Mathematical analysis of the effective viscosity of dilute suspensions

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(based on works with M. Hillairet, R. Höfer, A. Mecherbet)

Context

Starting point :

Suspension of $n \gg 1$ small solid spheres in a viscous flow.

- The solid particles induce resistance to strain.

- Can it be seen at a macroscopic scale as an extra viscosity ?

Hope :

- Averaging to take place as $n \to \infty$

- Suspension to be described by a single fluid model with some effective viscosity.

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Topic of great interest in rheology.
Many experiments (lab or computer) with sheared suspensions.

Measurement of the effective viscosity (assuming it exists !) :

$$\mu_{eff,exp} = \frac{\text{energy dissipation of the suspension}}{\text{energy dissipation of the fluid alone}}$$

Crucial parameter : solid volume fraction ϕ.

- ϕ small : dilute suspensions.
- $\phi \sim \phi_c$, maximal flowable volume fraction : dense suspensions.

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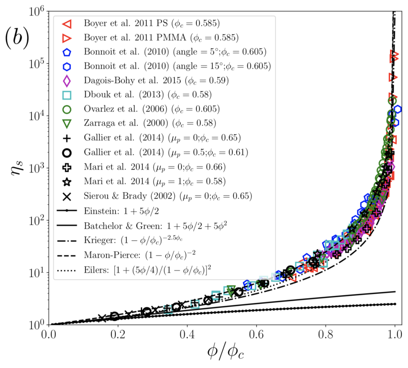
[Guazzelli-Pouliquen'18]



Suggests a universal behaviour : $\mu_{eff} = \mu_{eff}(\phi/\phi_c)$.

But far from understood, notably at large ϕ :

- Contact between particles plays a role
- Confinement plays a role as well.
- Non-newtonian behaviour.

Even in idealized models, difficult mathematical questions, related to percolation/graph theory :

- see [Berlyand et al'05] for finite n.
- Ongoing PhD thesis of Alexandre Girodroux-Lavigne.

Mathematical analysis of dilute suspensions

A simple model, with pure hydrodynamic interactions:

- n spherical particles $B_i = B(x_i, r_n)$.

- Stokes flow in $\Omega_n = \mathbb{R}^3 - \cup_{i=1}^n B_i$:

$$-\mu \Delta u_n + \nabla p_n = f, \quad \text{div } u_n = 0 \quad \text{in } \Omega_n$$

with f in $L^p(\mathbb{R}^3)$ for p large enough.

- Particles are neutrally buoyant (no sedimentation).

No inertia, no thermal fluctuation.

Force- and torque-free. For all i,

$$\int_{\partial B_i} \sigma_\mu(u_n, p_n)\nu \, ds = \int_{\partial B_i} \sigma_\mu(u_n, p_n)\nu \times (x - x_i) \, ds = 0$$

- Particles are rigid, with no-slip at the boundary: for all i

$$u_n|_{\partial B_i} = u_i + \omega_i \times (x - x_i), \quad u_i, \omega_i \in \mathbb{R}^3.$$

- Decay of u_n at infinity.

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Remark : Snapshot at a given time t.

In fact : $x_i = x_i(t)$, $u_i = u_i(t)$, $\dot{x}_i = u_i$.

Assumptions made on $(x_i)_{1 \leq i \leq n}$ preserved through time ?

This question is left aside here.

Can we approximate it by an effective fluid equation ?

$$-\mathrm{div}\,(2\mu_{eff} D(u_{eff})) + \nabla p_{eff} = (1-\phi)f, \quad \mathrm{div}\, u_{eff} = 0 \quad \text{in } \mathbb{R}^3$$

with $\mu_{eff} = \mu_{eff}(x)$, $\mu_{eff} \neq \mu$ in the region $\mathcal{O}$ of the particles.

We focus on the dilute regime. With $|\mathcal{O}| = 1$, we assume that

$$\phi = \frac{4\pi}{3} n r_n^3 \text{ is small but independent of } n$$

Two subquestions :

Q1 : **Exact effective viscosity** ?

$$\lim_n u_n = u_{eff} \quad \text{for some } \mu_{eff} \text{ ?}$$

See [Duerinckx-Gloria'20], [Duerinckx'20], [Jikov et al'1994].

