SCREENING IN INTERACTING PARTICLE SYSTEMS

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ABSTRACT.- We consider the Green's function of the Laplace operator in domains with spherical holes (particles). Under natural assumptions on the distribution of particles we show that the Green's function decays exponentially over distances larger than the screening length. This result is fundamental for example when deriving effective equations for coarsening systems in unbounded domains.

1 Introduction

In numerous applications, such as heat diffusion in a material with many inclusions, sedimentation [6] or electric fields in the presence of screens [15], one has to solve the Laplace equation with Dirichlet boundary conditions on many small holes (particles). It is by now a classical result that for regularly distributed particles the effective operator in the continuum limit is $-\Delta + \frac{1}{\xi^2} Id$, where $\frac{1}{\xi^2}$ is the capacity density of the particles (cf. e.g. [16, 3, 14, 4] and the references therein). In the present paper we show that already on the discrete level the corresponding Green's function decreases exponentially over distances larger than ξ. This is done under natural assumptions on the distribution of particles, which are satisfied in particular by randomly distributed particles.

This result is crucial in order to rigorously derive in arbitrarily large domains effective equations for particle systems which undergo coarsening by diffusional mass exchange. We briefly sketch the application of our result to this problem in Section 2 before we present the proof in Section 3. We concentrate in the present paper mainly on the three dimensional case. The two-dimensional case, which is also of importance to applications, can be treated analogously (cf. Section 3.4).

2 Mean-field models for coarsening

We consider the last stage of a first order phase transformation where particles of a new phase interact by diffusional mass exchange to reduce their total interfacial energy. In the case when the volume fraction of the particles is small they quickly become radially symmetric and do essentially not drift in space. Subsequently,

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to reduce the surface energy, large particles grow, smaller particles shrink and disappear, a scenario known as Ostwald Ripening.

In order to predict the statistics of a large system one is interested in deriving reduced models for this process. A suitable starting point for such a derivation is a modified version of the Mullins-Sekerka model (see [1, 17] for a justification). Within this model the particles are given by balls $B_i = B(x_i, R_i(t))$, with small total volume fraction $\varepsilon \ll 1$, and number density N_ε. The evolution of the particle radii is given by

$$\dot{R}_i = \frac{1}{|\partial B_i(t)|} \int_{\partial B_i(t)} \frac{\partial u}{\partial n} \quad \text{as long as } R_i > 0, \tag{2.1}$$

where for some domain $\Omega \subset \mathbb{R}^3$,

$$\Delta u = 0 \text{ in } \Omega \setminus \bigcup_i B_i(t), \tag{2.2}$$

$$u = \frac{1}{R_i} \text{ on } \partial B_i(t), \tag{2.3}$$

with periodic or Neumann boundary conditions on $\partial\Omega$. Here, u is a diffusion potential, assumed to be in local equilibrium given the distribution of phases. Equation (2.3) is the well-known Gibbs-Thomson law of local equilibrium, which accounts for surface tension. This evolution preserves the total volume fraction of particles and reduces their total surface area.

The characteristic length scales in this problem are the typical radius $r_\varepsilon = (\varepsilon N_\varepsilon)^{1/3}$ and the typical distance between particles $N_\varepsilon^{-1/3}$. However, as has been observed long ago, there is a crucial intrinsic length scale, the so-called screening length $\xi_\varepsilon = \frac{1}{\sqrt{r_\varepsilon N_\varepsilon}}$, which is the characteristic length over which particles interact. This will become apparent in the following asymptotic analysis of (2.1)-(2.3) for small ε. For the solution u of (2.2), (2.3) we choose the following ansatz:

$$u\,(x,t) = \sum_j \frac{\left(1 - \frac{R_j(t)\bar{u}(x_j,t)}{r_\varepsilon}\right)}{|x - x_j|} \tag{2.4}$$

where we assume that $\bar{u}(x,t)$ is a smoothly varying function in the macroscopic variable x and r_ε is a characteristic radius.

The ansatz (2.4) is motivated by an electrostatic analogy. First, the terms $\frac{1}{|x-x_j|}$ are the potentials created by the single particles. On the other hand, in each particle there is an additional contribution $\frac{R_j\bar{u}(x_j,t)}{r_\varepsilon}$ which takes the effect of particles different from x_j into account. Here, R_j is the capacity of the particles, $\bar{u}/r_\varepsilon$ is a normalized mesoscopic potential, and thus $\frac{R_j\bar{u}(x_j,t)}{r_\varepsilon}$ is roughly the charge induced by particle j on particle i. Due to the large number of particles we expect that the mesoscopic potential $\bar{u}$ varies slowly, that is on length scales which are much larger than the typical distance between neighboring particles.

