Quantum Mechanics in a Glass of Water

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The momentum distribution of the protons participating in hydrogen bonds is quite different from a classical Maxwell distribution, even at temperatures higher than room temperature. Thus the equilibrium structure of liquid water is directly influenced by quantum mechanics. From the space and momentum distributions, accessible from neutron diffraction and deep inelastic scattering experiments, one can extract the effective potential experienced by the protons in condensed phases. Analysis of Path Integral simulation data shows that often the proton environment is nearly harmonic but anisotropic. In those cases semi-classical approximations should be valid, but in presence of tunneling, such as e.g. in ice under high pressure, a full quantum treatment is needed. Then interplay between quantum mechanical tunneling and ice-rule correlations leads to distinct observable effects.