

# McKean–Vlasov diffusion and the well-posedness of the Hookean bead-spring chain model

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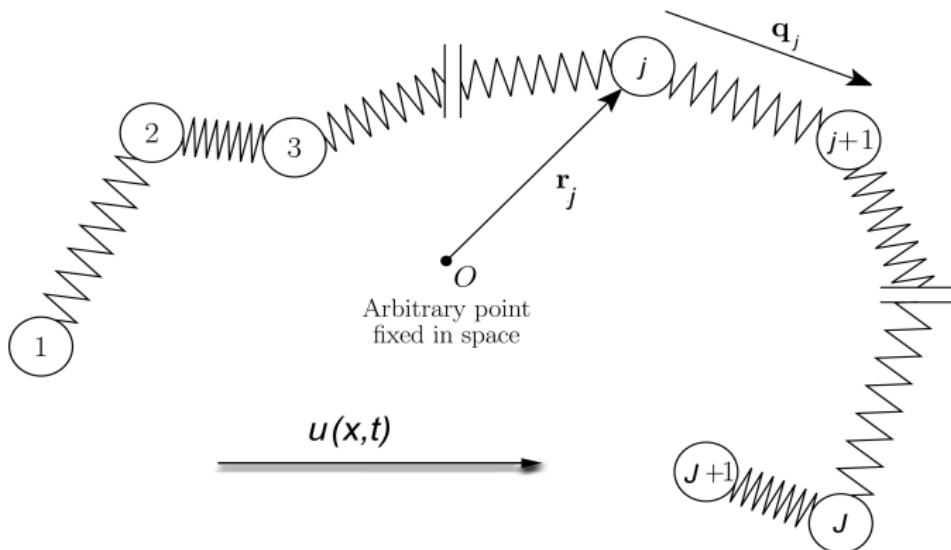
Joint work with Ghozlane Yahiaoui (Oxford)

Prague

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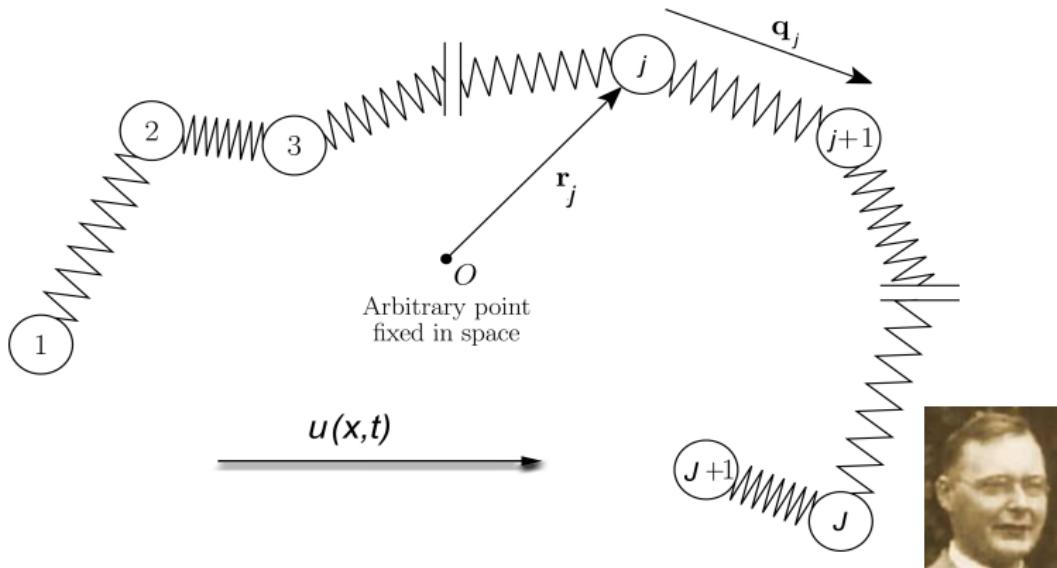
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The Hookean bead-spring-chain model describes the conformational dynamics of an ideal polymer chain. A polymer molecule is modelled as a linear chain of massless beads connected with Hookean springs, subjected to Brownian noise.



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H. A. Kramers. Het gedrag van macromoleculen in een stroomende vloeistof, Physica 11 (1944), 1–19. [← Werner Kuhn (1934), J.J. Hermans (1943)]

-  P. E. Rouse. A Theory of the Linear Viscoelastic Properties of Dilute Solutions of Coiling Polymers, J. Chem. Phys. 21, 1272 (1953).
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-  E. Süli and G. Yahiaoui. McKean–Vlasov diffusion and the well-posedness of the Hookean bead-spring-chain model for dilute polymeric fluids: small-mass limit and equilibration in momentum space. 85 pages. [cf. arXiv].

## Main results

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### Conclusions:

- If the flow domain  $\Omega$  is bounded, then the configuration space domain  $D^J = \underbrace{D \times \cdots \times D}_J$ , where  $D = \Omega - \Omega = \{r - \hat{r} : r, \hat{r} \in \Omega\}$ , is also bounded.



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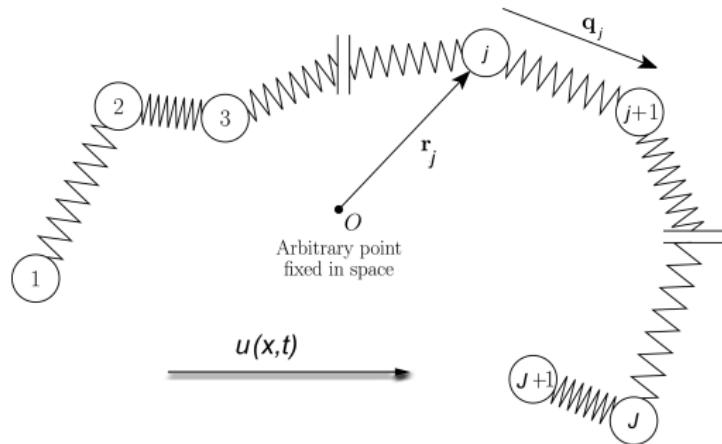