Combining (2.4) with the boundary condition (2.3) we easily obtain to leading order:

$$\frac{1}{R_i} = \frac{\left(1 - \frac{R_i \bar{u}(x_i,t)}{r_\varepsilon}\right)}{R_i} + \sum_{j \neq i} \frac{\left(1 - \frac{R_j \bar{u}(x_j,t)}{r_\varepsilon}\right)}{|x_i - x_j|}$$

or equivalently:

$$0 = -\bar{u}\left(x_i, t\right) + r_\varepsilon \sum_{j \neq i} \frac{\left(1 - \frac{R_j \bar{u}(x_j,t)}{r_\varepsilon}\right)}{|x_i - x_j|}.$$

It is convenient to rescale the radii with the typical radius r_ε. Namely, we define $\hat{R}_j = \frac{R_j}{r_\varepsilon}$. Using the fact that $\xi_\varepsilon = \frac{1}{\sqrt{r_\varepsilon N_\varepsilon}}$ we obtain

$$0 = -\bar{u}\left(x_i, t\right) + \frac{1}{\left(\xi_\varepsilon\right)^2} \sum_{j \neq i} \frac{\left(1 - \hat{R}_j \bar{u}\left(x_j, t\right)\right)}{|x_i - x_j|} \cdot \frac{1}{N_\varepsilon} \tag{2.5}$$

The spatial volume for a particle is $\frac{1}{N_\varepsilon}$. Suppose that in the limit $\varepsilon \to 0$ the number of particles in the differential of volume $x + dx$ with radius in the interval $[r, r+dr]$ is given by $\nu(x,r)dxdr$. We can then formally approximate the sum in (2.5) by means of an integral

$$0 = -\bar{u}\left(x, t\right) + \frac{1}{\left(\xi_\varepsilon\right)^2} \int \frac{\left[\rho\left(y\right) - \mu\left(y\right) \bar{u}\left(y, t\right)\right]}{|x - y|} dy \tag{2.6}$$

where we have used the assumption that $\bar{u}\left(\cdot, t\right)$ is smooth and where $\rho\left(y\right) = \int_0^\infty \nu(y,r)dr$, $\mu\left(y\right) = \int_0^\infty r\nu\left(y, r\right) dr$. Taking the Laplacian of (2.6) we obtain:

$$-\left(\xi_\varepsilon\right)^2 \Delta \bar{u} + 4\pi\mu\bar{u} = 4\pi\rho$$

This equation for the effective potential $\bar{u}$ shows that $\bar{u}$ varies over length scales of order ξ_ε. Since in the regime of small volume fraction ξ_ε is much larger than the typical distance between particles, this justifies a posteriori our assumption that $\bar{u}$ is slowly varying.

To derive the equation for the evolution of the radii we deduce from (2.4) and (2.1) that

$$\dot{R}_i = \frac{1}{|\partial B_i\left(t\right)|} \int_{\partial B_i(t)} \frac{\partial u}{\partial n} = -\frac{\left(1 - \hat{R}_i \bar{u}\left(x_i, t\right)\right)}{R_i^2}$$

or, using the natural time scale $\hat{t} = \frac{t}{r_\varepsilon^3}$,

$$\frac{d\hat{R}_i}{d\hat{t}} = -\frac{1}{\hat{R}_i^{\,2}} + \frac{\bar{u}\left(x_i, t\right)}{\hat{R}_i}. \tag{2.7}$$

In terms of the distribution of radii $\nu_t(r,x)$, equation (2.7) is equivalent to

$$\partial_t \nu_t + \partial_r \Big(\big(\frac{\bar{u}(t,x)}{r} - \frac{1}{r^2}\big)\nu_t \Big) = 0, \tag{2.8}$$

where $\bar{u}(t,x)$, after rescaling space with respect to ξ_ε, is given for each time t by

$$-\Delta \bar{u} + 4\pi\mu\bar{u} = 4\pi\rho \tag{2.9}$$

The model (2.8), (2.9) is an inhomogeneous extension of the classical model for Ostwald ripening, first considered by Lifshitz and Slyozov [7] and by Wagner [18]. The inhomogeneous extension has first been rigorously derived in [8] in the case that the system size is of the order of the screening length and for a regular distribution of particles. In [11, 12], these results are extended to the more realistic case, that the screening length is much smaller than the system size and that the particles are randomly distributed. A main technical difficulty is that the underlying domains become unbounded after rescaling with respect to the screening length. Thus we cannot use the techniques used in [8], but need mathematical tools which enable us to localize the analysis. To that aim the result of the present paper is crucial. It gives that the Green's function of the Laplace operator in domains with holes decreases exponentially over distances larger than the screening length. This allows to make the approach sketched above rigorous, since, roughly speaking, it avoids diverging sums in the above ansatz.

We refer to [11, 12] and the references therein for more details and also for a discussion on further issues in the analysis of models for Ostwald Ripening.

