

Stochastic models for joint elastic and inelastic scattering data analyses

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Models available for scattering data analysis are often specialized to one specific type of data. For examples, a wide array of form- and structure-factors have been developed for analyzing specifically elastic small-angle scattering of x-rays or neutrons (SAXS or SANS). However, when it comes to analyzing inelastic scattering data on the very same systems - say neutron spin-echo (NSE) data - one often has to use different models. Ideally, one would use a single model to jointly analyze all the scattering data available. This would enable one to build on the structural insight from elastic scattering to better understand the dynamical information from inelastic scattering, and vice versa. This presentation illustrates how time-dependent stochastic models can be used for that purpose.

Two classes of models are discussed, namely time-dependent Gaussian-field and Boolean models. They are illustrated on scattering data analysis from micro emulsions (SANS with two contrasts and NSE) 1, from phospholipid membranes subject to bending and thickness fluctuations (SAXS, SANS and NSE) 2, as well as from silica aerogels (SANS and NSE) 3. In all these examples, the data analysis proceeds in two steps: the structural parameters of the model are first inferred from the SAXS or SANS, and the dynamical parameters are identified afterwards from NSE. In other words, inelastic scattering data analysis is used to characterize the time-dependence of the static structures identified through elastic scattering.

1 C.J. Gommès, R. Zorn, S. Jaksch, H. Frielinghaus, O. Holderer. Inelastic neutron scattering analysis with time-dependent Gaussian-field models. *J. Chem. Phys.* 2021, 155, 024121;

2 C.J. Gommès, P. Dubey, A. Stadler, B. Wu, O. Czakkel, L. Porcar, S. Jaksch, S. Frielinghaus, O. Holderer. Gaussian model of fluctuating membrane and its scattering properties. *Phys. Rev. E* 2024, 110, 034608;

3 C.J. Gommès. Time-Dependent Hierarchical Model for Elastic and Inelastic Scattering Data Analysis of Aerogels and Similar Soft Materials. *Gels* 2022, 8, 236.

Abstract Title

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