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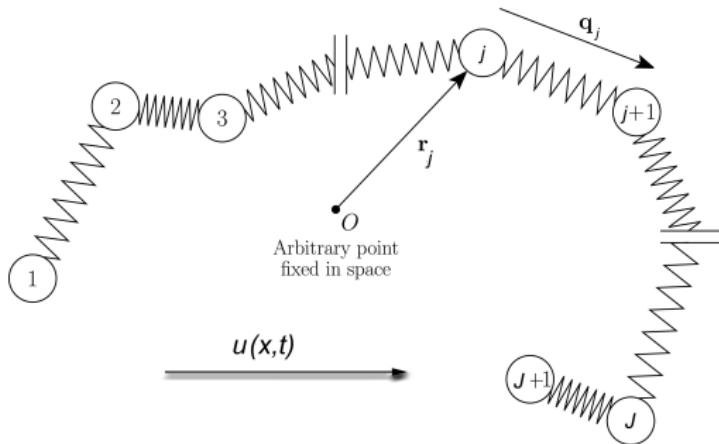
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⇒ FP eq. has center-of-mass diffusion ⇒ Oldroyd-B has stress-diffusion
- We rigorously prove an assertion, deduced by Schieber & Öttinger (1988) using formal asymptotics, that:

passage to the small-mass limit    ⇒    equilibration in momentum space.

## Formulation of the model



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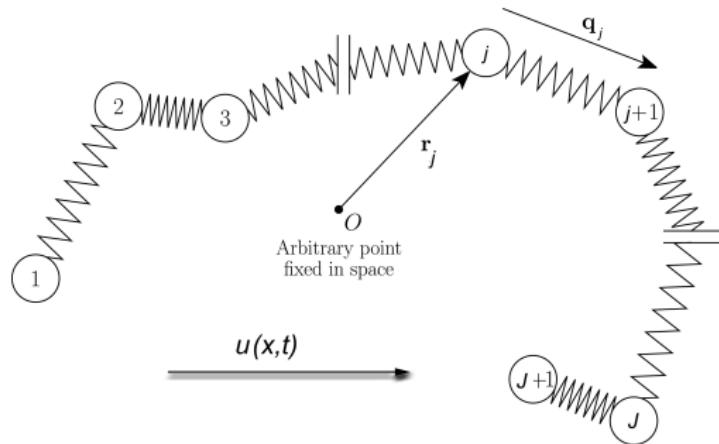


$$r := (r_1^T, \dots, r_{J+1}^T)^T, \quad r_j \in \Omega \quad \text{for } j = 1, \dots, J+1,$$

$$v := (v_1^T, \dots, v_{J+1}^T)^T, \quad v_j \in \mathbb{R}^d \quad \text{for } j = 1, \dots, J+1,$$

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$$q_j \in D := \Omega - \Omega = \{r - \hat{r} : r, \hat{r} \in \Omega\}, \quad \text{for } j = 1, \dots, J;$$

**Condition:**  $x := \frac{1}{J+1} \sum_{j=1}^{J+1} r_j.$

# Hydrodynamic interaction

**Oseen system** on the space-time domain  $\overline{\Omega} \times [0, T]$ , where  $\Omega$  is a bounded open convex  $C^2$  domain in  $\mathbb{R}^d$ ,  $d \in \{2, 3\}$ ,  $0 \in \Omega$ ,  $b \in L^\infty(\Omega \times (0, T))$ ,  $\nabla \cdot b = 0$ :

$$\begin{aligned}\partial_t u + (b \cdot \nabla) u - \mu \Delta u + \nabla \pi &= \nabla \cdot \mathbb{K} && \text{for } (x, t) \in \Omega \times (0, T], \\ \nabla \cdot u &= 0 && \text{for } (x, t) \in \Omega \times (0, T], \\ u(x, t) &= 0 && \text{for } (x, t) \in \partial\Omega \times (0, T], \\ u(x, 0) &= u_0(x) && \text{for } x \in \Omega,\end{aligned}$$

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with the non-Newtonian extra-stress tensor (Kramers–Kirkwood stress tensor)

$$\mathbb{K}(x, t; \varrho) := \sum_{j=1}^J \mathbb{E}^x (\lambda q_j \otimes q_j) \quad \text{for } (x, t) \in \Omega \times (0, T], J \geq 1,$$

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$$\mathcal{U}(r, t; \varrho) := \left( u(r_1, t; \varrho)^T, \dots, u(r_{J+1}, t; \varrho)^T \right)^T.$$

SDE :  $\epsilon^2 \ddot{r} = \underbrace{\mathcal{L}r}_{\text{Hookean spring force}} + \underbrace{\zeta(\mathcal{U}(r, t; \varrho) - \dot{r})}_{\text{Stokes drag force}} + \underbrace{\sqrt{2\beta} \dot{W}}_{\text{Brownian force}}$ .

$\epsilon^2 > 0$  is the mass of a bead in the chain,  $\beta = kT\zeta > 0$ , where  $k$  is the Boltzmann constant,  $T$  is the absolute temperature and  $\zeta$  is the drag coefficient;  $\mathcal{L}$  is the following  $(J+1) \times (J+1)$  block-matrix:

$$\mathcal{L} := \lambda \begin{pmatrix} -\mathbb{I} & \mathbb{I} & \mathbb{O} & \dots & \mathbb{O} \\ \mathbb{I} & -2\mathbb{I} & \mathbb{I} & \ddots & \mathbb{O} \\ \mathbb{O} & \mathbb{I} & -2\mathbb{I} & \mathbb{I} & \mathbb{O} \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \mathbb{O} & \dots & \mathbb{I} & -2\mathbb{I} & \mathbb{I} \\ \mathbb{O} & \dots & \mathbb{O} & \mathbb{I} & -\mathbb{I} \end{pmatrix} \in \mathbb{R}^{(J+1)d \times (J+1)d},$$

where  $\lambda > 0$  is a constant stiffness of the Hookean springs. W.l.o.g., we set  $\zeta = 1$ .

The SDE may then be rewritten as the first-order system

$$\epsilon \dot{r} = v,$$

$$\epsilon \dot{v} = \mathcal{L}r + \mathcal{U}(r, t; \varrho) - \epsilon^{-1}v + \sqrt{2\beta} \dot{W}.$$

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Let

$$\varrho : (r, v, t) \in \Omega^{J+1} \times \mathbb{R}^{(J+1)d} \times [0, T] \mapsto \varrho(r, v, t) \in \mathbb{R}_{\geq 0}$$

be the probability density function of the diffusion process  $(r, v)$ .

