakly anharmonic systems: the quantum harmonic ascilator, the heat capacity of a MgO crystal, and the isotope effects in LiH and LiD.

Unfortunately, QTB is subject to the problem of zero-point energy leakage (ZPEL) in highly anharmonic systems, which is inherent in the use of classical mechanics. Indeed, a part of the energy of the high-frequency modes is transferred to the low-frequency modes leading to a wrong energy distribution. We have shown that in order to reduce or even eliminate ZPEL, it is sufficient to increase the value of the frictional coefficient [4]. Another way to solve the ZPEL problem is to combine the QTB and PIMD techniques [5]. It requires the modification of the power spectral density of the random force within the QTB. This combination can also be seen as a way to speed up the PIMD.

Results obtained by QTB-MD and QTB-PIMD calculations on *i*) the ferroelectric-phase transitions in $BaTiO_3$, and *ii*) and proton position-disorder in molecules will be presented.

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[4] F. Brieuc, Y. Bronstein, H. Dammak, P. Depondt, F. Finocchi, M. Hayoun J. Chem. Theory Comput. 12 (2016) 5688.

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