Short-time dynamics of concentrated suspensions of permeable particles

Gustavo Abade

Department of Mechanical Engineering
University of Brasília, Brazil

B. Cichocki M. L. Ekiel-Jezewska G. Nägele E. Wanjryb

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Publications

Authors: G. Abade, B. Cichocki, M. L. Ekiel-Jezewska, G. Nägele, E. Wanjryb

Part I

- Short-time dynamics of permeable particles in concentrated suspensions. *J. Chem. Phys.* **132**, 014503 (2010)

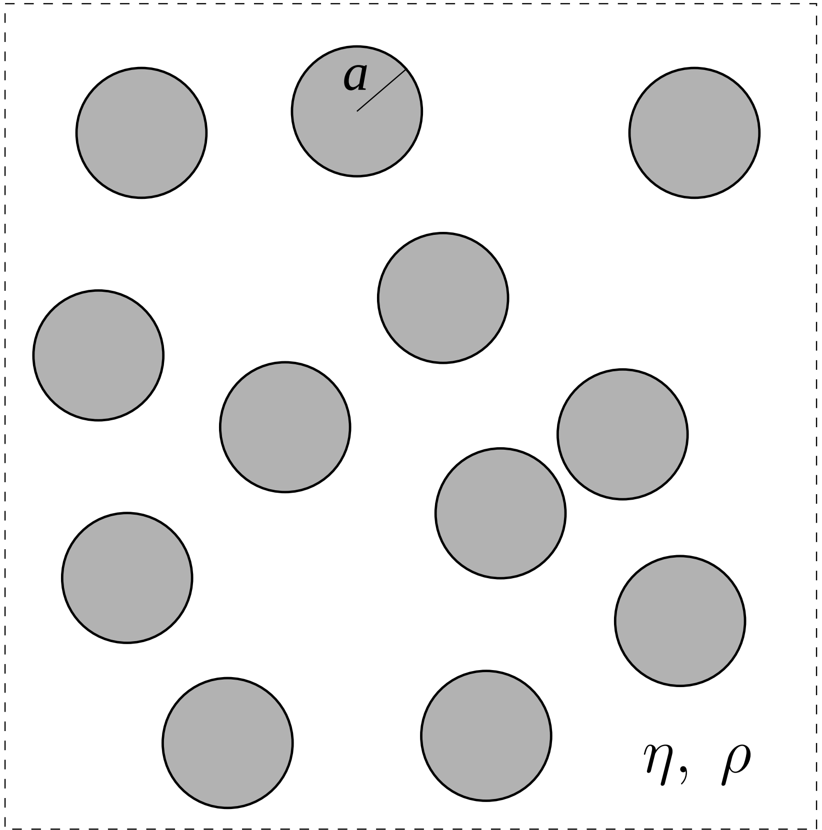
- Dynamics of permeble particles in concentrated suspensions, *Phys. Rev. E* **81**, 20404(R) (2010)

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 — $t \gg a^2 \frac{\rho}{\eta}$ viscous relaxation

Fluid flow

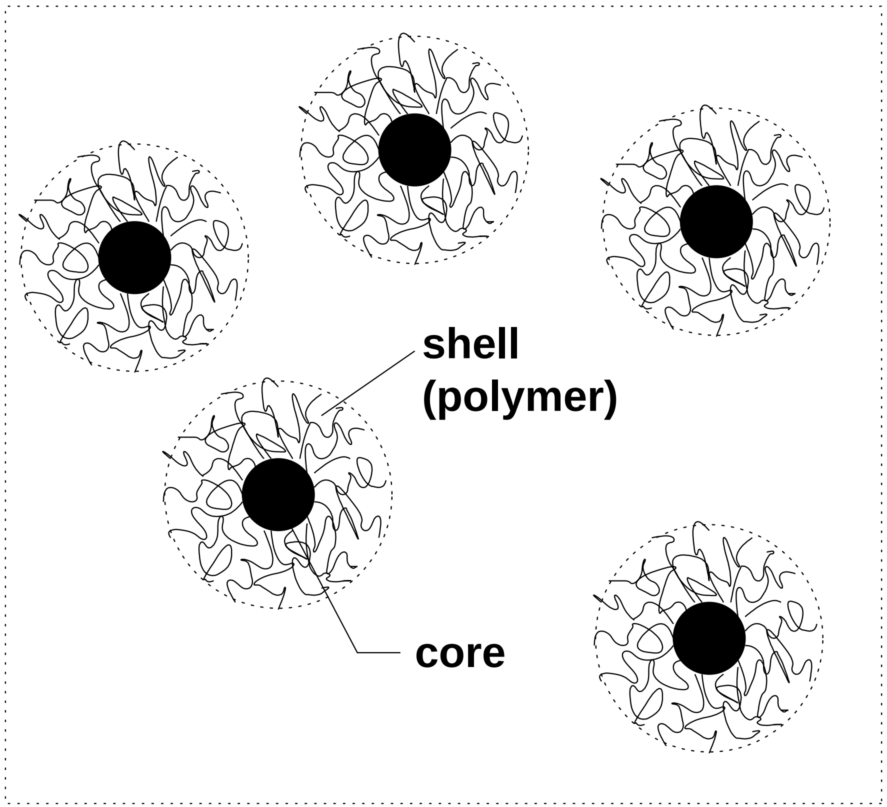
$$\eta \nabla^2 \mathbf{v} - \nabla p = 0, \qquad \nabla \cdot \mathbf{v} = 0$$