The law of  $(r, v)$  depends on  $\varrho$  itself through the function  $\mathcal{U}$ , and it is therefore a **McKean–Vlasov** diffusion process.

## Definition of the polymeric extra stress tensor $\mathbb{K}$

We define

$$\mathbb{E} \left( \sum_{j=1}^J \lambda q_j \otimes q_j \right) (t) := \int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} \left( \sum_{j=1}^J \lambda q_j(r) \otimes q_j(r) \right) \varrho(r, v, t) \, dr \, dv$$

and perform a change of variables, replacing integration over  $r \in \Omega^{J+1}$  by integration over  $(q, x) \in D^J \times \Omega$  via the linear bijection

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Then, for  $(x, t) \in \Omega \times (0, T]$ , the Kramers–Kirkwood stress tensor is:

$$\mathbb{K}(x, t; \varrho) = \mathbb{E}^x \left( \sum_{j=1}^J \lambda q_j \otimes q_j \right) (x, t) = \frac{\int_{D^J \times \mathbb{R}^{(J+1)d}} \left( \sum_{j=1}^J \lambda q_j \otimes q_j \right) \varrho(B(q, x), v, t) \, dq \, dv}{\int_{D^J \times \mathbb{R}^{(J+1)d}} \varrho(B(q, x), v, t) \, dq \, dv}$$

## Fokker–Planck equation for $\varrho$

$$\partial_t \varrho - \frac{\beta}{\epsilon^2} \left( \sum_{j=1}^{J+1} \partial_{v_j} \cdot (v_j \varrho) + \beta \partial_{v_j}^2 \varrho \right) + \frac{1}{\epsilon} \left( \sum_{j=1}^{J+1} v_j \cdot \partial_{r_j} \varrho + ((\mathcal{L}r)_j + u(r_j, t)) \cdot \partial_{v_j} \varrho \right) = 0$$

for all  $(r, v, t) \in \Omega^{J+1} \times \mathbb{R}^{(J+1)d} \times (0, T]$ ,

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$$\partial\Omega^{(j)} := \Omega \times \cdots \times \Omega \times \partial\Omega \times \Omega \times \cdots \times \Omega, \quad j = 1, \dots, J+1,$$

with  $\partial\Omega$  at the  $j$ -th position in this  $(J+1)$ -fold Cartesian product, and

$$\nu^{(j)}(r) := (0^T, \dots, 0^T, (\nu(r_j))^T, 0^T, \dots, 0^T)^T \in \mathbb{R}^{(J+1)d}.$$

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**Specular boundary condition:**

$$\varrho(r, v, t) = \varrho(r, v_*^{(j)}, t)$$

for all  $(r, v, t) \in \partial\Omega^{(j)} \times \mathbb{R}^{(J+1)d} \times (0, T]$ , with  $v \cdot \nu^{(j)}(r) < 0$ , where

$$v_*^{(j)} := v - 2(v \cdot \nu^{(j)}(r)) \nu^{(j)}(r), \quad j = 1, \dots, J+1.$$

## Existence of solutions

Define the Maxwellian

$$M(v) := (2\pi\beta)^{-\frac{J+1}{2}} \exp(-|v|^2/2\beta), \quad v \in \mathbb{R}^{(J+1)d},$$

and rescale:

$$\hat{\varrho} := \frac{\varrho}{M} \quad \text{and} \quad \hat{\varrho}_0 := \frac{\varrho_0}{M}.$$

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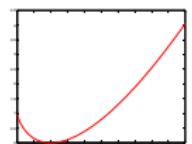
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Consider the nonnegative strictly convex function with superlinear growth:

$$\mathcal{F}(s) := s(\log s - 1) + 1, \quad s \in \mathbb{R}_{>0}, \quad \text{with } \mathcal{F}(0) := 1.$$



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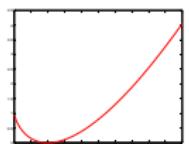
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The initial datum  $\varrho_0 = \varrho_0(r, v) \geq 0$  is assumed to satisfy

$$\begin{aligned} \varrho_0 &\in L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}), \quad \int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} \varrho_0(r, v) dr dv = 1, \\ M\mathcal{F}(\hat{\varrho}_0) &\in L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}); \end{aligned}$$

i.e.  $\varrho_0 \geq 0$  is assumed to have finite relative entropy with respect to  $M$ .

## Existence of solutions to FP, for $u$ fixed

### STEP 1.

We perform a parabolic regularization of FP equation by adding  $-\alpha\Delta_r\varrho$  to it, with homogeneous Neumann boundary condition on  $\partial\Omega^{J+1}$ .

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### STEP 2.

The assumption on the initial datum is strengthened by assuming *additionally* that

$$\hat{\varrho}_0 \in L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0}).$$

### STEP 3.

For  $u \in L^2(0, T; W_0^{1,\sigma}(\Omega)^d)$  for some  $\sigma > d$ , fixed, use linear parabolic theory based on Galerkin approximation to prove the existence of a unique weak solution to the  $\alpha$ -regularized FP eq.:

$$\hat{\varrho}_\alpha \in \mathcal{C}([0, T]; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})) \cap L^2(0, T; W_{*,M}^{1,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})),$$

$$\hat{\varrho}_\alpha \in W^{1,2}(0, T; (W_{*,M}^{1,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))').$$

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$$\hat{\varrho}_\alpha \in W^{1,2}(0, T; (W_{*,M}^{1,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))').$$

### STEP 4.

We then define  $\varrho_\alpha := M\hat{\varrho}_\alpha$ , and prove that

$$\int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} \varrho_\alpha(r, v, t) \, dr \, dv = 1 \quad \forall t \in [0, T].$$

Using Stampacchia's cut-off method, we prove that  $\varrho_\alpha(r, v, t) \geq 0$ .

