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Interface motion driven by curvature and potential and its homogenization limit

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1 Introduction

Homopolymer molecules are the chain of one kind of monomers, which can be made by polymerization, while diblock copolymer molecules consist of subchains of two different type of monomers. Due to repulsive forces between unlike monomers, say A- and B-monomers, the different homopolymers tend to segregate. This is called phase separation. On the other hand, in the case of copolymers, since the subchains are chemically bonded, two polymer chains can be forced to mix on a macroscopic scale. However on a microscopic scale, the two polymer chains still segregate, and micro-domains rich in A- and B-monomers respectively form patterns. This is called the micro phase separation. For more physical background on this phenomenon we refer to [3, 11].

Energetically favorable configurations have been characterized in the Ohta–Kawasaki theory [24] by minimizers of an energy functional of the form

$$I_\epsilon(u) = \int_\Omega \frac{\epsilon^2}{2}|\nabla u|^2 + W(u) + \frac{\gamma}{2}|(-\Delta)^{-1/2}(u-\rho)|^2\,dx\,.$$

Here $\Omega = (0,L)^N$ $(N = 2,3)$ is the domain covered by the copolymers and u denotes the local density of one of the two monomers. The function W is a double well potential with two global minima at 0 and 1, $\epsilon \in \mathbb{R}_+$ a small parameter depending on the size and mobility of monomers, $\frac{1}{L^N}\int_{(0,L)^N} u\,dx = \rho \in (0,1)$ the average density and $\gamma \in \mathbb{R}_+$ is a parameter related to the polymerization index. The first term in the energy prefers large blocks of monomers, the second favors segregated monomers and the third term prefers a uniform state or a very fine mixture. The parameter ϵ expresses the width of the transition layer between the two segregated states $u \sim 0$ and $u \sim 1$. Competition between these terms leads to minimizers of I_ϵ which represent micro-phase separation. Indeed, minimizers u_ε of the energy functional I_ϵ oscillate more and more rapidly as $\epsilon \to 0$.

On the other hand, the energy functional of the form

$$J_\epsilon(u) = \int_\Omega \frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u) + \frac{\gamma}{2}|(-\Delta)^{-1/2}(u-\rho)|^2\,dx$$

has the following sharp interface limit in the sense of Γ-convergence as $\epsilon \to 0$:

$$J_0(G) = \mathcal{H}^{N-1}(\partial G \cap \Omega) + \frac{\gamma}{2}\int_\Omega \left|(-\Delta)^{-1/2}(\chi_G - \rho)\right|^2 dx\,, \tag{1}$$

where $G \subset [0,L)^N$ denotes the region covered by, say, A-monomers, χ_G the characteristic function of G, $\rho = \frac{|G|}{L^N} \in (0,1)$ the volume fraction, and $\mathcal{H}^{N-1}$ denotes $N-1$ dimensional Hausdorff measure. We observe also on the level of the sharp interface model the competition between phase separation on the large scale, which is preferred by the first term, and fine mixtures that are preferred by the nonlocal term. Indeed,

$$0 = \inf_{G\in M}\int_{(0,L)^N} \left|(-\Delta)^{-1/2}(\chi_G - \rho)\right|^2 dx, \quad M = \{G \subset [0,L)^N\,;\, |G| = \rho L^N\}$$

is not attained on M since its minimizing sequence oscillates more and more rapidly. Thus this variational problem of characterizing minimizers of I_ϵ or J_ϵ can be considered as a prototype model of periodic pattern formation.

Starting with the pioneering work [21], where the Ohta–Kawasaki theory is formulated on a bounded domain as a singularly perturbed problem and the limiting sharp interface problem as $\varepsilon \to 0$ is identified, there has been a bulk of analytical work. The related minimization problems have been studied in [1, 4, 5, 7, 27].

