Extracting Interaction Potentials in Colloidal Monolayers via the Inversion of 2D Pair Correlation Functions

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The structure and stability of colloidal monolayers depends crucially on the effective pair interaction potential $u(r)$ between colloidal particles. In this study, we construct a novel method for extracting $u(r)$ from the 2D pair correlation function $g(r)$ of dense colloidal monolayers (the so-called inverse problem). The method is based on the Ornstein-Zernicke relation and the HMSA closure first proposed by Zerah and Hansen [1] which interpolates between the Hypernetted Chain (HNC) and the soft core Mean Spherical Approximation (SMSA) closures. The HMSA closure contains a single fitting parameter which is determined by requiring thermodynamic consistency between the virial and compressibility equations of state. The accuracy of the HMSA inversion scheme is compared to the conventional 'one-step' inversion methods of HNC and Percus-Yevick (PY). Specifically the accuracy of all three schemes is tested against $g(r)$ Monte Carlo simulation data from colloidal monolayers interacting via a range of commonly encountered potentials, including both purely repulsive potentials as well as potentials containing an attractive well. For all the potentials studied, we find the performance of the HMSA scheme to be superior to HNC and PY and crucially, we find that the HMSA scheme is able to faithfully distinguish between potentials with and without an attractive well. We also apply the HMSA scheme to experimental $g(r)$ data and find encouraging preliminary results. The proposed HMSA scheme is therefore a robust and more accurate alternative to conventional one-step inversion schemes.

References:

[1] G. Zerah and J.-P. Hansen Self-consistent integral equations for fluid pair distribution functions: Another attempt. J. Chem. Phys. 84, 2336 (1986)