Complexity Science 12-week research project proposal

Project title: Can we extract useful information from scattering artefacts in flow oriented spectroscopy experiments?

Supervisor (the person who will be doing the day to day supervision of the mini-project):
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Project proposal

A. Background to project

Whenever light interacts with a sample it is either absorbed (and perhaps later emitted) or scattered. In most spectroscopy applications we hope that scattering artefacts are minimal and we can focus on the absorbance. However, for particles whose size is within an order of magnitude of the wavelength of light this is often wishful thinking. The aim of this project is to turn this around and determine what information we can extract from the scattering effects in Couette flow cell experiments. It is anticipated that the emphasis will be on turbidity linear dichroism, which is the different in scattering of light polarized parallel to the flow direction and perpendicular to it. This project will require some mastery of fluid dynamics to determine orientation distributions as well as light scattering literature. It has the potential to be directly applicable in a number of current projects taking place at Warwick and at Birmingham. Follow-on work which could form an exciting and challenging PhD project would relate to more complex flow geometries, techniques with different optical factors, and more challenging overlapping experimental data systems than are proposed for this mini-project. Semi-rigid systems provide another layer of challenge and more complex size distributions than anticipated in the MSc project will be important for real systems.

B. Programme of work

The programme of work will proceed in stages

B.1 Removing the scattering from LD absorbance spectra

With fibres and membrane structures, one of the challenges is to determine what component of a measured spectroscopic signal is due to scattering and what to the spectroscopic signal of interest. We have previously had reasonable success in removing scattering following the method of Nordén and Nordh, which involves fitting an $a\lambda^{-k}$ functional form (Figure 1). However, scattering is a complicated function of particle size (being an overlap of Rayleigh and Mei scattering for nonspherical particles) in the regime in which we work. In this work we shall extend the approach used in our previous work (based on an appendix by Berne¹) to polarized light. Flow dynamics and size distributions will also be considered.

B.2 Testing the predictions

Data on a range of rigid particles will be collected to test the calculations. These may include off-theshelf particles with no absorbance as well as biological systems such as bacteriophage of varying dimensions and various protein fibre systems.

C. Skills to be learned

Theory: Basic fluid dynamics, scattering theory, MatLab programming, spectroscopic data analysis. **Experiment:** LD spectroscopy, absorbance spectroscopy, fluorescence spectroscopy, sample preparation, perhaps molecular biology methods to make phage and protein fibres.

D. Outline of a literature review, including starting references.

The simple starting point is provided by the discussions of scattering in 2 (available from AR). A more challenging group of references is provided by $^{3-5}$. The balance between theory and experiment on this project will determine exactly what literature is required.

- Berne, B. J. J. Mol. Biol. 1974, 89, 755. (1)
- (2)Nordén, B.; Rodger, A.; Dafforn, T. R. Linear dichroism and circular dichroism: a textbook on polarized spectroscopy; Royal Society of Chemistry: Cambridge, 2010.

 (3) Takahashi, M.; Kubista, M.; Nordén, B. Biochimie 1991, 73, 219.

 (4) Miakti, N.; Nordh, J.; Nordén, B. J. Phys. Chem. 1987, 91, 6048.

 - Nordh, J.; Deinum, J.; Nordén, B. Eur. Biophys. J. 1986, 14, 113. (5)