Vibrational dynamics and tunneling of water in beryl

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The vibrational dynamics of ultra-confined water in single crystals of beryl ($Be_3Al_2Si_3O_{18}$) [1], the structure of which contains 4.86 Å diameter channels parallel to the *c*-axis, was studied with inelastic (INS) and quasi-elastic (QENS) neutron scattering. The results reveal significantly anisotropic dynamical behavior of confined water, and, somewhat counterintuitively, show that effective potential experienced by water along the channels is significantly steeper than perpendicular to them. QENS data show evidence of single-file diffusion of water molecules along the channels at higher temperatures (up to 370 K), but below 150 K this diffusion is strongly suppressed. No such suppression, however, has been observed in the channel-perpendicular direction.

Further high resolution INS measurements of beryl at low temperature (1.5 K) show 7 peaks at energies between 0.25 and 15 meV. The intensity of these peaks strongly decreases with increasing temperature (up to 40 K), contrarily to the expected behavior of vibrational excitations, which show an increase of intensity with temperature due to the thermal population. Therefore, these peaks must be explained by transitions between the split states of energy levels for water in beryl due to water tunneling between the 6-fold equivalent positions across the channels of the beryl crystal. This is the first direct observation of tunneling of macroscopic particle like water molecule by neutron spectroscopy.

[1] L.M. Anovitz, E. Mamontov, P. ben Ishai and A.I. Kolesnikov (2013), *Phys. Rev. E* **88**, 052306.