+

boundary conditions

Motivation

Suspensions of core−shell particles

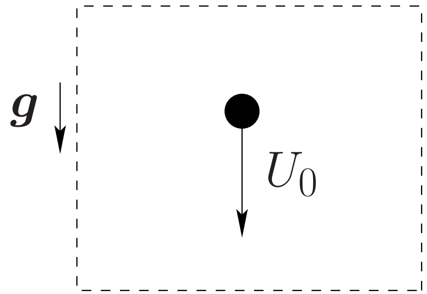


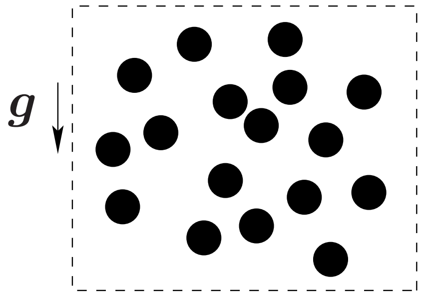
Little is known about transport properties of these systems

weaker hydrodynamic interactions

Transport processes

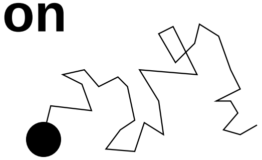
1. Sedimentation



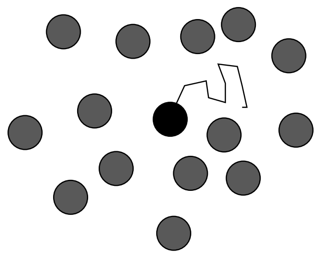


$$K = \frac{U}{U_0} < 1$$

2. Brownian diffusion



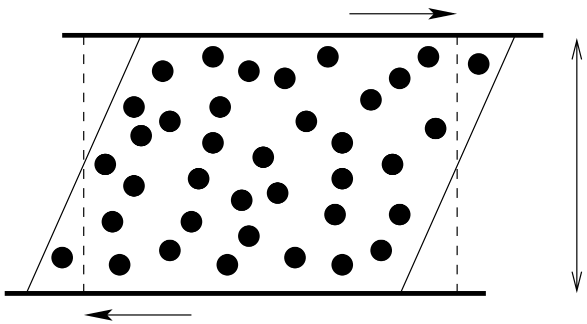
$$\langle |\mathbf{r}(t) - \mathbf{r}(0)|^2 \rangle \sim D_0\, t$$



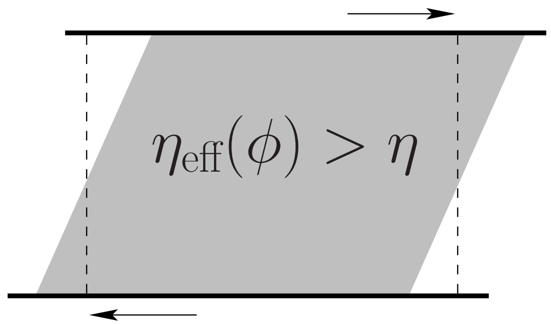
$$D_s(\phi) < D_0$$

self−diffusivity

3. Effective viscosity



$$\ell \gg a$$



Outline

- Hydrodynamic interactions
- Diffusion coefficients
- Effective viscosity
- Generalized Stokes-Einstein relations

Hydrodynamic interactions

(e.g. translational problem)

external forces

$$\mathbf{U}_i = \sum_{j=1}^{N} \boldsymbol{\mu}_{ij}(1\ldots N)\cdot\boldsymbol{\mathfrak{F}}_j$$

particle velocities

mobility matrix
(central entity)

Main difficulties while evaluating $\boldsymbol{\mu}(\mathbf{X})$

- **long−range**

$$\boldsymbol{\mu}_{ij} \sim \frac{1}{r_{ij}}$$

- **many−body character**

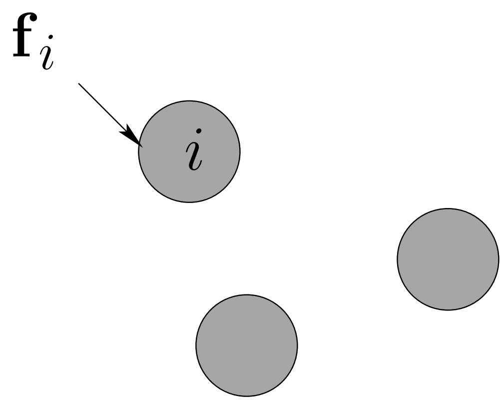
$$\boldsymbol{\mu}_{ij}(1\ldots N) \neq \boldsymbol{\mu}_{ij}(ij)$$

- **lubrication effects**

HYDROMULTIPOLE algorithm
(Cichocki, Felderhof, Jones, Schmitz, Wajnryb...)
$O(N^3)$