The Euler–Lagrange equation for J_ϵ is

$$-\epsilon\Delta u + \tfrac{1}{\epsilon}W'(u) + \gamma\mu = \text{const.} \quad \text{in } (0,L)^N, \tag{2}$$

$$-\Delta\mu = u - \rho \quad \text{in } (0,L)^N, \tag{3}$$

$$\frac{1}{L^N}\int_{(0,L)^N} u\,dx = \rho\,, \tag{4}$$

and its sharp interface limit is

$$\kappa + \gamma\mu = \text{const.} \quad \text{on } \partial G, \tag{5}$$

$$-\Delta\mu = \chi_G - \rho \quad \text{in } (0,L)^N, \tag{6}$$

$$\frac{|G|}{L^N} = \rho, \tag{7}$$

where κ is the mean curvature (the sum of the principal curvatures) of ∂G. Here we impose Neumann or periodic boundary conditions for u, μ on $\partial(0,L)^N$. The existence and stability of stationary solutions has been investigated in [22, 23, 25, 26, 28, 29, 30]. In what follows we will consider a periodic setting and hence always require that u and the potential μ are $(0,L)^N$-periodic.

A time dependent model has been considered in [10, 12]. A natural way to set up a model for the evolution of the copolymer configuration that decreases energy and preserves the average density is to consider the gradient flow of the energy.

The H^{-1} inner product $(\cdot,\cdot)_{H^{-1}}$ is given by

$$(u^1,u^2)_{H^{-1}} = \int_{(0,L)^N} \nabla w^1 \cdot \nabla w^2 \, dx\,,$$

where w^α is $(0,L)^N$-periodic and solves

$$-\Delta w^\alpha = u^\alpha$$

for functions u^α with mean value 0 ($\alpha = 1,2$). Hence the nonlocal energy can be expressed in terms of H^{-1} norm $\|u\|_{H^{-1}} = \sqrt{(u,u)_{H^{-1}}}$, that is,

$$J_\epsilon(u) = \int_\Omega \frac{\epsilon}{2}|\nabla u|^2 + \frac{1}{\epsilon}W(u)\,dx + \frac{\gamma}{2}\|u-\rho\|^2_{H^{-1}},$$

$$J_0(G) = \mathcal{H}^{N-1}(\partial G \cap \Omega) + \frac{\gamma}{2}\|\chi_G - \rho\|^2_{H^{-1}}.$$

Then the gradient flow equation of J_ϵ with respect to this inner product is the following fourth order parabolic equation

$$u_t = \Delta(-\epsilon\Delta u + \tfrac{1}{\epsilon}W'(u)) - \gamma(u-\rho)\,,$$

which is an extension of the Cahn–Hilliard equation for phase separation in binary alloys. The sharp interface limit of this evolution equation is the following extension of the Mullins–Sekerka evolution [14, 15]. The interface $\partial G = \partial G(t)$ evolves according to the law

$$V = \left[\nabla w \cdot \vec{n}\right] \qquad \text{on } \partial G, \tag{8}$$

$$-\Delta w = 0 \qquad \text{in } (0,L)^N \backslash \partial G, \tag{9}$$

$$w = \kappa + \gamma\mu \qquad \text{on } \partial G, \tag{10}$$

$$-\Delta\mu = \chi_G - \rho \qquad \text{in } (0,L)^N, \tag{11}$$

where V denotes the normal velocity of ∂G, $\vec{n}$ the unit outer normal to G, and $\left[\nabla w \cdot \vec{n}\right]$ denotes the jump of the normal component of the gradient of the potential w across the interface. Here $[f]$ denotes

$$[f] = \lim_{\substack{x\notin G \\ x\to\partial G}} f(x) - \lim_{\substack{x\in G \\ x\to\partial G}} f(x).$$

We see that the volume of $G(t)$ is preserved in time under the periodic boundary condition for μ, w on $\partial(0,L)^N$. In what follows we will require that the potentials μ, w, and the phase domain G are $(0,L)^N$-periodic. Local well-posedness of this evolution has been established in [9].

The evolution defined by (8)-(11) has an interpretation as a gradient flow of the energy (1) on a Riemannian manifold. To define a metric tensor, consider the manifold of $(0,L)^N$-periodic subsets of $\mathbb{R}^N$ with fixed volume, that is,

$$\mathcal{M} = \{G \subset \mathbb{R}^N \,;\, G \text{ is } (0,L)^N\text{-periodic},\ |G \cap [0,L)^N| = \mathrm{Vol}\},$$

whose tangent space $T_G\mathcal{M}$ at an element $G \in \mathcal{M}$ is described by all kinematically admissible normal velocities of ∂G, that is,

$$T_G\mathcal{M} = \left\{ V\colon \partial G \to \mathbb{R} \,;\, V \text{ is } (0,L)^N\text{-periodic}, \int_{\partial G \cap [0,L)^N} V\, dS = 0 \right\}.$$