## STEP 5.

As  $\alpha \rightarrow 0_+$ , parabolic energy estimates and relative entropy estimates yield uniform bounds on  $\widehat{\varrho}_\alpha$ , which imply that

$$\begin{aligned}
 \widehat{\varrho}_\alpha &\rightharpoonup \widehat{\varrho} && \text{weakly* in } L^\infty(0, T; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \\
 \nabla_v \widehat{\varrho}_\alpha &\rightharpoonup \nabla_v \widehat{\varrho} && \text{weakly in } L^2(0, T; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \\
 \alpha \nabla_r \widehat{\varrho}_\alpha &\rightarrow 0 && \text{strongly in } L^2(0, T; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \\
 M \partial_t \widehat{\varrho}_\alpha &\rightharpoonup M \partial_t \widehat{\varrho} && \text{weakly in } L^2(0, T; (W^{s,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))'), \\
 v_j \widehat{\varrho}_\alpha &\rightharpoonup v_j \widehat{\varrho} && \text{weakly in } L^2(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \\
 ((\mathcal{L}r)_j + u(r_j, \tau)) \widehat{\varrho}_\alpha &\rightharpoonup ((\mathcal{L}r)_j + u(r_j, \tau)) \widehat{\varrho} && \text{weakly in } L^2(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})),
 \end{aligned}$$

for  $j = 1, \dots, J+1$  and  $s > (J+1)d + 1$ . Furthermore,

$$\varrho := M\widehat{\varrho} \geq 0 \quad \text{and} \quad \int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} \varrho(r, v, t) \, dr \, dv = 1 \quad \forall t \in [0, T].$$

## STEP 6.

$\widehat{\varrho}$  solves FP and by weak lower-semicontinuity satisfies the energy inequality:

$$\begin{aligned} & \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}(t)) dv dr + \frac{2\beta^2}{\epsilon^2} \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) |\partial_{v_j} \sqrt{\widehat{\varrho}}|^2 dv dr d\tau \\ & \leq \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}_0) dv dr + \frac{16d}{\beta} (J+1) [\text{diam}(\Omega)]^2 T + \frac{J+1}{\beta} \|u\|_{L^2(0,T;L^\infty(\Omega))}^2 \end{aligned}$$

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### Note:

We supposed that  $\widehat{\varrho}_0 \in L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0})$ , but the bound only depends on the  $L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})$  norm of  $\mathcal{F}(\widehat{\varrho}_0)$ , the  $L^2(0,T;L^\infty(\Omega)^d)$  norm of  $u$ , and the constants  $d, \beta, J, L, T$ , all of which are independent of  $\epsilon$ .

# Existence of solutions to the Oseen–Fokker–Planck system

## STEP 7.

We formulate an iterative process, by defining the sequence of functions  $(u^{(k)}, \hat{\varrho}^{(k)})$ , for  $k = 1, 2, \dots$ , and let  $k \rightarrow \infty$ .

# Existence of solutions to the Oseen–Fokker–Planck system

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We set  $u^{(1)} \equiv 0$ . Given a divergence-free  $u^{(k)} \in L^2(0, T; W_0^{1,\sigma}(\Omega)^d)$ , for some  $k \geq 1$  and  $\sigma > d$ , we define  $\hat{\varrho}^{(k)}$  as the weak solution of the FP eq.:

$$M\partial_t \hat{\varrho}^{(k)} - \frac{\beta^2}{\epsilon^2} \left( \sum_{j=1}^{J+1} \partial_{v_j} \cdot (M\partial_{v_j} \hat{\varrho}^{(k)}) \right) + \frac{1}{\epsilon} \left( \sum_{j=1}^{J+1} Mv_j \cdot \partial_{r_j} \hat{\varrho}^{(k)} + ((\mathcal{L}r)_j + u^{(k)}(r_j, t)) \cdot \partial_{v_j} (M\hat{\varrho}^{(k)}) \right) = 0,$$

for all  $(r, v, t) \in \Omega^{J+1} \times \mathbb{R}^{(J+1)d} \times (0, T]$ ,

$$\hat{\varrho}^{(k)}(r, v, 0) = \hat{\varrho}_0^{(k)}(r, v) \quad \text{for all } (r, v) \in \Omega^{J+1} \times \mathbb{R}^{(J+1)d},$$

subject to a (weakly imposed) specular boundary condition w.r.t.  $r$ .

## STEP 8.

Given  $\widehat{\varrho}_0$  as in our *original* assumption, consider

$$G_k(s) := \frac{s}{1 + k^{-\frac{1}{4}} \sqrt{s}}, \quad s \in [0, \infty),$$

and define the renormalized initial condition

$$\widehat{\varrho}_0^{(k)} := G_k(\widehat{\varrho}_0), \quad k = 1, 2, \dots$$

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Then:

$$\widehat{\varrho}_0^{(k)} \in L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0}) \quad \text{for each fixed } k \geq 1,$$

$$\widehat{\varrho}_0^{(k)} \in L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0}), \quad \text{for each fixed } k \geq 1,$$

$$M\mathcal{F}(\widehat{\varrho}_0^{(k)}) \in L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0}), \quad \text{for each fixed } k \geq 1,$$

$$\int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} M(v) \widehat{\varrho}_0^{(k)} \, dr \, dv \leq 1, \quad \text{for each fixed } k \geq 1,$$

$$\widehat{\varrho}_0^{(k)} \rightarrow \widehat{\varrho}_0 \quad \text{strongly in } L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}) \text{ as } k \rightarrow \infty,$$

$$\mathcal{F}(\widehat{\varrho}_0^{(k)}) \rightarrow \mathcal{F}(\widehat{\varrho}_0) \quad \text{strongly in } L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}) \text{ as } k \rightarrow \infty.$$

## STEP 9.

By STEP 6, the sequence  $\widehat{\varrho}^{(k)}$  satisfies the following energy inequality:

$$\begin{aligned}& \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}^{(k)}(t)) dv dr \\& + \frac{2\beta^2}{\epsilon^2} \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) |\partial_{v_j} \sqrt{\widehat{\varrho}^{(k)}}|^2 dv dr d\tau \\& \leq \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}_0^{(k)}) dv dr \\& + \frac{16d}{\beta} (J+1) [\text{diam}(\Omega)]^2 T + \frac{J+1}{\beta} \|u^{(k)}\|_{L^2(0,T;L^\infty(\Omega))}^2,\end{aligned}$$

and the sequence  $u^{(k)}$  will be shown (in STEP 13) to satisfy:

$$\|u^{(k)}\|_{L^2(0,T;L^\infty(\Omega))} \leq C,$$

where  $C$  is a positive constant, independent of  $k$ .