Dynamics of the fluid + particles

Induced force picture



Stationary Stokes equations

$$\eta \nabla^2 \mathbf{v} - \nabla p = - \sum_{i=1}^{N} \mathbf{f}_i(\mathbf{r}), \qquad \nabla \cdot \mathbf{v} = 0$$

force density

accounts for the presence
of the particles in the flow

Formal solution

Green propagator

$$\mathbf{v}(\mathbf{r}) = \mathbf{v}_0(\mathbf{r}) + [\mathbf{G}\mathbf{f}](\mathbf{r})$$

ambient
flow

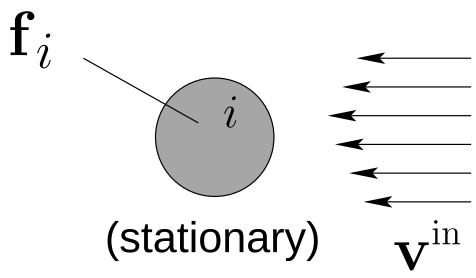
force density

Single sphere

$$\mathbf{f}_i = -\mathbf{Z}_0(i)\mathbf{v}^{\text{in}}$$

induced force density

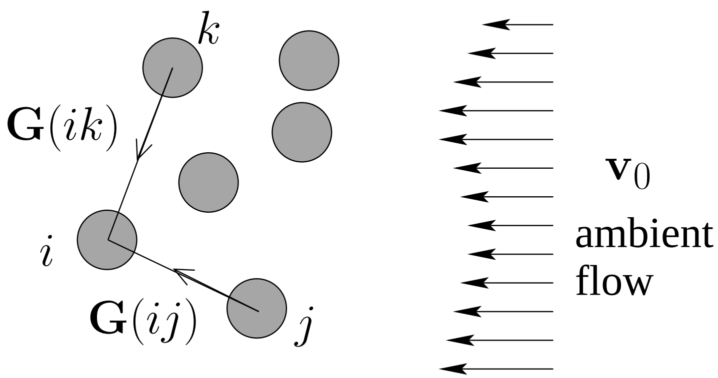
single−sphere resistance (boundary conditions)



Many spheres

$$\mathbf{v}_i^{\text{in}} = \mathbf{v}_0 + \sum_{j \neq i}^{N} \mathbf{G}(ij)\mathbf{f}_j$$

Green propagator
depends on the **fluid**



Formal solution

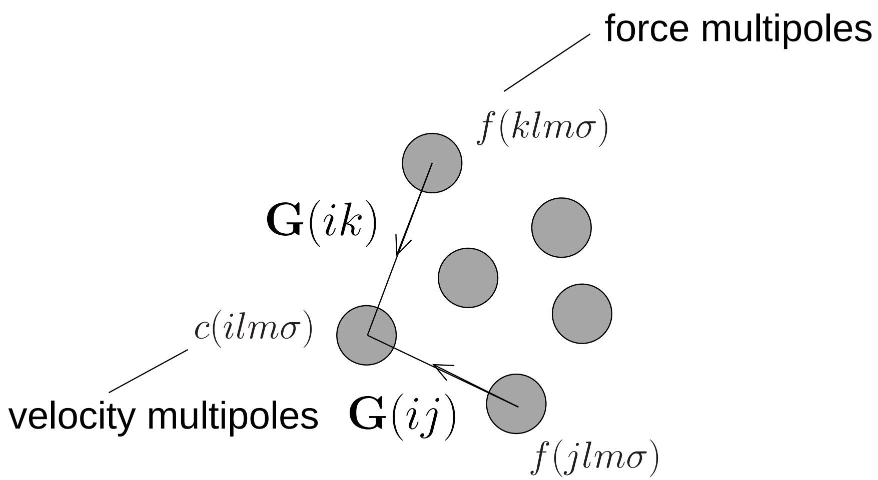
$$\mathbf{f} = -\mathbf{Z}\boldsymbol{v}_0 \qquad \mathbf{Z} = \left[\mathbf{Z}_0^{-1} + \mathbf{G}\right]^{-1}$$

many−sphere resistance

integral operators

Multipole description

Expansion in basis functions



solutions of the Stokes eqs.

$$\mathbf{v}^{+}_{lm\sigma}(\mathbf{r}) \sim r^{l+\sigma-1}$$

$$\mathbf{v}^{-}_{lm\sigma}(\mathbf{r}) \sim \frac{1}{r^{l+\sigma}}$$

Resistance matrix

$$\boldsymbol{\zeta} = \mathcal{P}\mathbf{Z}\mathcal{P}$$

projection onto physical multipoles

many−sphere resistance

Mobility matrix

$$\boldsymbol{\mu} = \boldsymbol{\zeta}^{-1}$$

Applications I.
Brownian diffusion at short−times

time scales

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

propagation of HIs

structural relaxation

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

autocorrelation of particle−density fluctuations

structure factor

diffusion function

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

hydrodynamic function (many−body HIs)

single−sphere diffusion coeff.

