

Anomalous quantum diffusion of hydrogen atoms in proteins

Wednesday, 6 September 2017 10:00 (30 minutes)

Gerald Kneller

Centre de Biophysique Moléculaire
CNRS/University of Orléans, France

Quasielastic neutron scattering (QENS) from biomolecular systems, such as proteins, probes essentially the diffusive single particle dynamics of the hydrogen atoms. As far as the internal dynamics is considered, the motion of the hydrogen atoms exhibits both multiscale and quantum properties. Starting from the definition for the mean square displacement of a quantum particle, it will be shown how both aspects can be combined within a theory of QENS experiments, which is asymptotically exact for long times/low frequencies and for moderate momentum transfers.

[1] G.R. Kneller, J Chem Phys 145, 044103 (2016)

[2] G.R. Kneller, J Chem Phys 134, 224106 (2011)

Primary author: KNELLER, Gerald (University of Orleans / CNRS)

Presenter: KNELLER, Gerald (University of Orleans / CNRS)

Session Classification: Session 8