The Riemannian structure is given by the following metric tensor on the tangent space:

$$g_G(V^1, V^2) = \int_{(0,L)^N} \nabla w^1 \cdot \nabla w^2 \, dx, \tag{12}$$

where w^α is $(0,L)^N$-periodic and solves

$$\begin{aligned} -\Delta w^\alpha &= 0 && \text{in } \mathbb{R}^N \backslash \partial G, \\ \left[\nabla w^\alpha \cdot \vec{n}\right] &= V^\alpha && \text{on } \partial G \end{aligned}$$

for $V^\alpha \in T_G\mathcal{M}$ $(\alpha = 1,2)$.

(8)-(11) can be regarded as the gradient flow of the energy (1) with respect to the metric g. In other words, V satisfies

$$g_{G(t)}(V, \tilde{V}) = -\langle DJ_0(G(t)), \tilde{V} \rangle \tag{13}$$

for all $\tilde{V} \in T_{G(t)}\mathcal{M}$.

2 Restriction to spherical particles

In what follows we are interested in the regime where the fraction of A-monomers is much smaller than the one of B-monomers. In this case the A-phase consists of a set of many small disconnected approximately spherical particles. This has been established in the sense of Γ-convergence for the sharp-interface functional in [6]. For our evolutionary problem it seems hence natural to restrict the evolution (8)-(11) to spherical particles by restricting the gradient flow to such morphologies.

For that purpose we define the submanifold $\mathcal{N} \subset \mathcal{M}$ of all sets G which are the union of disjoint balls

$$G = \bigcup_i B_{R_i}(X_i), \qquad \mathrm{mod}\ L\mathbb{Z}^N$$

where the centers $\{X_i\}_i$ and the radii $\{R_i\}_i$ are variables. Hence $\mathcal{N}$ can be identified with an open subspace of the hypersurface

$$\{\mathbf{Y} = \{R_i, X_i\}_i\,;\, (R_i, X_i) \in \mathbb{R}_+ \times [0,L)^N, \omega_N \sum_i R_i^N = \mathrm{Vol}\} \subset \mathbb{R}^{n(N+1)},$$

where ω_N is the volume of the unit ball in $\mathbb{R}^N$, n is the number and $i = 1, \cdots, n$ an enumeration of the particles with centers in the periodic box $[0,L)^N$. Since the normal velocity V satisfies $V = \frac{dR_i}{dt} + \frac{dX_i}{dt} \cdot \vec{n}$ on $\partial B_{R_i}(X_i)$, the tangent space can be identified with the hyperplane

$$T_{\mathbf{Y}}\mathcal{N} = \Big\{\mathbf{Z} = \sum_i (v_i \frac{\partial}{\partial R_i} + \xi_i \cdot \frac{\partial}{\partial X_i})\,;\, (v_i, \xi_i) \in \mathbb{R} \times \mathbb{R}^N, \sum_i R_i^{N-1} v_i = 0\Big\} \subset \mathbb{R}^{n(N+1)},$$

such that v_i describes the rate of change of the radius of particle i and ξ_i the rate of change of its center. We use the abbreviation $\mathbf{Z} = \{v_i, \xi_i\}_i$ for $\mathbf{Z} = \sum_i (v_i \frac{\partial}{\partial R_i} + \xi_i \cdot \frac{\partial}{\partial X_i})$.

It turns out to be notationally convenient to consider the normalized energy

$$E(\mathbf{Y}) = E_{\mathrm{surf}}(\mathbf{Y}) + \gamma E_{\mathrm{nl}}(\mathbf{Y}),$$

where

$$E_{\mathrm{surf}}(\mathbf{Y}) = 2\pi \sum_i R_i^{N-1},$$

$$E_{\mathrm{nl}}(\mathbf{Y}) = \frac{N}{2} \int_{(0,L)^N} |\nabla \mu|^2 \, dx$$

with $\mu = \mu(x)$ being $(0,L)^N$-periodic and solving

$$-\Delta \mu = \chi_G - \frac{\int_{(0,L)^N} \chi_G \, dx}{L^N}.$$

From now on we consider an arrangement of particles as described above which evolves according to the gradient flow equation.