Q2 : **Approximate effective viscosity of order** k ?

$$\limsup_n \|u_n - u_{eff}\|_{L^p} = o(\phi^k) \quad \text{for some } \mu_{eff}\text{, for some } p \text{ ?}$$

In this regime, the hope is to find μ_{eff} under the form

$$\mu_{eff} = \mu + \phi\mu_1 + \cdots + \phi^k\mu_k$$

where $\mu_i \in \mathrm{Sym}(\mathrm{Sym}_0(\mathbb{R}^3))$

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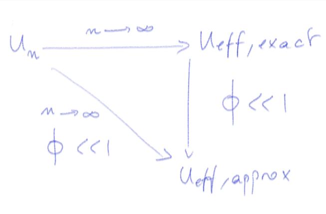

Q2 may require less assumptions than Q1 on the x_i's (e.g. for the derivation of Einstein's formula).

Useful as there is no canonical stationary measure.

First order approximation

[Einstein 1905] : If the suspension is homogeneously distributed in a (smooth bounded) domain $\mathcal{O}$, and if the interaction between the particles can be neglected, then a first order approx. is given by

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Mathematical justification ?

- [Sanchez Palencia, Levy et al, Haines et al]: x_i on a periodic grid.
- [Niethammer and Schubert, Hillairet and Wu]: under

$$\rho_n := \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i} \rightharpoonup \rho(x)dx, \quad \rho \text{ bounded}, \quad \text{supp}\rho = \overline{\mathcal{O}}. \qquad \text{(A1)}$$

$$d_n \geq cn^{-1/3}, \quad d_n = \inf_{i\neq j}|x_i - x_j|, \quad c \text{ independent of } \phi \qquad \text{(A2)}$$

Remark : (A1) includes the case of inhomogeneous distributions. Effective viscosity reads

$$\mu_{eff} = \mu(1 + \frac{5}{2}\phi\rho) \quad \text{in } \mathcal{O}$$

One recovers Einstein's formula for $\rho = 1_{\mathcal{O}}$.

Remark : The assumption that $d_n \geq cn^{-1/3}$ is stringent compared to the no-penetration condition, that reads

$$d_n \geq 2r_n = c'\phi^{1/3}n^{-1/3}$$

Theorem ([G-V and Höfer], see also [Duerinckx and Gloria])

Einstein's formula is still valid if (A2) is relaxed into a set of two conditions.

$$\exists \delta > 0, \quad \delta_n \geq (2+\delta) r_n \tag{A2'}$$

$$\exists C, \alpha > 0, s.t. \quad \forall \eta, \quad \sharp\{i, |x_i - x_j| \leq \eta n^{-1/3}\} \leq C \eta^{\alpha} n. \tag{A2''}$$

Remark :

(A2') could be even more relaxed.

(A2'') satisfied by i.i.d. random variables, points drawn from classical stationary ergodic processes...

Second order approximation

Can we go beyond Einstein's formula ? $o(\phi^2)$ approximation ?

Various formula in the literature, for periodic and random stationary distributions of particles: Nunan et al, O'Brien, Zuzovski et al, Ammari et al, Batchelor and Green, Hinch.... But ...

- Formulas do not always coincide !

- Some methods of derivation require mathematical clarity (like the renormalization technique of Batchelor and Green)

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Difficulties:

- Pairwise interactions must be taken into account.

- Microscopic structure plays a role: **knowing ρ is not enough**.

Mix of deterministic and probabilistic approaches.

Tools :

- Method of reflections

- Theory of Coulomb gases

- Stochastic homogenization

- Cluster expansions

Remark : **two extreme types of diluteness** (remind $\phi = \frac{4\pi}{3} n r_n^3$)

- play on the inter-particle distance. Example : periodic.

- play with thinning. No constraint on the minimal distance (except non-penetration condition). Example : point processes of Poisson type.

Suspensions with strong inter-particle distance

Main assumptions : (A1)-(A2)

Important object:

The 4-tensor field $\mathcal{M}(x) = D(\nabla \mathcal{U})$, with $\mathcal{U}$ the Oseen 2-tensor.

