Nuclear quantum effects: their relevance in topology of hydrogen bonded network and diffraction studies of hydrogen bonded liquids

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0It is well established for molecular liquids that can form hydrogen bonds (HB, H-bond) that their structutural and dynamical properties depend on nuclear quantum effects (NQE), too Differences in terms of density, dynamic and thermodynamic properties between deuterated and hydrogenated forms of many liquids are well known, while the nature of deviations in terms of the atomic structure can be quite complex. The main goal of the present work is to shed some light on the structural aspects at leas three different aspect.

1. The proper description of NQE effect on intra and intermolecular radial distribution function
2. Proper validation of isotopic substitution method in neutron diffraction.
3. NQE effect on different topological properties of Hydrogen bonded liquids. These properties can represented the local topological arrangements (Local structure index, tetrahedrality …) or the cooperative behaviour of hydrogen bonded network. It would be also shown a significantly different behaviour exist in the simulations, which are incorporated the effect of polarizability (AIMD, AMOEBA)

Additionally based on extensive benchmark studies between our newly developed method ('Generalized Smoothed Trajectory Analysis' (GSTA)1,2) GSTA filtered and PIMD simulation results, reasonably good agreement between the two methods is presented.

1. Berta, D., Ferenc, D., Bakó, I., Madarász, Á., Nuclear Quantum Effects from the Analysis of Smoothed Trajectories: Pilot Study for Water J. Chem. Theory Comput. 2020, 16, 3316
2. Imre Bakó, Ádám Madarász, László Pusztai Nuclear quantum effects: their relevance in neutron diffraction studies of liquid water J. Mol. Liq.2021, 325 115192