Let $w = w(x)$ be the $(0,L)^N$-periodic function which solves

$$\begin{aligned} -\Delta w &= 0 && \text{in } \mathbb{R}^N \backslash \partial G, \\ \left[\nabla w \cdot \vec{n}\right] &= v_i + \xi_i \cdot \vec{n} && \text{on } \partial B_{R_i}(X_i) \end{aligned}$$

for $\mathbf{Z} = \{v_i, \xi_i\}_i \in T_{\mathbf{Y}}\mathcal{N}$.

Then we see that w satisfies

$$\frac{1}{|\partial B_{R_i}(X_i)|} \int_{\partial B_{R_i}(X_i)} \left(w - \tfrac{1}{R_i} - N\gamma\mu\right) dS = \lambda(t) \tag{14}$$

and

$$\int_{\partial B_{R_i}(X_i)} (w - N\gamma\mu)\, \vec{n} \, dS = 0 \tag{15}$$

for all i such that $R_i > 0$, with a Lagrange parameter $\lambda(t)$ that ensures volume conservation. Here $|\partial B_{R_i}(X_i)|$ denotes the surface area of $\partial B_{R_i}(X_i)$. Equations (14) and (15) are the analogue of (10) in the restricted setting.

3 Mean field equations

We remark that in general one cannot expect that a smooth solution exists globally. In fact, if the initial configuration consists of a collection of nonoverlapping balls, short time existence and uniqueness of a smooth solution can be established as it has been done in [16] for a related case without nonlocal term. If a particle disappears, the evolution is not smooth; however one can extend the solution continuously by just starting again with the new configuration. The evolution cannot be extended further when particles collide.

The leading order asymptotics of the evolution have been identified by formal asymptotics in [8, 13]. If $\mathcal{R}$ denotes the average radius (see (19) for a precise definition) then it turns out that on a time scale $t_{\mathcal{R}} \sim \mathcal{R}^3$ migration of particles can be neglected and the evolution of the radii is governed by an extension of the classical LSW growth law for coarsening of particles. More precisely, in a dilute regime (see below for a precise definition), the radii of particles evolve according to

$$\frac{d}{dt}R_i \sim \frac{1}{R_i^2 \log(1/\rho)}\big(\lambda R_i - 1 - \gamma R_i^3 \log(1/\rho)\big), \tag{16}$$

when $N = 2$, and

$$\frac{d}{dt}R_i \sim \frac{1}{R_i^2}\big(\lambda R_i - 1 - \gamma R_i^3\big), \tag{17}$$

when $N = 3$, where $\lambda = \lambda(t)$ is determined by the condition that the volume fraction of the particles is conserved. In an early stage this means that larger particles grow while smaller ones shrink and disappear. However, the term γR_i^3 which comes from the nonlocal energy prevents infinite coarsening and leads to a stabilization of the remaining particles around a stable radius. The migration of particles typically leads to the self-organization of particles in lattice structures.

To describe the mean-field models for this time regime, we now introduce the relevant scales and parameters. In what follows we use the abbreviation $\sum_i = \sum_{i:R_i>0}$. We define the number density $\frac{1}{d^N}$ of particles by

$$d^N \sum_i 1 = L^N \tag{18}$$

and the average volume $\omega_N \mathcal{R}^N$ by

$$\sum_i R_i(0)^N = \mathcal{R}^N \sum_i 1. \tag{19}$$

We identify the evolution in the limit of vanishing volume fraction of particles. More precisely,

we consider a sequence of systems characterized by the parameter

$$\varepsilon := \begin{cases} \left(\log\left(\frac{d}{\mathcal{R}}\right)\right)^{-1/2} & \text{for } N = 2 \\ \left(\frac{\mathcal{R}}{d}\right)^{1/2} & \text{for } N = 3 \end{cases} \tag{20}$$

in the limit $\varepsilon \to 0$. Note that we define here the initial number density and the initial average volume. During the evolution d and $\mathcal{R}$ typically increase in time; the parameter ε is however preserved during the evolution. It is well-known that there is, analogous to electrostatics, a characteristic length scale, the screening length

$$L_{sc} := \begin{cases} d\left(\log\frac{d}{\mathcal{R}}\right)^{1/2} \sim d\left(\log\frac{1}{\rho}\right)^{1/2} & \text{for } N = 2 \\ \left(\frac{d^3}{\mathcal{R}}\right)^{1/2} & \text{for } N = 3 \end{cases} \tag{21}$$

which describes the effective range of particle interactions.