For all x, $\mathcal{M}(x) \in \mathrm{Sym}(\mathrm{Sym}_0(\mathbb{R}^3))$, with

$$\mathcal{M}(x)S = -\frac{3}{8\pi} D\Big(\frac{x \otimes x : S}{|x|^5} x\Big)$$

Mean field functionals : for any smooth φ,

$$W_n[\varphi] := \frac{25\mu}{2}\Big(\frac{1}{n^2}\sum_{i\neq j} \mathcal{M}(x_i - x_j)\varphi(x_i)\varphi(x_j) - \int_{\mathbb{R}^3\times\mathbb{R}^3} \mathcal{M}(x-y)\varphi(x)\varphi(y)\rho(x)\rho(y)dxdy\Big)$$

Theorem [GV-Hillairet], [GV-Mecherbet]

Assume (A1)-(A2). Let
$\mu_2 = \mu_2(x) \in L^\infty\big(\mathbb{R}^3), \mathrm{Sym}(\mathrm{Sym}_0(\mathbb{R}^3))\big)$.

Let $\mu_{eff} = \mu + \frac{5}{2}\mu\rho\phi + \mu_2\phi^2$. Then,

$$\limsup_n \|u_n - u_{eff}\|_{L^p} = O(\phi^{7/3}), \quad \forall p \leq 3.$$

if and only if for all smooth φ,

$$\lim_{n\to+\infty} W_n[\varphi] = \int_{\mathbb{R}^3} \mu_2(x)|\varphi(x)|^2 dx \qquad \text{(MF)}$$

Remark : $W_n[\varphi] \not\to 0$ as $n \to +\infty$! Due to the singularity of $\mathcal{M}$. $\mathcal{M}$ is a Calderon-Zygmund operator, which is crucial to us.

Remark : The convergence (MF) of the mean-field functional is necessary and sufficient to have a $O(\phi^2)$ effective model.

Quick ideas from the proof:

1. **Duality argument** : it is enough to show that

$$\forall q \geq 3, \quad \exists C > 0, \quad \Big| \int_{\mathbb{R}^3} v_n f \Big| \leq C\, \phi^{7/3} \|v\|_{W^{1,q}}, \quad \forall v \in \mathcal{D}_\sigma(\mathbb{R}^3),$$

where $v_n = v_n[v]$ is the solution of

$$\begin{aligned} -\mu \Delta v_n + \nabla q_n = 2\mathrm{div}\, \Big(\frac{5}{2}\rho\phi + \mu_2 \phi^2\Big) \quad & \text{in } \mathbb{R}^3 \setminus \cup B_i \\ \mathrm{div}\ \phi_n = 0 \quad & \text{in } \mathbb{R}^3 \setminus \cup B_i, \\ v_n = v + v_i + \omega_i \times (x - x_i) \quad & \text{in } B_i, \quad \forall 1 \leq i \leq n. \end{aligned}$$

$+$ consistent force and torque conditions.

2. **Method of reflections** to build an approximation of v_n.

$$v_{n,app} = v_{source} + v_{n,bc}$$

- $v_{source} = \mathcal{U} \star \text{div } \left(\frac{5}{2}\rho\phi + \mu_2\phi^2\right)$
- $v_{n,bc} = \sum_{i=1}^n V_{single,i}[A_i]$

where $V_{single,i}$ solves a one-sphere Stokes problem:

$$\begin{aligned} -\Delta V_{single,i} + \nabla P_i = 0, \text{ div } V_{single,i} = 0 \quad &\text{in} \quad \mathbb{R}^3 \setminus B_i, \\ V_{single,i} = A_i(x - x_i) \quad &\text{in } B_i. \end{aligned}$$

Matrices A_i are obtained in the form of an expansion, adding at each step a superposition of one-sphere solutions.

Last : - control $v_n - v_{n,app}$ strongly in $\dot{H}^1$

- control $\int v_{n,app} f$ through a duality argument.

