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New analysis frameworks for the analysis of inelastic measurements from neutron backscattering spectrometers

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Recent developments in the instrument design of neutron backscattering spectrometers allow to measure the total scattering function $S(q,\omega)$ with quasi-continous energy transfers but also with specific energy transfers - so called elastic fixed window scans (E/IFWS)- with a high energy resolution. While several models have been developed for the analysis of EFWS [1], there are only few approaches to analyze IFWS.

By reducing the number of energy transfers observed, the corresponding measuring time can be significantly reduced, allowing to investigate samples as a function of control parameters such as temperature-, pressure- or time-dependent samples.

In this contribution, several different approaches are presented to analyze the I/EFWS. This includes the combination of several IFWS as "sparse QENS" [2] , the extraction of generalized mean squared displacements [3] as well as the combination of EFWS and IFWS to extract global diffusion of dissolved proteins [4,5].

The different methods will be analyzed for their suitability for different neutron spectrometers taking into account their resolutions, energy transfers and momentum transfers. Results from modeled data of complex dynamics will be compared to measurements from IN16b (ILL).

[1] D. Zeller, J. Chem. Phys. 2018

[2] K. Pounot, JPCL, 2020

[3] Roosen-Runge et al, EPJ Web of Conf. 2015

[4] O. Matsarskaia et al, PCCP, 2020

[5] C. Beck, PhD Thesis, Univ. Tübingen, 2020

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