Dilute case

In the case that $L \ll L_{sc}$, that is in the very dilute case, in the limit of vanishing volume fraction as $\varepsilon \to 0$, the normalized number density of particles with radius r, denoted by $\nu(t,r)$, satisfies

$$\partial_t \nu + \partial_r \left[\frac{1}{r^2}\{\lambda(t) r - 1 - \gamma r^3\}\nu\right] = 0 \tag{22}$$

with

$$\lambda(t) = \frac{\int_{\mathbb{R}_+} \frac{1}{r}\,\nu\,dr + \gamma \int_{\mathbb{R}_+} r^2\,\nu\,dr}{\int_{\mathbb{R}_+} \nu\,dr} \tag{23}$$

when $N = 2$, and

$$\partial_t \nu + \partial_r \left[\frac{1}{r^2}\{\lambda(t) r - 1 - \gamma r^3\}\nu\right] = 0 \tag{24}$$

with

$$\lambda(t) = \frac{\int_{\mathbb{R}_+} \nu\,dr + \gamma \int_{\mathbb{R}_+} r^3\,\nu\,dr}{\int_{\mathbb{R}_+} r\,\nu\,dr} \tag{25}$$

when $N = 3$. We observe that this is just the formulation of (16) on the level of a size distribution.

Inhomogeneous extension

If $L \sim L_{sc}$ in the limit of vanishing volume fraction as $\varepsilon \to 0$, one obtains an inhomogeneous extension where λ is not constant in space but is replaced by a slowly varying function $\overline{u}(t,x) - \gamma K(t,x)$. The joint distribution of particle radii and centers $\nu = \nu(t,r,x)$ satisfies

$$\partial_t \nu + \partial_r \left[\frac{1}{r^2}\left\{r\,\overline{u}(t,x) - 1 - \gamma\left(r^3 + rK(t,x)\right)\right\}\nu\right] = 0\,, \tag{26}$$

where $K = K(t,x)$ is $(0,L)^N$-periodic and solves for each t that

$$\int_{(0,L)^N} K(t,x)\,dx = 0$$

and

$$-\Delta K = 2\pi\left(\int_{\mathbb{R}_+} r^2\,\nu\,dr - \frac{1}{L^2}\int_{\mathbb{R}_+\times\Omega} r^2\,\nu\,dr dy\right) \tag{27}$$

when $N = 2$,

$$-\Delta K = 4\pi\left(\int_{\mathbb{R}_+} r^3\,\nu\,dr - \frac{1}{L^3}\int_{\mathbb{R}_+\times\Omega} r^3\,\nu\,dr dy\right) \tag{28}$$

when $N = 3$, and $\overline{u} = \overline{u}(t,x)$ is $(0,L)^N$-periodic and solves for each t

$$-\Delta\overline{u} + 2\pi\left\{\overline{u}\int_{\mathbb{R}_+}\nu\,dr - \int_{\mathbb{R}_+}\frac{1}{r}\,\nu\,dr - \gamma\left(\int_{\mathbb{R}_+} r^2\,\nu\,dr + K(t,x)\int_{\mathbb{R}_+}\nu\,dr\right)\right\} = 0 \tag{29}$$

when $N = 2$,

$$-\Delta\overline{u} + 4\pi\left\{\overline{u}\int_{\mathbb{R}_+} r\,\nu\,dr - \int_{\mathbb{R}_+}\nu\,dr - \gamma\left(\int_{\mathbb{R}_+} r^3\,\nu\,dr + K(t,x)\int_{\mathbb{R}_+} r\,\nu\,dr\right)\right\} = 0 \tag{30}$$

when $N = 3$. In the case $L \sim L_{sc}$, the inhomogeneous mean-field model in the homogenization limit as $\varepsilon \to 0$ has been derived in [17]. The derivation of the dilute limit can be done along the same lines.