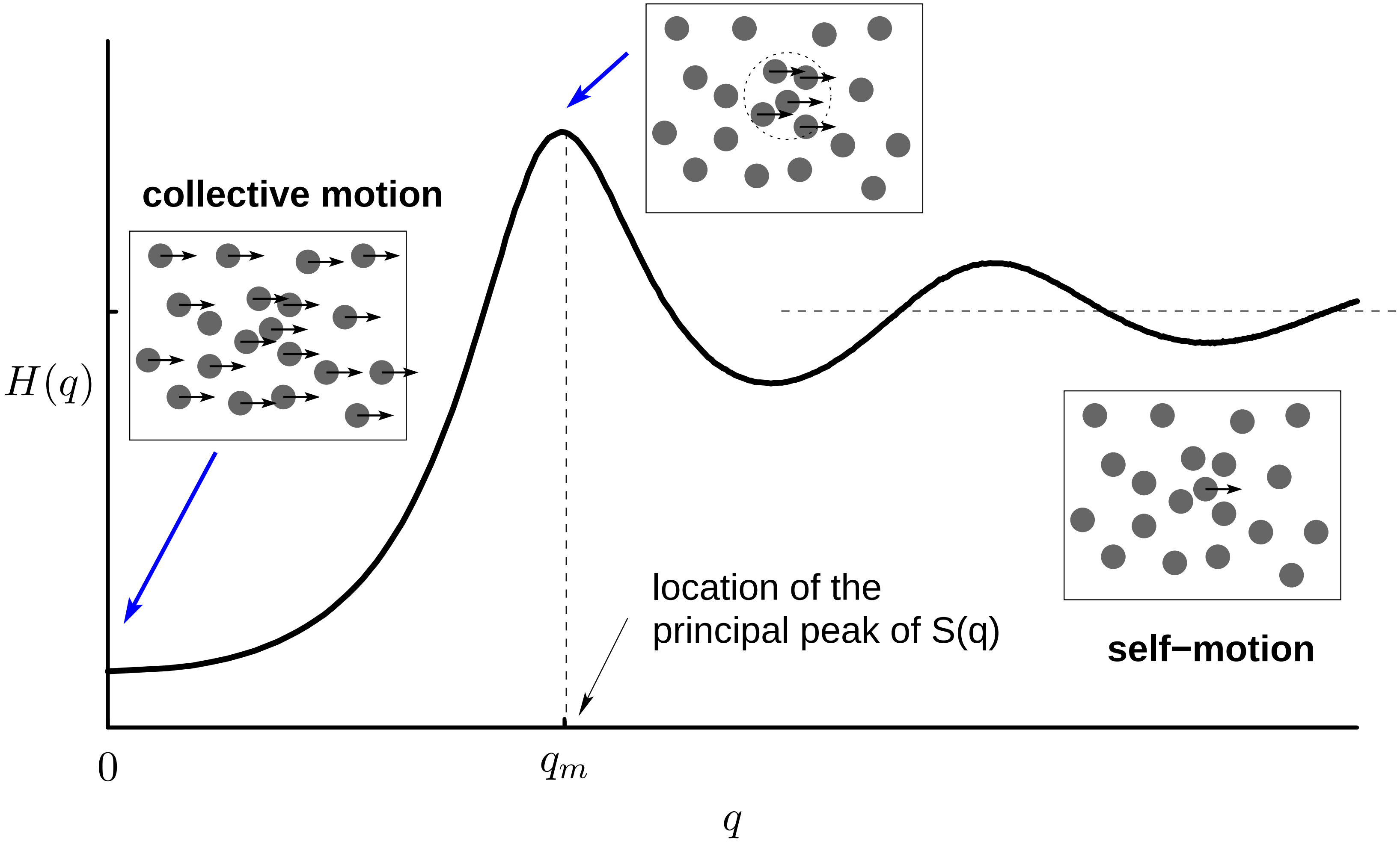
hard spheres equilibrium

$$H(q) = \left\langle \frac{k_B T}{N D_0} \sum_{i,j=1}^{N} \hat{\mathbf{q}} \cdot \boldsymbol{\mu}_{ij}^{tt} \cdot \hat{\mathbf{q}} \exp[i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)] \right\rangle$$

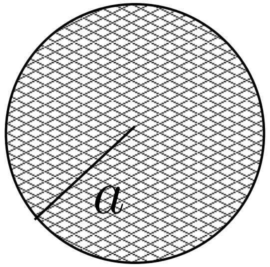
mobility matrix

Hydrodynamic function

generalized sedimentation coefficient



Suspension of permeable spheres



affects Z_0 only

Flow inside the spheres

(Debye−Bueche−Brinkman)

