Hydrodynamics of concentrated suspensions of permeable and core-shell particles using a precise multipole method

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Introduction

We report on equilibrium (short-time) and non-equilibrium (long-time) simulations of the hydrodynamics of suspensions of hard spheres. Equilibrium simulations are focused on diffusion properties of colloidal suspensions of permeable and core-shell particles [1, 2]. Non-equilibrium simulations address the sedimentation of a dilute suspension of non-Brownian impermeable spheres [3]. Many-body hydrodynamic interactions between spheres are evaluated using a precise multipole method, encoded in the HYDROMULTIPOLE and FAST-HYDROMULTIPOLE programs.

Equilibrium and non-equilibrium simulations

An individual permeable particle is modeled as a solvent-permeable sphere of interaction radius a and uniform permeability κ, with the fluid flow inside the particle described by the Debye-Bueche-Brinkman equation, and outside by the Stokes equation. Numerical results are presented for the hydrodynamic function (Fig. 1, left panel), $H(q)$, and its characteristic values: the short-time self-diffusion coefficient, the sedimentation coefficient, and the collective diffusion coefficient. It is found that for a given volume fraction, the wavenumber dependence of a reduced hydrodynamic function (Fig. 1, right panel) , $h(q)$, can be estimated by a single master curve, independent of the particle permeability, given by the hard-sphere impermeable model.

A core-shell particle is composed of a rigid, spherical dry core of radius a surrounded by a uniformly permeable shell of outer radius b and permeability κ. Numerical results are presented for the high-frequency shear viscosity, η_∞, and diffusion coefficients. The hydrodynamic influence of the core in concentrated systems is discussed.

As an application to a non-equilibrium problem, we consider sedimentation of a non-Brownian suspension of impermeable hard spheres. Attention is focused on the mean settling velocity and the structure of particles distribution as the suspension attains a non-equilibrium steady sedimentation state. With the complete neglect of Brownian motion, the sedimentation velocity and the particles configurational distribution in the steady state differ measurably from their equilibrium counterparts. Simulations reproduce short-range particle correlations in good agreement with the statistical description of sedimentation formulated by Cichocki and Sadlej [4].

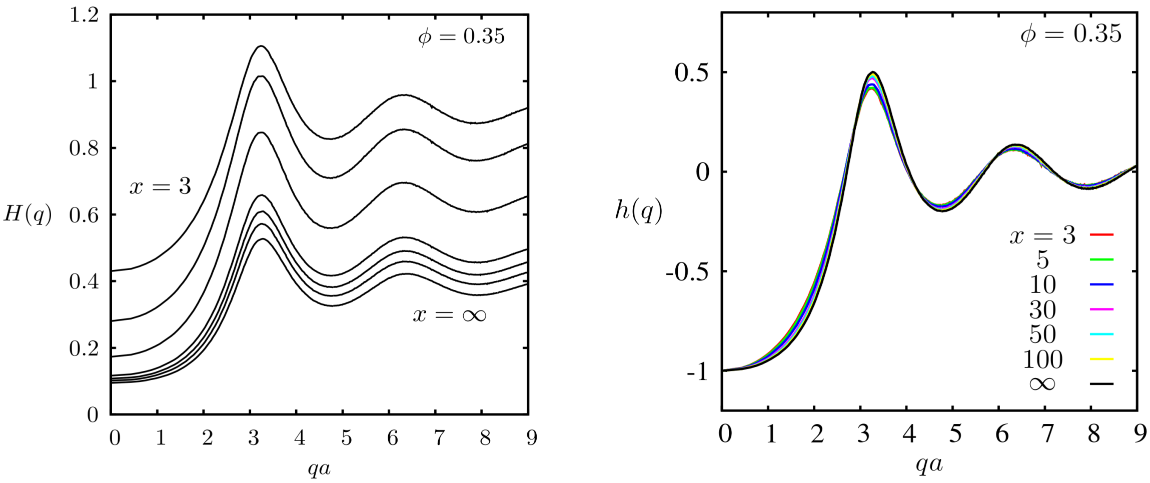

Figure 1: Hydrodynamic function, $H(q)$, and its reduced counterpart $h(q)$, for a volume fraction $\phi = 0.35$ and different values of the dimensionless hydrodynamic penetration depth x.

References

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