## STEP 10.

Define  $(u^{(k+1)}, \pi^{(k+1)})$ , with

$$\begin{aligned} u^{(k+1)} &\in L^\infty(0, T; L^2(\Omega)^d) \cap L^2(0, T; W_0^{1,2}(\Omega)^d), \\ \pi^{(k+1)} &\in \mathcal{D}'(0, T; L^2(\Omega)/\mathbb{R}), \end{aligned}$$

as the weak solution of the Oseen system:

$$\begin{aligned} \partial_t u^{(k+1)} + (b \cdot \nabla) u^{(k+1)} - \mu \Delta u^{(k+1)} + \nabla \pi^{(k+1)} &= \nabla \cdot \mathbb{K}^{(k)} && \text{for } (x, t) \in \Omega \times (0, T], \\ \nabla \cdot u^{(k+1)} &= 0 && \text{for } (x, t) \in \Omega \times (0, T], \\ u^{(k+1)}(x, 0) &= u_0(x) && \text{for } x \in \Omega, \end{aligned}$$

$u_0 \in W_0^{1-2/z, z}(\Omega)^d$ , with  $z = d + \vartheta$ ,  $\vartheta \in (0, 1)$ , is divergence-free, and

$$\mathbb{K}^{(k)}(x, t) := \frac{\int_{D^J \times \mathbb{R}^{(J+1)d}} (\sum_{j=1}^J \lambda q_j \otimes q_j) M \widehat{\varrho}^{(k)}(B(q, x), v, t) dq dv}{\int_{D^J \times \mathbb{R}^{(J+1)d}} M \widehat{\varrho}^{(k)}(B(q, x), v, t) dq dv}.$$

## STEP 11.

Clearly,

$$\|\mathbb{K}^{(k)}\|_{L^\infty(0,T;L^\infty(\Omega))} \leq \lambda d \max_{q \in D^J} \|q\|^2 =: C,$$

where  $C$  is a positive constant, independent of  $k$ . Thus, there exists a  $\mathbb{K} \in L^\infty(0,T;L^\infty(\Omega;\mathbb{R}_{\text{symm}}^{d \times d}))$  (to be identified), such that

$$\mathbb{K}^{(k)} \rightarrow \mathbb{K} \quad \text{weak* in } L^\infty(0,T;L^\infty(\Omega;\mathbb{R}_{\text{symm}}^{d \times d})) \text{ as } k \rightarrow \infty.$$

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We would like to show that

$$\mathbb{K}(x,t) := \frac{\int_{D^J \times \mathbb{R}^{(J+1)d}} (\sum_{j=1}^J \lambda q_j \otimes q_j) M \widehat{\varrho}(B(q,x), v, t) dq dv}{\int_{D^J \times \mathbb{R}^{(J+1)d}} M \widehat{\varrho}(B(q,x), v, t) dq dv}$$

but this is **far from trivial**. [We shall return to this in STEPS 15–17.]

## STEP 12.

As  $W_0^{1-2/z,z}(\Omega)^d \hookrightarrow L^2(\Omega)^d$  for  $z = d + \vartheta$  and some  $\vartheta \in (0, 1)$ , there exists a unique weak solution  $(u^{(k+1)}, \pi^{(k+1)})$  to the Oseen system with

$$\|u^{(k+1)}\|_{L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;W^{1,2}(\Omega))} \leq C(1 + \|u_0\|_{L^2(\Omega)}),$$

where  $C$  is independent of  $k$ .

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where  $C$  is independent of  $k$ . Hence, by function space interpolation,

$$\|u^{(k+1)}\|_{L^{2+\frac{4}{d}}(Q_T)} \leq C$$

where  $Q_T := \Omega \times (0, T)$ .

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where  $Q_T := \Omega \times (0, T)$ . Therefore, also,

$$\|b \otimes u^{(k+1)}\|_{L^{2+\frac{4}{d}}(Q_T)} \leq C,$$

whereby

$$\|\mathbb{K}^{(k)} - b \otimes u^{(k+1)}\|_{L^{2+\frac{4}{d}}(Q_T)} \leq C.$$

### STEP 13.

By maximal regularity theory for the Stokes system [Koch–Solonnikov (2001)], there is a positive constant  $C = C_\sigma$ , independent of  $k$ , s.t.

$$\|u^{(k+1)}\|_{W_\sigma^{1,\frac{1}{2}}(Q_T)} \leq C \left( \|\mathbb{K}^{(k)} - b \otimes u^{(k+1)}\|_{L^\sigma(Q_T)} + \|u_0\|_{W^{1-\frac{2}{\sigma},\sigma}(\Omega)} \right),$$

where  $\sigma = \min(\hat{\sigma}, z) > d$ ,  $\hat{\sigma} := 2 + \frac{4}{d}$ , with  $z = d + \vartheta$  for some  $\vartheta \in (0, 1)$ ,

$$W_\sigma^{1,\frac{1}{2}}(Q_T) := L^\sigma(0, T; W_0^{1,\sigma}(\Omega)^d) \cap W^{1/2,\sigma}(0, T; L^\sigma(\Omega)^d).$$

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$$W_\sigma^{1,\frac{1}{2}}(Q_T) := L^\sigma(0, T; W_0^{1,\sigma}(\Omega)^d) \cap W^{1/2,\sigma}(0, T; L^\sigma(\Omega)^d).$$

As  $W_\sigma^{1,\frac{1}{2}}(Q_T) \hookrightarrow L^2(0, T; W_0^{1,\sigma}(\Omega)^d)$ , it follows that by STEP 12 that

$$\|u^{(k+1)}\|_{L^2(0, T; W^{1,\sigma}(\Omega))} \leq C(1 + \|u_0\|_{W^{1-\frac{2}{\sigma},\sigma}(\Omega)}), \quad \sigma > d,$$

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$$\|u^{(k+1)}\|_{L^2(0, T; W^{1,\sigma}(\Omega))} \leq C(1 + \|u_0\|_{W^{1-\frac{2}{\sigma},\sigma}(\Omega)}), \quad \sigma > d,$$

and therefore, by Sobolev embedding,

$$\|u^{(k+1)}\|_{L^2(0, T; L^\infty(\Omega))} \leq C(1 + \|u_0\|_{W^{1-\frac{2}{\sigma},\sigma}(\Omega)}).$$