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

inverse permeability

Two parameters characterizing the model

$$x = \kappa a$$

reduced inverse permeability

$$\phi = \frac{4}{3}\pi a^3 n$$

particle volume fraction

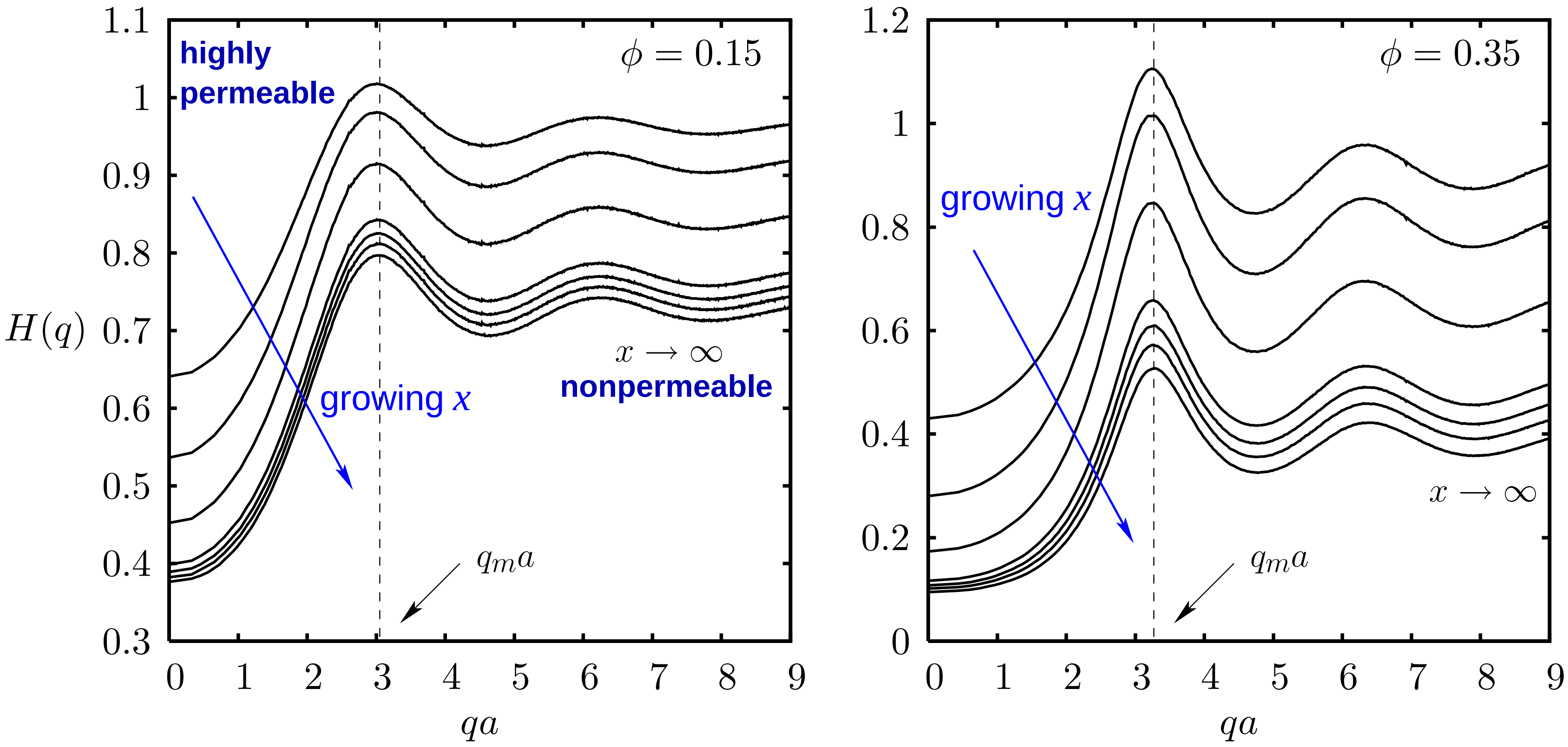
$x \to \infty$

nonpermeable sphere

well−explored in the literature!

Hydrodynamic function

(generalized sedimentation coefficient)