Connection to theory of Coulomb gases

How to show that convergence (MF) **holds and how to compute the limit** μ_2 **?**

Inspiration taken from the lecture notes of Sylvia Serfaty.

Example: homogeneous setting : $\rho = 1_{\mathcal{O}}$. We restrict to

$$W_n[1] = \frac{25\mu}{2}\Big(\frac{1}{n^2}\sum_{i\neq j}\mathcal{M}(x_i - x_j) - \int_{\mathbb{R}^3\times\mathbb{R}^3}\mathcal{M}(x-y)\rho(x)\rho(y)dxdy\Big)$$

1. We prove that for $S \in \mathrm{Sym}_0(\mathbb{R}^3)$, with $g_s(x) := \frac{25\mu}{2}\mathcal{M}(x)S : S$,

$$W_n[1]S : S$$
$$= \underbrace{\int_{x\neq y} g_S(x-y)(\rho_n(dx) - \rho(x)dx)(\rho_n(dy) - \rho(y)dy)}_{:=V_n} + o_n(1).$$

2. To understand V_n, we express it as an energy.

Proposition

For all $f \in L^2(\mathbb{R}^3)$,

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} g_S(x-y) f(x) f(y) dy = 25 \int_{\mathbb{R}^3} |D(u_f)|^2$$

$$\text{where} \quad -\Delta u_f + \nabla p_f = \text{div}\,(Sf), \quad \text{div}\ u_f = 0 \quad \text{in } \mathbb{R}^3$$

Idea : replace f by $\rho_n - \rho$ to find

$$'' \int_{\mathbb{R}^3 \times \mathbb{R}^3} g_S(x-y)(\delta_n(dx) - \rho(x)dx)(\delta_n(dy) - \rho(y)dx) = 25 \int_{\mathbb{R}^3} |D(h_n)|^2 ''$$

with $h_n = u_{\rho_n - \rho}$

$$"\int_{\mathbb{R}^3\times\mathbb{R}^3} g_S(x-y)(\delta_n(dx)-\rho(x)dx)(\delta_n(dy)-\rho(y)dx) = 25\int_{\mathbb{R}^3}|D(h_n)|^2"$$

Problem: both terms are infinite !

- the left-hand side is infinite because of the diagonal (which was excluded in the definition of V_n).

- the right-hand side is infinite because $\rho_n - \rho$ is not in H^{-1}.

But there is a way to make sense of this equality and use it, through **regularization and renormalization** : see [Serfaty'14].

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At the end of the day : one needs for a fixed value of a regularization parameter η, to understand the limit in n of $\int_{\mathbb{R}^3} |D(h_n^\eta)|^2$, with

$$-\Delta h_n^\eta + \nabla p_n^\eta = \mathrm{div}\,\Big(S(\rho_n^\eta - \rho)\Big), \quad \mathrm{div}\; h_n^\eta = 0$$

More precisely,

$$-\Delta h_n^\eta + \nabla p_n^\eta = \mathrm{div}\,\left(\sum_{i=1}^{n} \psi^\eta(n^{1/3}(x - x_i)) - S\rho\right)$$

with ψ^η compactly supported.

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with ψ^η compactly supported.

Idea : Evokes the following baby model :

$$-\Delta h^\varepsilon + \nabla p^\varepsilon = \mathrm{div}\,\big(F(x/\varepsilon)\big), \quad \mathrm{div}\ h^\varepsilon = 0 \tag{1}$$

with $F = F(y)$ $\mathbb{Z}^3$-periodic in y, with zero average.

In this analogy:

- $F(x/\varepsilon)$ corresponds to $\sum_{i=1}^n \psi^\eta(n^{1/3}(x-x_i)) - S\rho$.

- It oscillates at typical scale $\varepsilon = n^{-1/3}$.

Bottom line : Possible to understand the limit of the energy, and eventually compute μ_2, in classical homogenization settings.

Example 1 : Cubic lattice.