## STEP 14.

We deduce that

$$u^{(k)} \rightarrow u \quad \text{weakly in } L^2(0, T; W_0^{1,\sigma}(\Omega)^d) \text{ as } k \rightarrow \infty, \quad \sigma > d,$$

$$u^{(k)} \rightarrow u \quad \text{weakly in } W^{1,2}(0, T; W^{-1,\sigma}(\Omega)^d) \text{ as } k \rightarrow \infty,$$

$$u^{(k)} \rightarrow u \quad \text{strongly in } L^2(0, T; \mathcal{C}^{0,\gamma}(\overline{\Omega})^d) \text{ as } k \rightarrow \infty, \quad 0 < \gamma < 1 - \frac{d}{\sigma}, \quad \sigma > d,$$

where the last result follows, via the Aubin–Lions lemma, thanks to the compact embedding of  $W_0^{1,\sigma}(\Omega)^d$  into  $\mathcal{C}^{0,\gamma}(\overline{\Omega})^d$  for  $0 < \gamma < 1 - \frac{d}{\sigma}$ ,  $\sigma > d$ .

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It is now straightforward to pass to the limit in the Oseen system:

$$\begin{aligned} \partial_t u + (b \cdot \nabla) u - \mu \Delta u + \nabla \pi &= \nabla \cdot \mathbb{K} && \text{for } (x, t) \in \Omega \times (0, T], \\ \nabla \cdot u &= 0 && \text{for } (x, t) \in \Omega \times (0, T], \\ u(x, t) &= 0 && \text{for } (x, t) \in \partial\Omega \times (0, T], \\ u(x, 0) &= u_0(x) && \text{for } x \in \Omega. \end{aligned}$$

## STEP 15.

It remains to identify the weak\* limit  $\mathbb{K}$  of the sequence  $(\mathbb{K}^{(k)})_{k \geq 0}$  in terms of the limit  $\widehat{\varrho}$  of the sequence  $(\widehat{\varrho}^{(k)})_{k \geq 0}$ .

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We rewrite FP equation as

$$\begin{aligned} M\partial_t \widehat{\varrho}^{(k)} - \frac{\beta^2}{\epsilon^2} \left( \sum_{j=1}^{J+1} \partial_{v_j} \cdot (M\partial_{v_j} \widehat{\varrho}^{(k)}) \right) + \frac{1}{\epsilon} \left( \sum_{j=1}^{J+1} Mv_j \cdot \partial_{r_j} \widehat{\varrho}^{(k)} \right) \\ = -\frac{1}{\epsilon} \sum_{j=1}^{J+1} \left( ((\mathcal{L}r)_j + u^{(k)}(r_j, t)) \cdot \partial_{v_j} (M\widehat{\varrho}^{(k)}) \right) \\ \text{in } \mathcal{D}'(\Omega^{J+1} \times \mathbb{R}^{(J+1)d} \times (0, T)), \end{aligned}$$

$$\widehat{\varrho}^{(k)}(r, v, 0) = \widehat{\varrho}_0^{(k)}(r, v) = G_k(\widehat{\varrho}_0(r, v)),$$

and note that the differential operator on the left-hand side is hypoelliptic.

## STEP 16.

(A) Boundedness of the sequence of initial data:

$$\sup_{k \geq 1} \|M \hat{\varrho}_0^{(k)}\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} \leq C.$$

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(B) Equiboundedness of the sequence of initial data:

$$\sup_{k \geq 1} \|\chi_{|v| \geq R}(\cdot) M \hat{\varrho}_0^{(k)}\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} \leq \frac{C}{R^2} \quad \forall R \geq 1.$$

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$$\sup_{k \geq 1} \|\chi_{|v| \geq R}(\cdot) M \widehat{\varrho}_0^{(k)}\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} \leq \frac{C}{R^2} \quad \forall R \geq 1.$$

(C) Boundedness of the sequence of right-hand sides:

$$\sup_{k \geq 1} \int_0^T \left(1 + \|u^{(k)}(\cdot, t)\|_{L^\infty(\Omega)}\right) \|M \partial_{v_j} \widehat{\varrho}^{(k)}(\cdot, \cdot, t)\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} dt \leq C.$$

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$$\sup_{k \geq 1} \|\chi_{|v| \geq R}(\cdot) M \widehat{\varrho}_0^{(k)}\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} \leq \frac{C}{R^2} \quad \forall R \geq 1.$$

(C) Boundedness of the sequence of right-hand sides:

$$\sup_{k \geq 1} \int_0^T \left(1 + \|u^{(k)}(\cdot, t)\|_{L^\infty(\Omega)}\right) \|M \partial_{v_j} \widehat{\varrho}^{(k)}(\cdot, \cdot, t)\|_{L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})} dt \leq C.$$

(D) Equiboundedness of the sequence of right-hand sides:

$$\lim_{R \rightarrow \infty} \sup_{k \geq 1} \|\chi_{|v| \geq R}(\cdot) ((\mathcal{L}r)_j + u^{(k)}) \cdot \partial_{v_j} (M \widehat{\varrho}^{(k)})\|_{L^1(0, T; L^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))} = 0.$$

## STEP 17.

By an argument of R. DiPerna & P.-L. Lions (1988), (A)–(D) imply that

$$\widehat{\varrho}^{(k)} \rightarrow \widehat{\varrho} \quad \text{strongly in } L^1(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})) \quad \text{as } k \rightarrow \infty.$$

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This then (eventually, after a further technical argument,) implies that

$$\mathbb{K}^{(k)}(x, t) := \frac{\int_{D^J \times \mathbb{R}^{(J+1)d}} (\sum_{j=1}^J \lambda q_j \otimes q_j) M \widehat{\varrho}^{(k)}(B(q, x), v, t) dq dv}{\int_{D^J \times \mathbb{R}^{(J+1)d}} M \widehat{\varrho}^{(k)}(B(q, x), v, t) dq dv}$$

converges to

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weakly\* in  $L^\infty(\Omega \times (0, T))$ .

