Approximate method of calculation of transport coefficients for suspensions.

Karol Makuch, Bogdan Cichocki

Institute of Theoretical Physics, Warsaw University, Poland

Suspension of spherical particles.

Stokes equations for N spheres (stick boundary conditions).

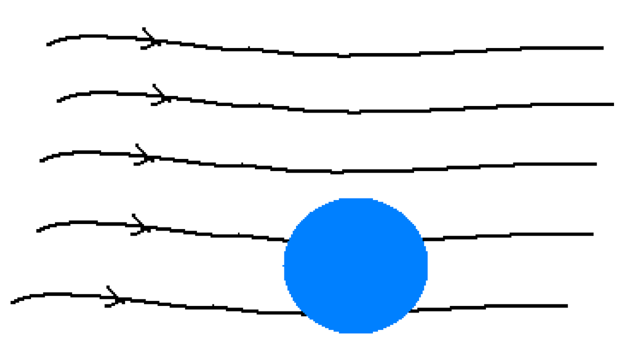
$$\nu\Delta\vec{v}(\vec{r}) - \vec{\nabla}p(\vec{r}) = -\sum_{i=1}^{N}\vec{f}_i(\vec{r})$$

$$\vec{\nabla}\cdot\vec{v} = 0$$

$$\left.\begin{array}{l}\vec{v}(\vec{r}) = \vec{u}_i + \vec{\Omega}_i \times (\vec{r} - \vec{R}_i)\\ p_i(\vec{r}) = 0\end{array}\right\} \vec{r} \in S_i$$

$\vec{v}(\vec{r})$ - velocity field of suspension,
$\vec{u}(\vec{r})$, $\vec{\Omega}(\vec{r})$ - velocity and angle velocity of i-th particle,
$\vec{f}_i(\vec{r})$ - induced forces (on the surface of i-th particle).

One particle problem



One particle in an ambient flow $\vec{v}_0(\vec{r})$.

One-particle friction kernel

$$\vec{f}(\vec{r}) = \int d\vec{r}'\ Z_0(\vec{r}, \vec{r}')\vec{v}_0(\vec{r}')$$

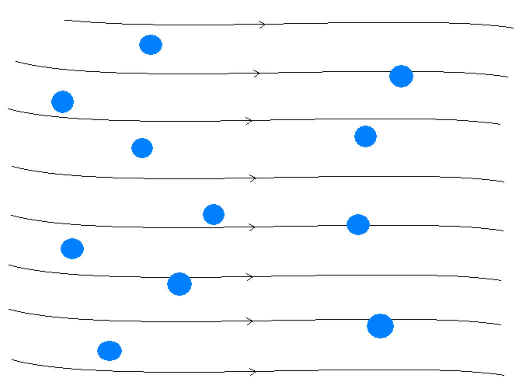
Forces induced on the surface of particle

Solution:

$$\vec{v}(\vec{r}) = \vec{v}_0(\vec{r}) + \int d\vec{r}'\ G(\vec{r} - \vec{r}')\vec{f}(\vec{r}')$$

$G(\vec{r}) = \frac{1}{8\pi\eta r}(1 + \hat{r}\hat{r})$ - Oseen tensor.

Many particle problem.



Suspension velocity field

$$\vec{v}(\vec{r}) = \vec{v}_0(\vec{r}) + \sum_{i=1}^{N}\int d\vec{r}'\ G(\vec{r} - \vec{r}')\vec{f}_i(\vec{r}')$$

The flow acting on particle i (induced by remaining particles)

$$\vec{v}_i^{\mathrm{act}}(\vec{r}) = \vec{v}_0(\vec{r}) + \sum_{j\neq i}\int d\vec{r}'\ G(\vec{r} - \vec{r}')\vec{f}_j(\vec{r}')$$

Multipole expansion: $v_i^{\mathrm{act}} = v_{0i} + \sum_{j\neq i} G(ij)f_j$ $\qquad f_i = Z_0(i)v_i^{\mathrm{act}}$

$$f_i = Z_0(i)v_{0i} + \sum_{j\neq i} Z_0(i)G(ij)f_j$$

Solution $\Longrightarrow$ Scattering series:

$$f_i = Z_0(i)v_{0i} + \sum_{j\neq i} Z_0(i)G(ij)Z_0(j)v_{0j} + \sum_{k\neq i}\sum_{j\neq k} Z_0(i)G(ik)Z_0(k)G(kj)f_j$$