Energy for the mean-field models

The mean-field model has a gradient flow structure. More precisely, the mean field equation is the gradient flow of the energy functional defined below. In the dilute case, we define

$$E(\nu) = 2\pi\int_{\mathbb{R}_+}\left(\frac{\gamma}{4}r^4 + r\right)\nu\,dr \tag{31}$$

when $N = 2$, and

$$E(\nu) = 4\pi\int_{\mathbb{R}_+}\left(\frac{\gamma}{5}r^5 + \frac{r^2}{2}\right)\nu\,dr \tag{32}$$

when $N = 3$. In the inhomogeneous case, we define

$$E(\nu) = 2\pi\int_{\mathbb{R}_+\times\Omega}\left(\frac{\gamma}{4}r^4 + r\right)\nu\,drdx + \frac{\gamma}{4}\int_\Omega |\nabla K|^2\,dx \tag{33}$$

when $N = 2$,

$$E(\nu) = 4\pi\int_{\mathbb{R}_+\times\Omega}\left(\frac{\gamma}{5}r^5 + \frac{r^2}{2}\right)\nu\,drdx + \frac{\gamma}{6}\int_\Omega |\nabla K|^2\,dx \tag{34}$$

when $N = 3$, where $K = K(x)$ is an $(0,L)^N$-periodic function solving $\int_{(0,L)^N} K\,dx = 0$, (27) when $N = 2$, and (28) when $N = 3$.

4 The derivation of mean-field models

The inhomogeneous mean-field model for the evolution of the size distribution of particles in the limit of vanishing volume fraction has been rigorously derived in [17], and show that particles, if initially well separated, remain separated over the time span we are considering and thus well-posedness is ensured. We denote the joint distribution of particle centers and radii at a given time t by ν or ν_t. The natural space for ν is the space of nonnegative bounded Borel measures on $\mathbb{R}_+ \times \mathbb{T}$. Here $\mathbb{T}$ denotes the N dimensional flat torus, and we identify functions on $\mathbb{T}$ with $(0, L)^N$-periodic functions on $\mathbb{R}^N$. By introducing suitably rescaled variables, setting up the equation in the rescaled variables, under the appropriate assumption on our initial particle arrangement, the mean-field models (26)-(30) can be derived. We will state the derivation results and describe the main ideas of the proof.

We assume from now on that $L = L_{sc}$ and for the ease of presentation, we will rescale the spatial variables by L_{sc} such that $L_{sc} = L = 1$. Hence in two dimensional case, $d = \varepsilon$, $\mathcal{R} = \alpha_\varepsilon := \varepsilon \exp(-1/\varepsilon^2)$. Notice that $\rho = \pi\alpha_\varepsilon^2\varepsilon^{-2}$ and $\log(1/\rho) \sim \varepsilon^{-2}$. We introduce $\hat{R}_i$, $\hat{t}$, $\hat{w}$, $\hat{v}_i$, $\hat{\xi}_i$, $\hat{\gamma}$ and $\hat{\mu}$ via

$$
\begin{aligned}
&R_i(t) = \alpha_\varepsilon \hat{R}_i(\hat{t}), \qquad t = \alpha_\varepsilon^3 \log(1/\rho)\hat{t}, \qquad w(t,x) = \alpha_\varepsilon^{-1}\hat{w}(\hat{t},x),\\
&v_i(t) = \frac{1}{\alpha_\varepsilon^2 \log(1/\rho)}\hat{v}_i(\hat{t}) \sim \frac{\varepsilon^2}{\alpha_\varepsilon^2}\hat{v}_i(\hat{t}), \qquad \xi_i(t) = \frac{\varepsilon}{\alpha_\varepsilon^2}\hat{\xi}_i(\hat{t}),\\
&\gamma = \frac{1}{\alpha_\varepsilon^3 \log(1/\rho)}\hat{\gamma} \sim \frac{\varepsilon^2}{\alpha_\varepsilon^3}\hat{\gamma}, \qquad \mu(t,x) = \frac{\alpha_\varepsilon^2}{\varepsilon^2}\hat{\mu}(\hat{t},x).
\end{aligned}
$$