$q_m a$ 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

$$\mathbf{J} = -D_c \nabla \phi \qquad D_c = \frac{D_0}{S(0)} K$$

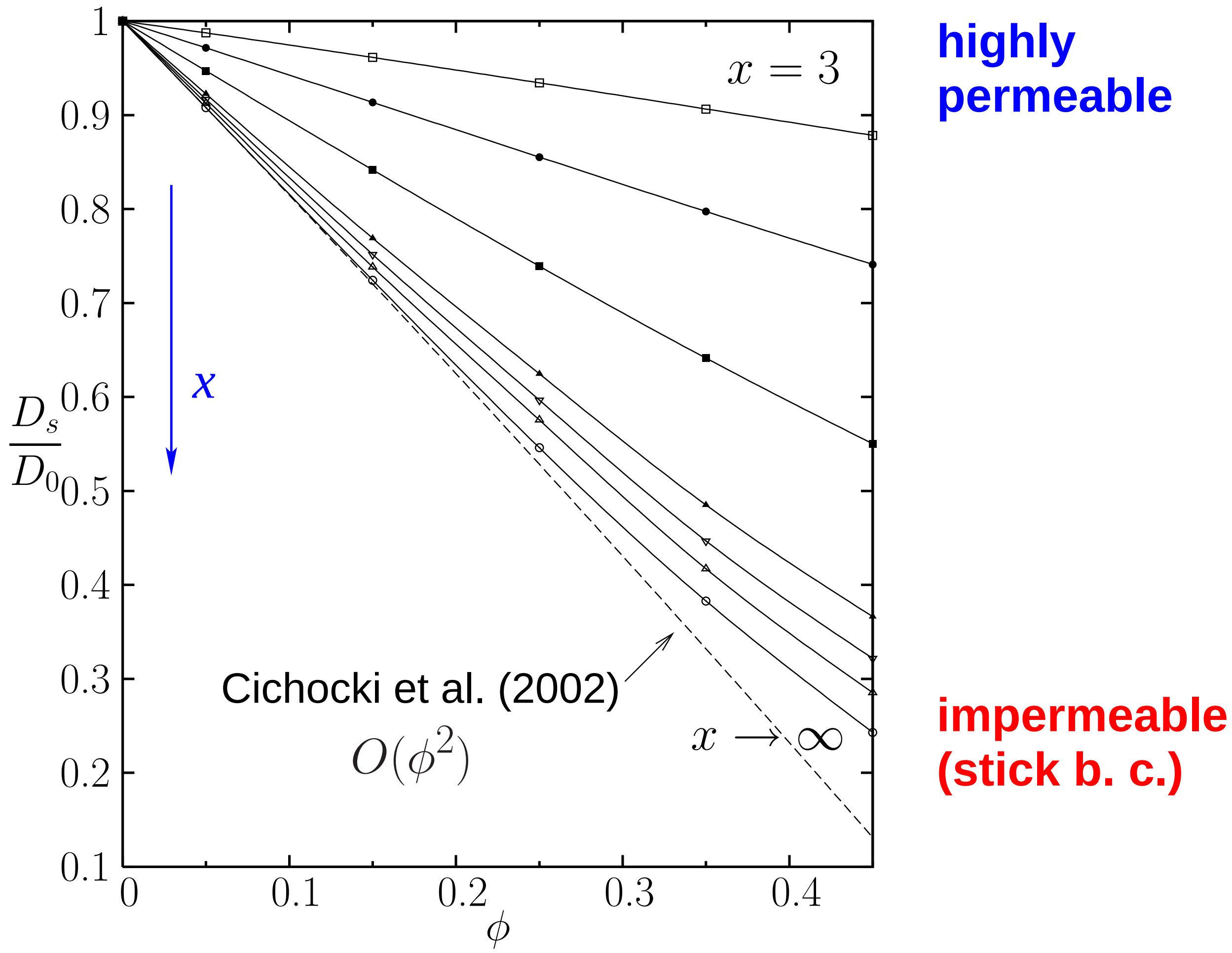
particle flux

Diffusion at q_m

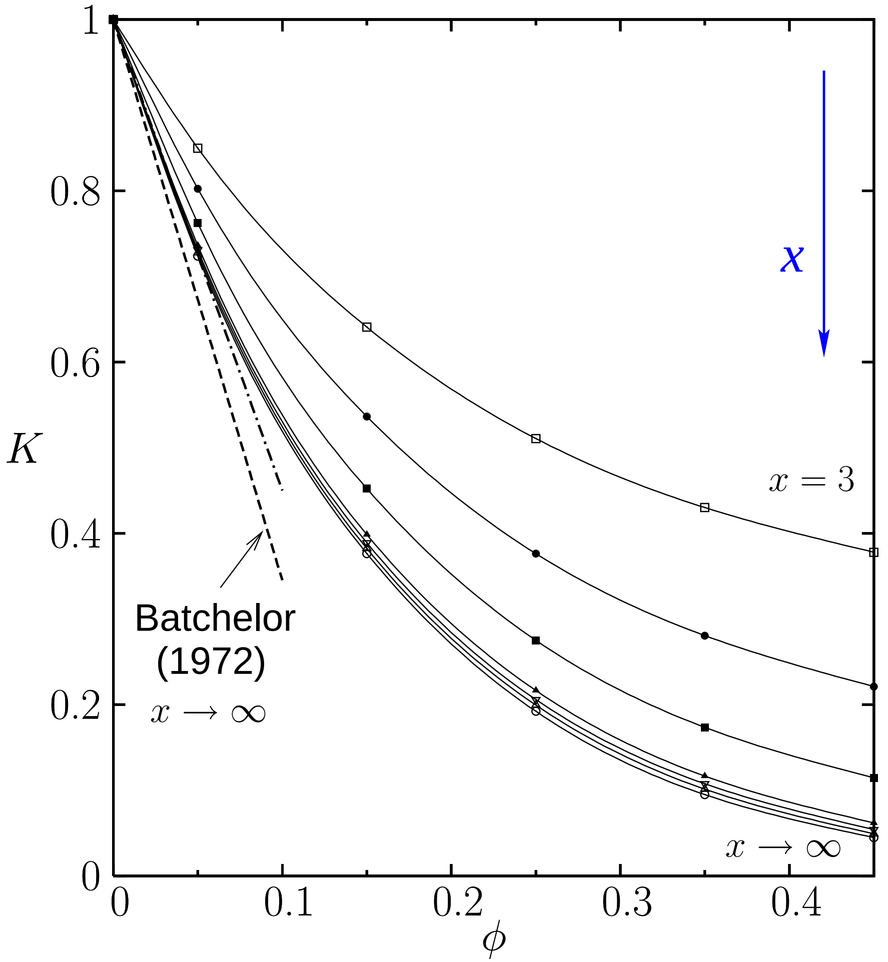