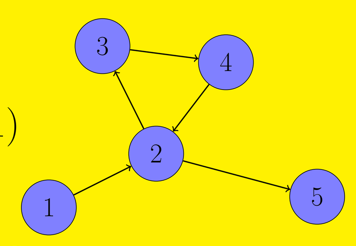
Many-particle friction kernel:

$$f_i = \sum_j \hat{Z}_{ij}(1,\ldots,N)v_{oj}$$

Series of scattrering sequences

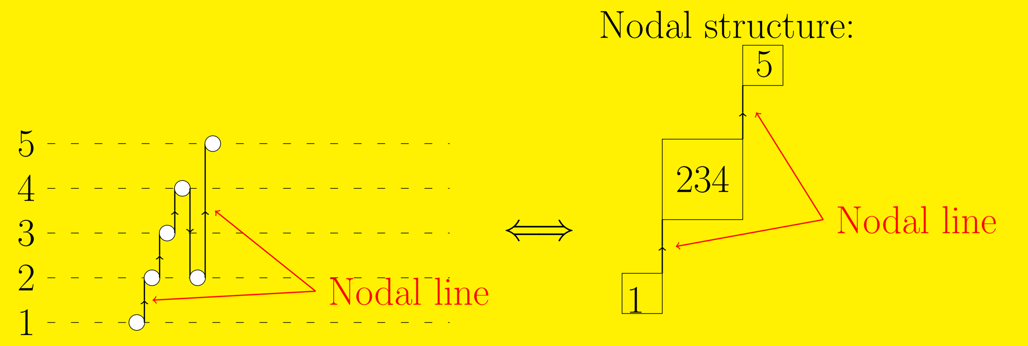
Scattering sequences.

Exemplary sequence:
$Z_0(5)G(52)Z_0(2)G(24)Z_0(4)G(43)Z_0(3)G(32)Z_0(2)G(21)Z_0(1)$



Diagramatic representations of scattering sequences.:

Nodal structure:



Average over probability distribution for configurations of particles.

Averaged force density: $\langle f(\vec{R})\rangle = \int d\,\vec{R}'\langle\hat{Z}(\vec{R}, \vec{R}')\rangle v_o(\vec{R}')$

$f(\vec{R}) = \sum_{i=1}^{N}\delta(\vec{R} - \vec{R}_i)f_i$ $\qquad$ Average friction kernel $\qquad \hat{Z}(\vec{R}, \vec{R}') = \sum_{i,j=1}^{N}\delta(\vec{R} - \vec{R}_i)\hat{Z}_{ij}\delta(\vec{R}' - \vec{R}_j)$

Effective viscosity.

Relation between induced forces density and the average flow.

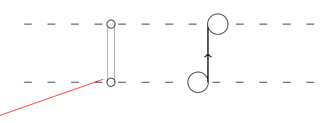
$$\langle v\rangle = v_0 + G\langle f\rangle \qquad \langle f\rangle = \langle\hat{Z}\rangle v_0 \qquad \Longrightarrow \qquad \langle f\rangle = \underbrace{\langle\hat{Z}\rangle\left(1 + G\langle\hat{Z}\rangle\right)^{-1}}_{\langle\hat{Z}\rangle^{\mathrm{irr}}}\langle v\rangle$$

Effective viscosity is given immediately by matrix element of $\langle\hat{Z}\rangle^{\mathrm{irr}}$.

Exemplary term in $\langle\hat{Z}\rangle^{\mathrm{irr}}$

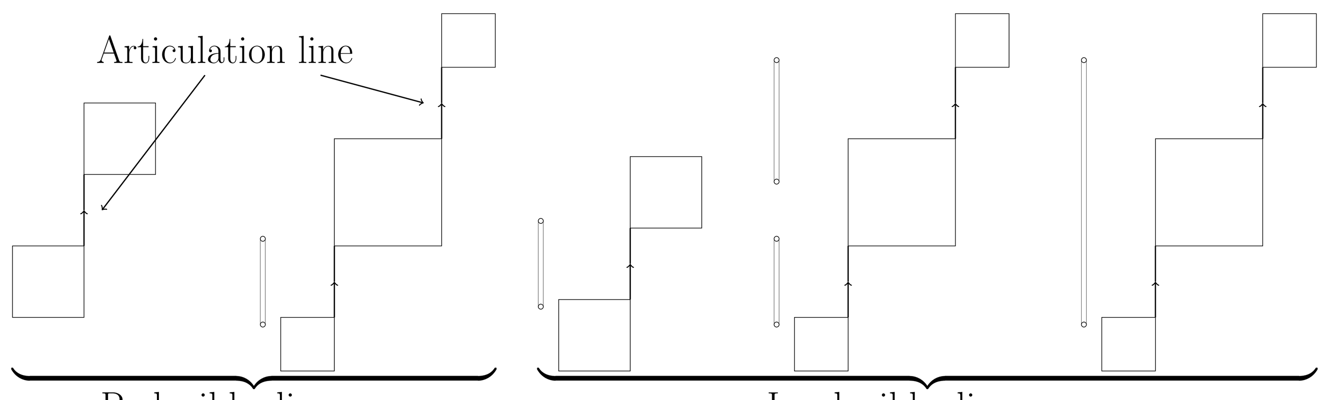
$$\langle\hat{Z}\rangle^{\mathrm{irr}}(\vec{R}, \vec{R}') \ni Z_0G(\vec{R} - \vec{R}')Z_0n_2(\vec{R} - \vec{R}') - Z_0G(\vec{R} - \vec{R}')Z_0n_1^2$$