Theorem

If the x_i are distributed according to a cubic lattice:

$$\mu_2 S : S = \mu(\alpha \sum_i |S_{ii}|^2 + \beta \sum_{i \neq j} |S_{ij}|^2), \quad \alpha \approx 9.48,\ \beta \approx -2.5.$$

Example 2 : Stationary ergodic point process. Given a small ϕ:

- We start from a point process with intensity ϕ, $\{y_k\} = \{y_k(\omega)\}$ satisfying $|y_k - y_{k'}| \geq c\phi^{-1/3}$ a. s. for some fixed $c > 0$.

- We introduce a small parameter $0 < \varepsilon \ll 1$.

- We set $\{x_1, \dots, x_n\} = \{\varepsilon y_k\} \cap \mathcal{O}$.

Remark : n is now random.

By the ergodic theorem, goes to infinity almost surely as $\varepsilon \to 0$, with $n \sim \phi\varepsilon^{-3}$.

The resulting set $\{x_1, \dots, x_n\}$ satisfies (A2) almost surely.

Theorem

$$\mu_2 = \frac{25}{2}\mu \lim_n \frac{1}{n} \int_{B_n \times B_n} \mathcal{M}(x-y) g_2(x,y) dxdy$$

with B_n the ball of volume n and $g_2(x,y) = g(x-y)$ the two-point correlation function of the process (y_k).

If furthermore the point process is isotropic and if $g \to 1$ fast enough,

$$\mu_2 = \frac{5}{2}\mu.$$

Remark: for $|x-y| \to \infty$:

- $g_2(x, y) \sim 1$

- $\mathcal{M}(x-y)$ scales like $\frac{1}{|x-y|^3}$ (borderline integrable)

Not obvious to show that the limit exists.

[Batchelor-Green'1972] : solve the problem by the so-called **renormalization technique**.

They add artificially in the expression for μ_2 an expression which has zero expectation, and exhibits the same kind of divergence.

Actually not needed ! As $\mathcal{M}$ is of Calderon-Zygmund type, it vanishes on spheres, and this is enough to circumvent the problem.

Suspensions dilute through thinning

Same stochastic model as before, but:

- we relax the assumption (A2) into (A2')

- we assume boundedness and decorrelation properties at large distances of k-point correlation functions g_k, $0 \leq k \leq 5$. (consistent with Poisson type processes).

Exemple: $g_2(x, y) = 1 + R(x - y), \quad R \in L^q \cap L^\infty$ for some q

Theorem

$$\mu_2 = \frac{25}{2}\mu \lim_{n \to +\infty} \frac{1}{n} \int_{B_n \times B_n} \mathcal{N}(x - y) g_2(x, y)\, dx dy$$

with $\mathcal{N}(x)$ explicit in terms of solutions of two-sphere Stokes problems, and behaving like $\mathcal{M}$ at infinity.

Vague idea of the proof :

Relies from the start on stochastic homogenization.

We use the expression of effective viscosity given by homogenization.

We show that it can be rewritten as

$$\mu_{eff} S : S = \mathbb{E} \lim_n \mathcal{L}_n[u_n^S]$$

where $\mathcal{L}_n$ is a linear functional, and u_n^S satisfies the same system as before, replacing the source term with inhomogeneous b.c.

$$u_n^S = Sx + u_i + \omega_i \times (x - x_i) \quad \text{on} \quad B_i.$$

To compute the $O(\phi^2)$ term in μ_{eff}, we use a **cluster expansion** of u_n^S. Substitute to the method of reflections.

Idea [Felderhof'82] : for any function $f = f(I)$ defined on finite subsets of $\mathbb{N}$, we can always decompose

$$f(I) = \sum_{J \subset I} g(J), \quad \text{with } \; g(I) := \sum_{J \subset I} (-1)^{\sharp I - \sharp J} f(J) \qquad \text{(CE)}$$

Expansion (CE) allows to distinguish in the value of f the contribution of subsets of one element, two elements, ...

Here : we take $f(I) = u_I^s$, with $I \subset \{1, \ldots, n\}$ and u_I^S the Stokes solution outside the balls with centers whose indices are in I.

$$u_I^S = u_\emptyset^S + \sum_k u_{\{k\}}^S + \sum_{k \neq l} u_{\{k,l\}}^S$$

The k-th term in the expansion provides the ϕ^k term in the effective viscosity.