¨cage¨ diffusion

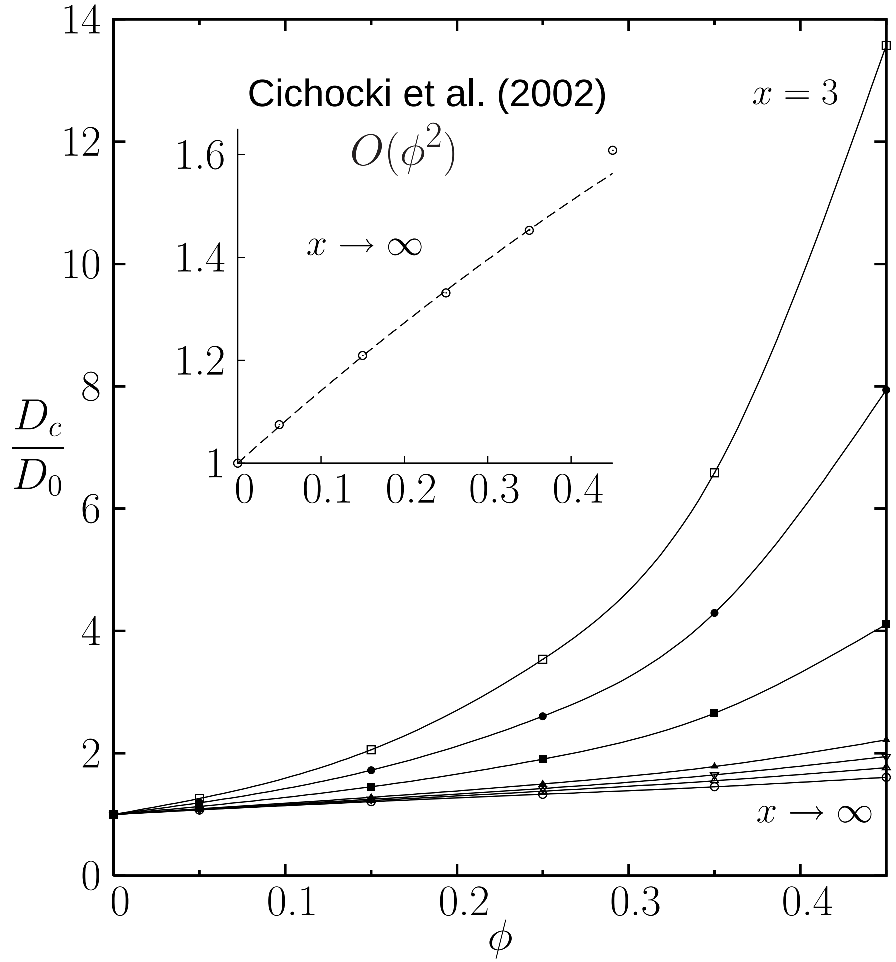
obtained from $H(q_m)$

Self−diffusion coefficient



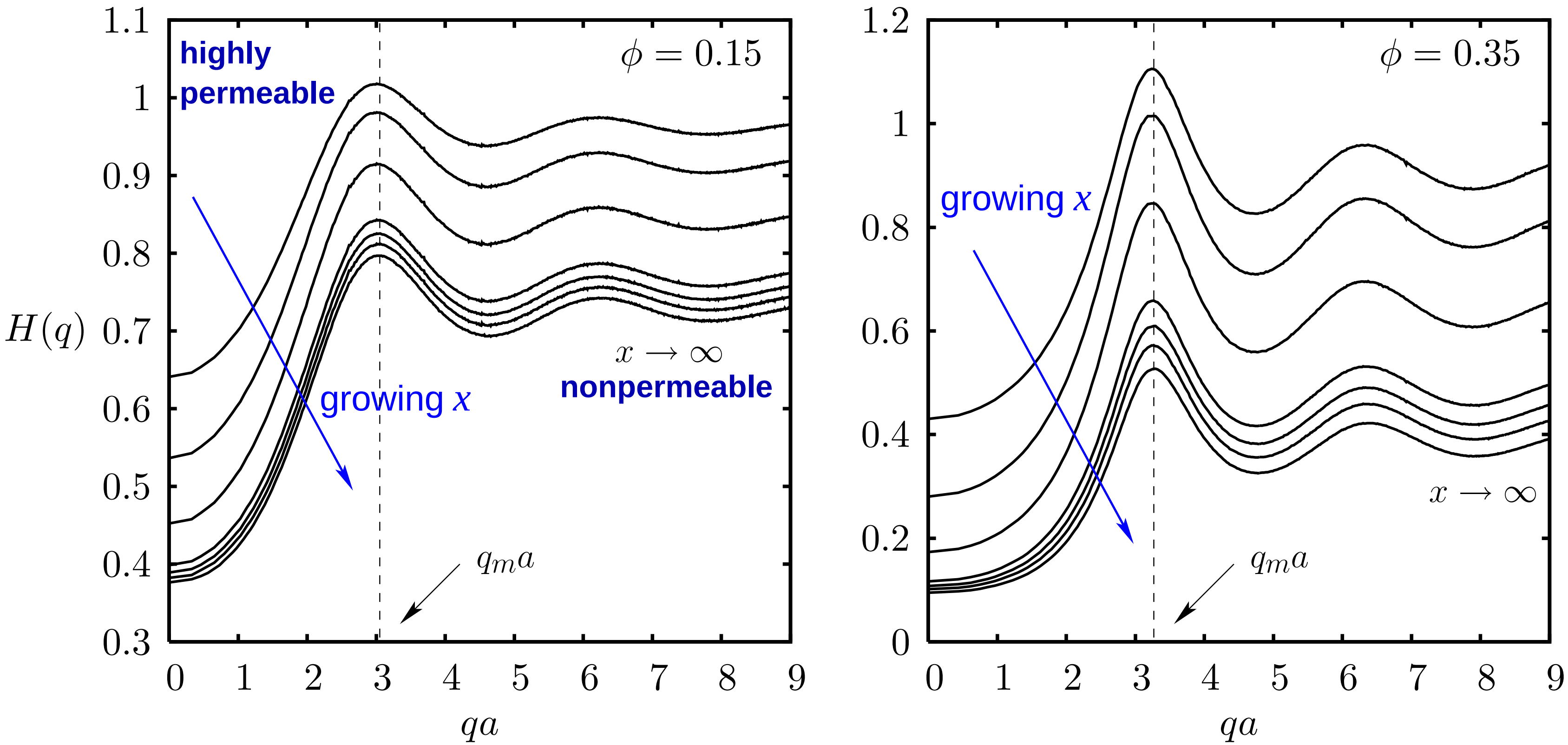
Sedimentation and collective diffusion coefficients