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weakly\* in  $L^\infty(\Omega \times (0, T))$ . Thus we have shown the existence of a weak solution to the coupled Oseen–Fokker–Planck system with the bead-mass  $\epsilon > 0$  fixed.  $\square$

## Small-mass limit and equilibration in momentum space

We showed the existence of functions  $u = u_\epsilon$  and  $\hat{\varrho} = \hat{\varrho}_\epsilon$ , such that

$$u_\epsilon \in \mathcal{C}([0, T]; L^\sigma(\Omega)^d) \cap L^2(0, T; W_0^{1,\sigma}(\Omega)^d) \cap W^{1,2}(0, T; W^{-1,\sigma}(\Omega)^d),$$

with  $\sigma = \min(\hat{\sigma}, z) > d$ ,  $\hat{\sigma} := 2 + \frac{4}{d}$  and  $z = d + \vartheta$  for some  $\vartheta \in (0, 1)$ , is a weak solution to the Oseen system,

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$$\mathcal{F}(\hat{\varrho}_\epsilon) \in L^\infty(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}; \mathbb{R}_{\geq 0})),$$

$$\nabla_v \sqrt{\hat{\varrho}_\epsilon} \in L^2(0, T; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})),$$

$$\nabla_v \hat{\varrho}_\epsilon \in L^2(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})),$$

$$M \partial_t \hat{\varrho}_\epsilon \in L^2(0, T; (W^{s,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))'), \quad s > (J+1)d + 1,$$

satisfies the following weak form of the Fokker–Planck equation:

$$\begin{aligned}
& \int_0^t \langle M \partial_\tau \widehat{\varrho}_\epsilon(\cdot, \cdot, \tau), \varphi(\cdot, \cdot, \tau) \rangle d\tau \\
& + \frac{\beta^2}{\epsilon^2} \left( \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \partial_{v_j} \widehat{\varrho}_\epsilon \cdot \partial_{v_j} \varphi dv dr d\tau \right) \\
& - \frac{1}{\epsilon} \left( \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) v_j \widehat{\varrho}_\epsilon \cdot \partial_{r_j} \varphi dv dr d\tau \right) \\
& - \frac{1}{\epsilon} \left( \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) ((\mathcal{L}r)_j + u_\epsilon(r_j, \tau)) \widehat{\varrho}_\epsilon \cdot \partial_{v_j} \varphi dv dr d\tau \right) = 0
\end{aligned}$$

$\forall \varphi \in L^2(0, T; W_{*,M}^{1,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}) \cap W_*^{s,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \quad s > (J+1)d + 1.$

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& \int_0^t \langle M \partial_\tau \widehat{\varrho}_\epsilon(\cdot, \cdot, \tau), \varphi(\cdot, \cdot, \tau) \rangle d\tau \\
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\end{aligned}$$

Furthermore  $\widehat{\varrho}_\epsilon(\cdot, \cdot, 0) = \widehat{\varrho}_0(\cdot, \cdot)$ ,

$$\int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} M \widehat{\varrho}_\epsilon(r, v, t) dr dv = \int_{\Omega^{J+1} \times \mathbb{R}^{(J+1)d}} M \widehat{\varrho}_0(r, v) dr dv = 1 \quad \forall t \in (0, T].$$

In addition,  $\widehat{\varrho}_\epsilon$  satisfies the following energy inequality:

$$\begin{aligned} \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}_\epsilon(t)) dv dr + \frac{2\beta^2}{\epsilon^2} \sum_{j=1}^{J+1} \int_0^t \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) |\partial_{v_j} \sqrt{\widehat{\varrho}_\epsilon}|^2 dv dr d\tau \\ \leq C \left[ 1 + \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) \mathcal{F}(\widehat{\varrho}_0) dv dr \right], \end{aligned}$$

where  $C = C(\|u_0\|_{W^{1-\frac{2}{\sigma}, \sigma}(\Omega)}, \|b\|_{L^\infty(0, T; L^\infty(\Omega))})$ ,  $\sigma = \min(\hat{\sigma}, z) > d$ ,  $\hat{\sigma} := 2 + \frac{4}{d}$  and  $z = d + \vartheta$  for some  $\vartheta \in (0, 1)$ ;  $C$  is independent of  $\epsilon > 0$ .

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Hence,

$(\mathcal{F}(\widehat{\varrho}_\epsilon))_{\epsilon>0}$  is bounded in  $L^\infty(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))$ ,

$(\nabla_v \sqrt{\widehat{\varrho}_\epsilon})_\epsilon$  is bounded in  $L^2(0, T; L_M^2(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))$ ,

$(M \partial_t \widehat{\varrho}_\epsilon)_{\epsilon>0}$  is bounded in  $L^2(0, T; (W^{s,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))')$ ,

for  $s > (J+1)d + 1$ .

## STEP 18.

$$\begin{aligned}\widehat{\varrho}_\epsilon &\rightharpoonup \widehat{\varrho}_{(0)} && \text{weakly in } L^p(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})) \quad \forall p \in [1, \infty), \\ M \partial_t \widehat{\varrho}_\epsilon &\rightharpoonup M \partial_t \widehat{\varrho}_{(0)} && \text{weakly in } L^2(0, T; (W^{s,2}(\Omega^{J+1} \times \mathbb{R}^{(J+1)d}))'), \quad s > (J+1)d + 1, \\ v_j \widehat{\varrho}_\epsilon &\rightharpoonup v_j \widehat{\varrho}_{(0)} && \text{weakly in } L^2(0, T; L_M^1(\Omega^{J+1} \times \mathbb{R}^{(J+1)d})), \quad j = 1, \dots, J+1.\end{aligned}$$

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Also, because

$$\|u_\epsilon\|_{L^2(0, T; W^{1,\sigma}(\Omega)) \cap W^{1,2}(0, T; W^{-1,\sigma}(\Omega))} \leq C(1 + \|u_0\|_{W^{1-\frac{2}{\sigma}, \sigma}(\Omega)}),$$

with  $\sigma > d$ , whereby

$$u_\epsilon \rightharpoonup u_{(0)} \quad \text{weakly in } L^2(0, T; W^{1,\sigma}(\Omega)) \cap W^{1,2}(0, T; W^{-1,\sigma}(\Omega)),$$

$$u_\epsilon \rightarrow u_{(0)} \quad \text{strongly in } L^2(0, T; \mathcal{C}^{0,\gamma}(\overline{\Omega})^d) \text{ as } \epsilon \rightarrow 0_+, \quad 0 < \gamma < 1 - \frac{d}{\sigma}.$$

## STEP 19.

Furthermore,

$$\sum_{j=1}^{J+1} \int_0^T \int_{\Omega^{J+1}} \int_{\mathbb{R}^{(J+1)d}} M(v) |\partial_{v_j} \sqrt{\hat{\varrho}(0)}|^2 \, dv \, dr \, d\tau \leq 0.$$

## STEP 19.

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Hence,

$$\hat{\varrho}_{(0)}(r, v, t) = \eta(r, t) \quad \text{a.e. in } \Omega^{J+1} \times \mathbb{R}^{(J+1)d} \times (0, T)$$

with  $\eta \in L^\infty(0, T; L^1(\Omega^{J+1}))$  to be determined.