On the other hand, in three dimensional case, $d = \varepsilon$, $\mathcal{R} = \alpha_\varepsilon := \varepsilon^3$. In this case, we introduce $\hat{R}_i$, $\hat{t}$, $\hat{v}_i$, $\hat{\xi}_i$, $\hat{w}$, $\hat{\mu}$, and $\hat{\gamma}$ via

$$
\begin{aligned}
&R_i(t) = \varepsilon^3\hat{R}_i(\hat{t}), \qquad t = \varepsilon^9\hat{t}, \qquad v_i(t) = \varepsilon^{-6}\hat{v}_i(\hat{t}), \qquad \xi_i(t) = \varepsilon^{-6}\hat{\xi}_i(\hat{t}),\\
&w(t,x) = \varepsilon^{-3}\hat{w}(\hat{t},x), \qquad \mu(t,x) = \varepsilon^6\hat{\mu}(\hat{t},x), \qquad \gamma = \varepsilon^{-9}\hat{\gamma}.
\end{aligned}
$$

We note that, over the time scales we are considering, ξ_i and hence also $\frac{dX_i}{dt}$, vanish in the limit. From now on we only deal with the rescaled quantities and drop the hats in the notation.

In rescaled variables the submanifold $\mathcal{N}^\varepsilon$ is given by

$$
\mathcal{N}^\varepsilon = \{\mathbf{Y}^\varepsilon = \{R_i, X_i\}_i \,;\, \sum_i \varepsilon^N R_i^N = 1\}
$$

and the tangent space by

$$
T_{\mathbf{Y}^\varepsilon}\mathcal{N}^\varepsilon = \left\{\tilde{\mathbf{Z}}^\varepsilon = \sum_i (\tilde{v_i}\frac{\partial}{\partial R_i} + \varepsilon^3\tilde{\xi_i}\cdot\frac{\partial}{\partial X_i}) \,;\, \sum_i R_i^2\tilde{v_i} = 0\right\}
$$

when $N = 3$, and

$$T_{\mathbf{Y}^\varepsilon}\mathcal{N}^\varepsilon = \Big\{\tilde{\mathbf{Z}}^\varepsilon = \sum_i (\tilde{v}_i \frac{\partial}{\partial R_i} + \varepsilon\alpha_\varepsilon \log(1/\rho)\tilde{\xi}_i \cdot \frac{\partial}{\partial X_i})\,;\, \sum_i R_i\tilde{v}_i = 0\Big\}$$

when $N = 2$.

We define the energy in rescaled variables as

$$E_\varepsilon(\mathbf{Y}^\varepsilon) = 2\pi \sum_i \varepsilon^N R_i^{N-1} + \frac{N\gamma}{2}\int_{(0,1)^N} |\nabla\mu^\varepsilon|^2\, dx,$$

where $\mu^\varepsilon = \mu^\varepsilon(t,x)$ is $(0,1)^N$-periodic and solves

$$-\Delta\mu^\varepsilon = \left(\frac{\varepsilon}{\alpha_\varepsilon}\right)^N \chi_{\cup B_i} - \omega_N$$

and $\int_{(0,1)^N} \mu^\varepsilon\, dx = 0$. Here $B_i := B_{\alpha_\varepsilon R_i}(X_i)$.

We denote the joint distribution of particle centers and radii at a given time t by $\nu_t^\varepsilon \in (C_p^0)^*$, which is given by

$$\int \zeta\, d\nu_t^\varepsilon = \sum_i \varepsilon^N \zeta\,(R_i(t), X_i(t)) \quad \text{for } \zeta \in C_p^0\,, \tag{35}$$

where C_p^0 stands for the space of continuous functions on $\mathbb{R}_+ \times \mathbb{T}$ which have compact support included in $\mathbb{R}_+ \times \mathbb{T}$. We identify functions $\zeta = \zeta(r,x) \in C_p^0$ with functions which are $(0,1)^N$-periodic in x. Note that since $\zeta(r,x) = 0$ for $r = 0$, particles which have vanished do not enter the distribution. Hence the natural space for ν_t^ε is the space $(C_p^0)^*$ of Borel measures on $\mathbb{R}_+ \times \mathbb{T}$, that is, the product of the positive half axis and the torus. In accordance with the notation in (35) we will use in what follows the abbreviation

$$\int \zeta\, d\nu_t := \int_{\mathbb{R}_+\times(0,1)^N} \zeta(r,x)\, d\nu_t(r,x) \quad \text{for } \zeta \in C_p^0,\ \nu_t \in (C_p^0)^*.$$

Otherwise the domain of integration is specified.