Hydrodynamic function

(generalized sedimentation coefficient)

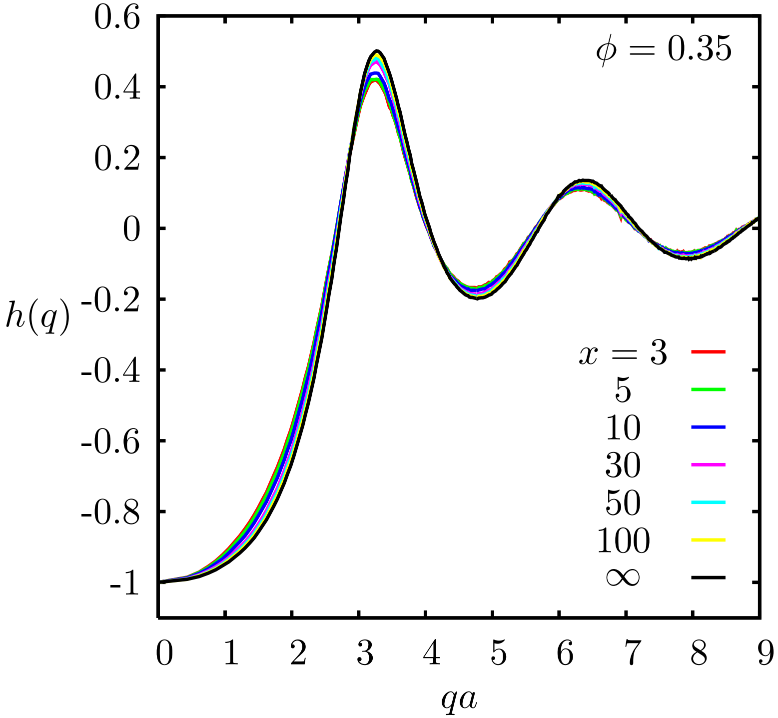


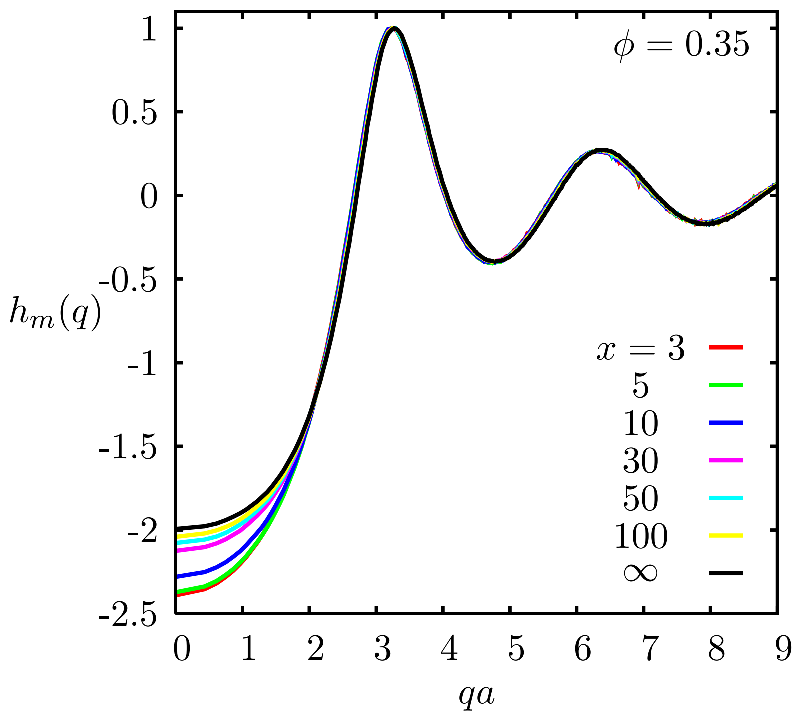
$q_m a$ location of the principal peak of S(q)

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 $D(q_m)$.