Bayesian estimation of aggregated nanoparticle dispersions from small-angle neutron scattering data

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Small-angle scattering (SAS) is widely used to characterize nanoscale structures noninvasively, including the size of nanoparticles, by fitting experimentally measured scattering intensities with theoretical models. Conventionally, the parameters are obtained by manually adjusting the model to achieve the best fit to the SAS data or by performing nonlinear least-squares fitting. However, a previous study has pointed out that these fitting procedures are heuristic in nature or tend to converge to local minima in the parameter space [1]. Furthermore, the uncertainty of the estimated parameters and the validity of the selected model are not always evaluated. Bayesian inference provides a systematic framework for addressing these issues. In the previous study [1], using artificial SAS data generated by numerical simulations, posterior probability distributions of model parameters were calculated based on Bayesian inference, which has been explored as a new methodological approach. These distributions allow the estimated parameters to be evaluated together with their credible intervals. Bayesian model comparison can also be used to assess which structural model most appropriately describes the scattering data.

In this study, a dilute dispersion of silica nanoparticles (1 vol%) in D_2O solution was analyzed as a simple test case, for which interparticle interactions were negligible. The posterior distributions provided estimates of the particle radius and polydispersity together with their credible intervals. The analysis was then extended to a dispersion containing 100 mM NaCl. Models with unimodal and multimodal radius distributions $P(R)$ were compared using Bayesian model comparison (Fig. 1). The smaller-radius component was comparable to the particle radius observed without NaCl, whereas the larger-radius component was consistent with the emergence of aggregates under increased ionic strength. These results demonstrate that Bayesian inference enables systematic parameter estimation and model selection for experimental SANS data.

[1] Y. Hayashi, S. Katakami, S. Kuwamoto, K. Nagata, M. Mizumaki and M. Okada *J Phys Soc Jpn* 92:094002 (2023).

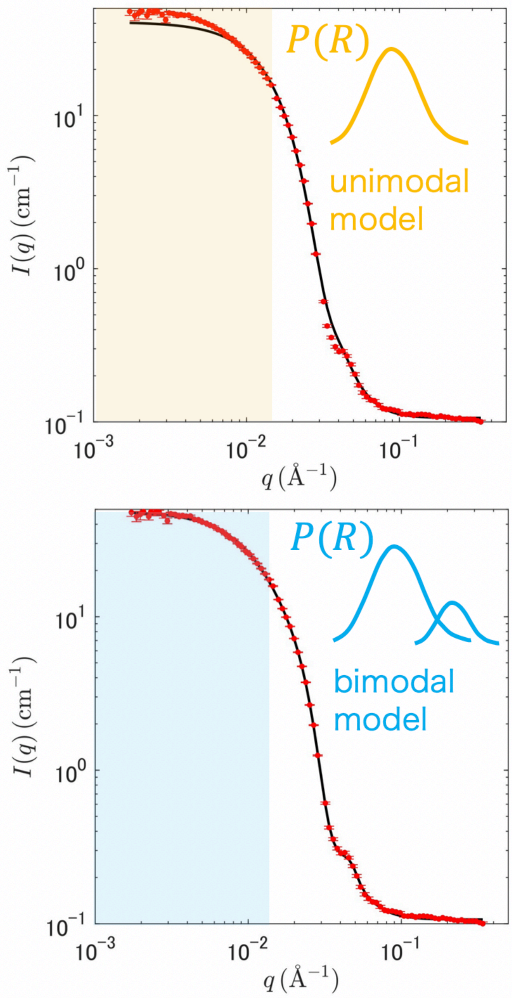

Fig. 1. Measured scattering intensity of silica nanoparticles dispersed at 1 vol% in D_2O containing 100 mM NaCl (red), and the fit obtained by Bayesian estimation (black).