Reduction of SAXS data into sets of structural moments

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How much information is encoded in a small-angle scattering (SAS) curve? What does it tell us about the structure of the scattering object? Many have provided insights to answer those questions in the past, and we provide here an approach that we hypothesize will help refine shape classification of scattering objects.

In this talk, I will briefly outline the foundational answers to these questions. Then I will show how one can exploit the invariant properties of the scattering intensity to expand the SAS curve to a simple sum over a basis of functions well separated in the scattering space. We call the weights of the basis functions Kn that, together with the radius R of the support of the scattering object, give a complete theoretical description of the SAS curve. Those weights also entirely describe the pair distance distribution function (PDDF) of the object, as they are related to its moments. Adding an overall constant, these parameters are easily fitted against experimental data giving a concise comprehensive description of the data.

In addition to the understanding they bring, these invariants can also be used to reliably estimate structural moments beyond the radius of gyration, thereby rigorously defining the actual set of model-free quantities one can extract from experimental SAS data. I will conclude on how these quantities can help narrow down possible structural models for the scattering object.

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