Main result

The main result is the following which informally says that ν_t^ε converges as $\varepsilon \to 0$ to a weak solution of (26)-(30).

Let $T > 0$ be given and assume some appropriate assumptions on initial particle arrangements. Then there exists a subsequence, again denoted by $\varepsilon \to 0$, and a weakly continuous map $[0,T] \ni t \mapsto \nu_t \in (C_p^0)^*$ with

$$\int \zeta\, d\nu_t^\varepsilon \to \int \zeta\, d\nu_t$$

uniformly in $t \in [0,T]$ for all $\zeta \in C^0_p$, and

$$\int r^N \, d\nu_t \;=\; 1$$

for all $t \in [0,T]$. Furthermore, there exists a measurable map $(0,T) \ni t \mapsto (\overline{u}(t), K(t)) \in (H^1_p)^2$ such that (26)-(30) hold in the following weak sense.

$$\frac{d}{dt}\int \zeta \, d\nu_t \;=\; \int \partial_r \zeta \, \frac{1}{r^2}\left(r\,\overline{u}(t,x) - 1 - \gamma(r^3 + rK(t,x))\right) d\nu_t \tag{36}$$

distributionally on $(0,T)$ for all $\zeta \in C^0_p$ with $\partial_r \zeta \in C^0_p$. Here

$$\int_{(0,1)^2} \nabla K(t,x) \cdot \nabla \zeta \, dx = 2\pi \left(\int r^2 \zeta \, d\nu_t - \int_{(0,1)^2} \zeta \, dx \right), \tag{37}$$

$$\int_{(0,1)^2} \nabla \overline{u}(t,x) \cdot \nabla \zeta \, dx + 2\pi \int \zeta \left(\overline{u}(t,x) - \frac{1}{r} - \gamma \left\{ r^2 + K(t,x) \right\} \right) d\nu_t = 0 \tag{38}$$

when $N = 2$,

$$\int_{(0,1)^3} \nabla K(t,x) \cdot \nabla \zeta \, dx = 4\pi \left(\int r^2 \zeta \, d\nu_t - \int_{(0,1)^3} \zeta \, dx \right), \tag{39}$$

$$\int_{(0,1)^3} \nabla \overline{u}(t,x) \cdot \nabla \zeta \, dx + 4\pi \int \zeta \left(\overline{u}(t,x)\, r - 1 - \gamma \left\{ r^3 + rK(t,x) \right\} \right) d\nu_t = 0 \tag{40}$$

when $N = 3$, for all $\zeta \in H^1_p$ and a.e. $t \in (0,T)$. Moreover the energy functional converges in the following sense.

$$\lim_{\varepsilon \to 0} E_\varepsilon(\mathbf{Y}^\varepsilon) = E(\nu_t), \quad \text{uniformly in } t \in [0,T].$$

Here $E(\nu)$ is the homogenized energy defined by (33) and (34).

The strategy of the proof is as follows. We first derive some simple a-priori estimates, and then homogenize within the variational principle of a gradient flow structure, also known as the Rayleigh principle. This follows the related analysis in [18] for the case $\gamma = 0$. In contrast to [18], since our particles move, we need to show that the particles remain separated over the time span we are considering. We also have to identify corresponding additional terms in the metric tensor. Furthermore, in order to prove the convergence of the differential of the energy, we need to prove that the tightness condition is preserved in time.

Rayleigh principle says that (13) can be reformulated as follows: for fixed t the direction of steepest descent v minimizes

$$\tfrac{1}{2} g_{G(t)}(\tilde{V}, \tilde{V}) + \langle DJ_0(G(t)), \tilde{V} \rangle \tag{41}$$

under all $\tilde{V} \in T_{G(t)}\mathcal{M}$. Since we will in general only deal with solutions which are piecewise smooth in time and globally continuous, it is convenient to have (41) in the time integrated version, that is v minimizes

$$\int_0^T \beta(t) \Big(\tfrac{1}{2} g_{G(t)}(\tilde{V}, \tilde{V}) + \langle DJ_0(G(t)), \tilde{V} \rangle \Big) \, dt \tag{42}$$

where $\beta = \beta(t)$ is an arbitrary nonnegative smooth function.

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