Short-time dynamics of concentrated suspensions of permeable particles

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Publications

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Part I


Part II

- High-frequency viscosity and generalized Stokes-Einstein relations in dense suspensions of porous particles (submitted to the Journal of Physics: Condensed Matter)
Physical system

Suspension: hard PERMEABLE spheres + fluid

Hydrodynamic interactions (HIs)
(coupling between the dynamics of the fluid and the particles)

Stationary Stokes hydrodynamics
(instantaneous HIs)

time scale of particles motion

Fluid flow

\[ \eta \nabla^2 \mathbf{v} - \nabla p = 0, \quad \nabla \cdot \mathbf{v} = 0 \]

+ boundary conditions
Motivation
Suspensions of core–shell particles

Little is known about transport properties of these systems

weaker hydrodynamic interactions
Transport processes

1. Sedimentation
\[ g \downarrow U_0 \]
\[ \eta_{\text{eff}}(\phi) > \eta_D(\phi) < D_0 \]

2. Brownian diffusion
\[ \langle |r(t) - r(0)|^2 \rangle \sim D_0 t \]
\[ K = \frac{U}{U_0} < 1 \]

3. Effective viscosity
\[ \ell \gg a \]
\[ \eta_{\text{eff}}(\phi) > \eta \]
Outline

- Hydrodynamic interactions
- Diffusion coefficients
- Effective viscosity
- Generalized Stokes-Einstein relations
Hydrodynamic interactions
(e.g. translational problem)

\[ U_i = \sum_{j=1}^{N} \mu_{ij}(1 \ldots N) \cdot F_j \]

Main difficulties while evaluating \( \mu(X) \)

- long–range
  \[ \mu_{ij} \sim \frac{1}{r_{ij}} \]

- many–body character
  \[ \mu_{ij}(1 \ldots N) \neq \mu_{ij}(ij) \]

- lubrication effects

HYDROMULTIPOLE algorithm
(Cichocki, Felderhof, Jones, Schmitz, Wajnryb...)
\[ O(N^3) \]
Dynamics of the fluid + particles

Induced force picture

Stationary Stokes equations

\[
\eta \nabla^2 \mathbf{v} - \nabla p = - \sum_{i=1}^{N} f_i(\mathbf{r}), \quad \nabla \cdot \mathbf{v} = 0
\]

- \( f_i \) represents the force density
- accounts for the presence of the particles in the flow

Formal solution

\[
\mathbf{v}(\mathbf{r}) = \mathbf{v}_0(\mathbf{r}) + \left[ \mathbf{Gf} \right](\mathbf{r})
\]

- Green propagator
- ambient flow
- force density
Single sphere

\[ f_i = -Z_0(i)v^{in} \]

induced force density

single-sphere resistance (boundary conditions)

Many spheres

\[ v_i^{in} = v_0 + \sum_{j \neq i}^N G(i,j)f_j \]

Green propagator depends on the fluid

Formal solution

\[ f = -Zv_0 \quad Z = \left[ Z_0^{-1} + G \right]^{-1} \]

many-sphere resistance

integral operators
Multipole description

Expansion in basis functions

\[ f_{ijkl} = f_{jkl} \]

\[ G_{ij} = G_{ji} \]

\[ c_{ilm\sigma} = c_{il\sigma m} \]

solutions of the Stokes eqs.

\[ v_{l m\sigma}^+(r) \sim r^{l+\sigma-1} \]

\[ v_{l m\sigma}^-(r) \sim \frac{1}{r^{l+\sigma}} \]

Resistance matrix

projection onto physical multipoles

\[ \zeta = \mathcal{P} \mathcal{Z} \mathcal{P} \]

Mobility matrix

\[ \mu = \zeta^{-1} \]

many-sphere resistance
Applications I. Brownian diffusion at short–times

\[ S(q, t) \approx S(q) \exp \left[ -q^2 D(q) t \right] \]

- autocorrelation of particle–density fluctuations
- structure factor
- diffusion function

\[
D(q) = D_0 \frac{H(q)}{S(q)}
\]

- single–sphere diffusion coeff.
- hydrodynamic function (many–body HIs)
- mobility matrix

\[
H(q) = \left\langle \frac{k_B T}{N D_0} \sum_{i,j=1}^{N} \hat{q} \cdot \mu_{ij}^{tt} \cdot \hat{q} \exp[iq \cdot (R_i - R_j)] \right\rangle
\]

- propagation of HIs
- structural relaxation

\[
\frac{\rho a^2}{\eta} \ll t \ll \frac{a^2}{D_0}
\]

- time scales
- hard spheres equilibrium

Applications I.
Hydrodynamic function

generalized sedimentation coefficient

$H(q)$

location of the principal peak of $S(q)$

collective motion

self-motion

$q_m$

$q$
Suspension of permeable spheres

Flow inside the spheres
(Debye–Bueche–Brinkman)

\[ \eta \nabla^2 \mathbf{v} - \eta \kappa^2 \mathbf{v} - \nabla p = 0, \quad \nabla \cdot \mathbf{v} = 0 \]

Two parameters characterizing the model

- \( x = \kappa a \) reduced inverse permeability
- \( \phi = \frac{4}{3} \pi a^3 n \) particle volume fraction

well-explored in the literature!
Hydrodynamic function
(generalized sedimentation coefficient)

$H(q)$

$q_m \alpha$ location of the principal peak of $S(q)$
Short–time transport coefficients

Self–diffusion coefficient

\[ D_s = D_0 H(q \to \infty) \]

Collective motions

**Sedimentation coefficient**

\[ K = \frac{U}{U_0} = \lim_{q \to 0} H(q) \]

**Gradient diffusion**

\[ J = -D_c \nabla \phi \quad D_c = \frac{D_0}{S(0)K} \]

**Diffusion at** \( q_m \)

"cage" diffusion

obtained from \( H(q_m) \)
Self–diffusion coefficient

Cichocki et al. (2002)

\[ O(\phi^2) \]

\[ \frac{D_s}{D_0} \]

\[ x \rightarrow \infty \]

highly permeable

impermeable (stick b. c.)
Sedimentation and collective diffusion coefficients

Batchelor (1972)

\[ x \rightarrow \infty \]

Cichocki et al. (2002)

\[ O(\phi^2) \]

\[ x \rightarrow \infty \]
Hydrodynamic function
(generalized sedimentation coefficient)

\[ q_m \alpha \] location of the principal peak of \( S(q) \)
**Reduced hydrodynamic function**

\[ h(q) = \frac{H(q) - H(\infty)}{H(\infty) - H(0)} \]

\[ h_m(q) = \frac{H(q) - H(\infty)}{H(q_m) - H(\infty)} \]

We can estimate \( H(q) \) in terms of the reduced functions for hard spheres with stick boundary conditions and the coefficients

\[ H(0) = K(x, \phi), \quad H(\infty) = D_s(x, \phi)/D_0(x), \quad H(q_m; x, \phi) \]
Summary

- Short-time dynamic properties of uniformly permeable spheres have been calculated as a function of permeability and concentration.

- The hydrodynamic function can be shifted and scaled to that of impermeable hard spheres.

- The short-time generalized Stokes-Einstein relations are valid to moderate accuracy only for $D(q_m)$. 