26. Neutron scattering kernel for light and heavy water including structure and molecular diffusion

J.I. Márquez Damian[1] and J.R. Granada[1,2]

[1] CONICET
[2] CNEA, Centro Atomico Bariloche, Av. Bustillo 9500, S.C. de Bariloche, 8400, Rio Negro, Argentina

The thermal neutron scattering kernels available for nuclear engineering applications in ENDF format over-predict the values of the total neutron cross sections in the cold energy range up to 100% and fail to reproduce the features observed by QENS and neutrondiffraction. These scattering kernels are based on only two essentially different models which contain a rough representation of the isolated molecule's dynamics, do not include collective vibrational modes or molecular diffusion, and do not consider the details of water structure. At the Neutron Physics Group of Centro Atomico Bariloche we are developing new scattering kernels for light and heavy water that include a better representation of cold neutron interactions using the standard numerical tool LEAPR/NJOY. In this poster we will present some results obtained by explicit inclusion of molecular diffusion and in the translational contribution to S(Q,w) for each liquid, as well as the coherent effects in the case of heavy water.