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Thus, we have **equilibration in momentum space**:

$$\varrho_{(0)} := M \hat{\varrho}_{(0)} = M \eta,$$

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## STEP 20.

The small-mass limit of the coupled Oseen–Fokker–Planck system satisfies

$$\begin{aligned}\partial_t u_{(0)} + (b \cdot \nabla) u_{(0)} - \mu \Delta u_{(0)} + \nabla \pi_{(0)} &= \nabla \cdot \mathbb{K}_{(0)} && \text{for } (x, t) \in \Omega \times (0, T], \\ \nabla \cdot u_{(0)} &= 0 && \text{for } (x, t) \in \Omega \times (0, T], \\ u_{(0)}(x, t) &= 0 && \text{for } (x, t) \in \partial\Omega \times (0, T], \\ u_{(0)}(x, 0) &= u_0(x) && \text{for } x \in \Omega.\end{aligned}$$

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The identification of  $\mathbb{K}_{(0)}$  (via the DIV-CURL Lemma) is (again) technical:

$$\mathbb{K}_{(0)}(x, t) := \frac{\int_{D^J} \sum_{j=1}^J (F(q_j) \otimes q_j) \eta(B(q, x), t) \, dq}{\int_{D^J} \eta(B(q, x), t) \, dq} \quad \text{for } (x, t) \in \Omega \times (0, T],$$

where  $B(x, q) = r$ ,

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where  $B(x, q) = r$ , and  $\eta \geq 0$ , with  $\int_{\Omega^{J+1}} \eta(r, t) \, dr = 1$  for all  $t \in [0, T]$ , solves

$$\partial_t \eta + \sum_{j=1}^{J+1} \partial_{r_j} \cdot \left( \eta ((\mathcal{L}r)_j + u_{(0)}(r_j, \cdot)) \right) - \beta \sum_{j=1}^{J+1} \partial_{r_j}^2 \eta = 0 \quad \text{in } \Omega^{J+1} \times (0, T],$$

$$\eta(\cdot, 0) = \widehat{\varrho}_0 \in L^2(\Omega^{J+1}; \mathbb{R}_{\geq 0}) \quad + \left\{ \begin{array}{l} \text{zero-flux boundary condition on} \\ \partial\Omega^{(j)} \times (0, T] \text{ for } j = 1, \dots, J+1. \end{array} \right.$$

Change variables in FP from  $r \in \Omega^{J+1}$  to  $(x, q) \in \Omega \times D^J$

Hence,  $\psi(x, q, t) := \eta(B(q, x), t) = \eta(r, t)$  solves on  $\Omega \times D^J \times [0, T]$ :

$$\begin{aligned} & \partial_t \psi + \nabla_x \cdot (u_{(0)} \psi) + \sum_{j=1}^J \partial_{q_j} \cdot ((\nabla_x u_{(0)}) q_j \psi) \\ & - \beta \sum_{i,j=1}^J \partial_{q_j} \cdot \left[ \mathcal{R}_{ij} \mathfrak{M}(q) \partial_{q_i} \left( \frac{\psi}{\mathfrak{M}(q)} \right) \right] - \frac{\beta}{J+1} \Delta_x \psi = 0, \end{aligned}$$

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with the initial condition  $\psi(x, q, 0) = \psi_0(x, q) := \hat{\varrho}_0(B(q, x))$ , and the bdry. cond.

$$\nabla_x \psi(x, q, t) \cdot n_x(x) = 0 \quad \text{for all } (x, q, t) \in \partial\Omega \times D^J \times (0, T],$$

where  $n_x$  is the unit outward normal vector to  $\partial\Omega$ , and

$$\sum_{i=1}^J \left[ \beta \mathcal{R}_{ij} \mathfrak{M}(q) \partial_{q_i} \left( \frac{\psi}{\mathfrak{M}(q)} \right) - (\nabla u_{(0)}) q_j \psi \right] \cdot n_{q_j} = 0$$

for all  $(x, q, t) \in \Omega \times (D \times \cdots \times \partial D \times \cdots \times D) \times (0, T]$ ,  $j = 1, \dots, J$ , where  $n_{q_j}$  is the unit outward normal vector to  $\partial D$  for the  $j$ th copy of  $D$ ; and

$$\mathfrak{M}(q) := (2\pi\beta)^{-\frac{1}{2}Jd} \exp(-|q|^2/2\beta), \quad q \in D^J.$$

**Note:** If the initial datum  $\psi_0$  is such that, for some constant  $n > 0$ ,

$$\int_{D^J} \psi_0(x, q) dq = n^{-1} \quad \text{for a.e. } x \in \Omega,$$

then it follows that

$$\int_{D^J} \eta(B(q, x), t) dq = \int_{D^J} \psi(x, q, t) dq = n^{-1} \quad \text{for a.e. } (x, t) \in \Omega \times [0, T],$$

so the expression for  $\mathbb{K}_{(0)}$  simplifies to the **Kramers' expression**:

$$\mathbb{K}_{(0)} = n \int_{D^J} \sum_{j=1}^J (F(q_j) \otimes q_j) \psi(x, q, t) dq.$$



The number  $n > 0$  is called the *polymer number density per unit volume*.



M. Dostálík, J. Málek, V. Průša, and E. Süli. A simple approach to thermodynamically consistent modelling of non-isothermal flows of dilute compressible polymeric fluids. *Fluids* 2020, Volume 5, Issue 3, 29 pp.; DOI:10.3390/fluids5030133.