$n_2(\vec{R} - \vec{R}') - n_1^2$ - two-particle correlation function

$Z_0G(\vec{R} - \vec{R}')Z_0\, h(\vec{R} - \vec{R}') =$ 

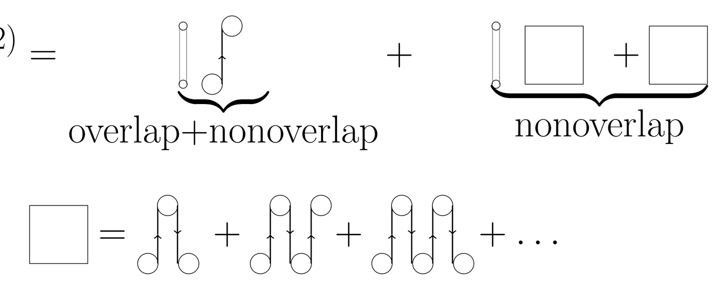
Correlation function.

Irreducibility.



$\langle\hat{Z}\rangle^{\mathrm{irr}}$ consists of all irreducible diagrams (without articulation line).
Morover all transport coefficients (sedimentation, self and collective diffusion) may be expressed by similar (with irreducible structure) kernels.

Two-particle terms.



Virial expansion.

Effective viscosity: $\eta_{\mathrm{eff}} = \eta\{1 + \frac{5}{2}\phi + \lambda\phi^2 + \nu\phi^3 + \ldots\}$

λ: nonoverlap $\approx 50\%$; overlap $\approx 50\%$

ν: three-particle nonoverlapping configurations $\approx 5\%$; overlap(three-particle)+ full two-particle $\approx 95\%$

Sedimentation coefficient: $K = 1 + \lambda_c\phi + b_c\phi^2 + \ldots$

For sequences, which starts and ends on different particles:

λ_c: nonoverlap $\approx 6\%$; overlap $\approx 94\%$

b_c: three-particle nonoverlapping configurations $\approx 1\%$; overlap(three-particle)+ full two-particle $\approx 99\%$

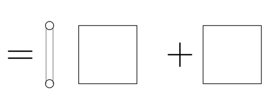
Remarks:
1) Overlapping configurations of particles give the dominant contribution to transport coefficients.
2) Negligible contribution from three-particle nonoverlapping configurations.

Approximated method.

Foundation:
We derived the exact relations, which allow to calculate $\langle\hat{Z}\rangle^{\mathrm{irr}}$ for overlapping configurations by means of $\langle\hat{Z}\rangle^{\mathrm{irr}}$ for nonoverlapping configurations.

$\langle\hat{Z}\rangle^{\mathrm{irr}}$ for nonoverlapping configurations $\Longrightarrow$ $\langle\hat{Z}\rangle^{\mathrm{irr}}$ for overlapping configurations.

The method consists in introducing closure relation, by the following approximation:

$\langle\hat{Z}\rangle^{\mathrm{irr}}_{nov} \approx \langle\hat{Z}\rangle^{\mathrm{irr}(2)} =$ 

Motivation for introducing this closure relation are remarks placed above (frame "Virial expansion"). Indeed, the relation implicates neglecting of three(and more)-particle contributions of nonoverlapping configurations. Moreover, by dint of the exact relations, one can calculate $\langle\hat{Z}\rangle^{\mathrm{irr}}$. Transport coefficients, may be expressed imediately by $\langle\hat{Z}\rangle^{\mathrm{irr}}$ kernel.