Nuclear Quantum Effects in high-pressure ice

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Because of their light mass, hydrogen nuclei are subjected to nuclear quantum effects (NQE), mainly tunneling and zero-point energy. They can be crucial to describe correctly the properties of hydrogen-containing systems, even at room temperature. One prototypical example of the importance of NQE is the transition from asymmetric hydrogen bonds in phase VII to symmetric bonds in phase X of high-pressure ice, in which the zero-point energy drastically reduces the transition pressure.[1] However, natural ice is rarely pure and it has been shown that even small concentrations of salt (LiCl or NaCl) in ice have a strong effect on the phase diagram: the VII to X transition is shifted to higher pressures, questioning the resilience of NQE in the presence of ionic impurities.[2]

We investigate these questions using the Quantum Thermal Bath[3] , that is, a semi-classical Langevin dynamics, in order to take into account both NQE and thermal effects in pure and salty ices. We show why NQE can be sensitive to the presence of impurities and that non-trivial phenomena could result, such as the spectacular upshift of the transition pressure and the peculiar motion of ions throughout the ice lattice.[4]

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