3 The screening property

3.1 Assumptions on the distribution of particles

We first go over to suitably rescaled variables. As we have seen in the previous section, the relevant length scale is the screening length ξ_ε, which describes the scale over which particles interact. Hence we introduce the following rescaled variables:

$$\hat{x} = \frac{x}{\xi_\varepsilon}, \quad \hat{r_\varepsilon} = \frac{r_\varepsilon}{\xi_\varepsilon}, \quad \hat{R}_i = \frac{R_i}{r_\varepsilon}, \quad \hat{N}_\varepsilon = N_\varepsilon \xi_\varepsilon^3 \approx \varepsilon^{-1/2}. \tag{3.1}$$

In the following we will always work with these rescaled variables and thus we drop the hats for convenience. We also denote by $B_i := B_{r_\varepsilon R_i}(x_i)$. In addition we notice for later reference that in these rescaled variables we have $r_\varepsilon = N_\varepsilon^{-1}$.

We will assume that there exist two sequences d_ε and l_ε which satisfy

$$r_\varepsilon \ll d_\varepsilon \leq N_\varepsilon^{-1/3} \ll l_\varepsilon \ll 1 \qquad \text{as } \varepsilon \to 0, \tag{3.2}$$

with the following properties.

There exists a constant $C_0 > 0$ such that

(H1) The density of particles is bounded. That is, each cube Q of volume 1 can be decomposed into disjoint cubes of size l_ε that will be denoted as Q_ε such that

$$n(Q_\varepsilon) \leq C_0 l_\varepsilon^3 N_\varepsilon, \tag{3.3}$$

where $n(Q)$ denotes the number of particles in a cube Q.

(H2) Particles are well separated; more precisely

$$\min_{i\neq j} |x_i - x_j| \geq \frac{1}{C_0} d_\varepsilon$$

(H3) Particles are on average homogeneously distributed. That is, there exists $\delta_\varepsilon \to 0$ as $\varepsilon \to 0$ such that for each cube Q_ε we have

$$\max_{Q_\varepsilon} \max_{x_i \in Q_\varepsilon} \sum_{x_j \in Q_\varepsilon,\, j\neq i} \frac{1}{|x_i - x_j|} \frac{1}{N_\varepsilon} \leq \delta_\varepsilon. \tag{3.4}$$

(H4) The average capacity in regions of the size of the screening length (now rescaled to one) is bounded below. More precisely, we assume that for any cube Q with volume 1

$$\frac{1}{N_\varepsilon} \sum_{x_i \in Q} R_i \geq \frac{1}{C_0} \tag{3.5}$$

(H5) All particles are of the same order of size. We assume

$$\max_i R_i \leq C_0. \tag{3.6}$$

Remark 3.1. Some of the above assumptions on the particles might seem on first glance a bit arbitrary. However, it is shown in [12] that they are basically satisfied with high probability for randomly distributed particles. Let us comment in more detail on each assumption.

(H1) By this assumption we avoid regions with very high particle concentration. In principle, this uniform assumption could be replaced by an assumption of integral type. We prefer however not to do so to avoid technicalities which are not relevant for the scope of this article.

(H2) This assumption mainly enables us to consider different particles as independent ones, such that – combined with the other assumptions – the capacity of the particles is basically additive. For randomly distributed particles assumption (H2) fails for a small fraction of particles (cf. [12]). However, this is not relevant for the result in this paper, since additional particles only improve the screening property. It is only crucial that the subset of particles which satisfies (H2) still satisfies (H4), but this is true with high probability.

In the context of the full problem (2.1)-(2.3) the particles which overlap give rise to some technical difficulties. In fact, one has to show that only very few particles come close during the evolution and that they do not have a significant impact on the other particles. That this is the case is again a consequence of the screening property. For details we again refer to [12].

(H3) Assumption (H3) is perhaps the least intuitive. It basically states that particles in each cube Q_ε are far enough between themselves. We easily check that (H3) is satisfied for periodic arrays of particles. In this case

$$\sum_{x_j \in Q_\varepsilon,\, j \neq i} \frac{1}{|x_i - x_j|\, N_\varepsilon} \leq C \int_{Q_\varepsilon} \frac{dy}{|x-y|} \leq C\delta_\varepsilon^2.$$

Another way to formulate the meaning of (H3) is again by electrostatic analogy. (H3) ensures that the electrostatic fields produced by charges close to a given particle are small compared to the ones generated by particles within the screening length. In Section 3.3 we will give an example of a particle distribution which satisfies all assumptions but (H3) and for which the screening property does not hold.

(H4) This assumptions implies that there are enough particles to ensure the screening effect in distances of order one. Obviously, this property is essential and cannot be weakened.

(H5) This assumption avoids that too many large particles are present. It could probably be relaxed to allow for radii distributions with a tail which is decaying fast enough. Then, however, we would need a slightly stronger version of (3.4), since we typically encounter terms of the form $\sum_{x_j \in Q_\varepsilon} \frac{R_j}{|x_j - x_i| N_\varepsilon}$ which need to be small.

3.2 Exponential screening

This section is the heart of the paper, where we prove the screening property.

For the following we define

$$\mathcal{U}_\varepsilon := \mathbb{R}^3 \setminus \bigcup_i B_i.$$

We also introduce the capacity density:

$$\mu_\varepsilon(x) = \frac{1}{N_\varepsilon l_\varepsilon^3} \sum_{x_i \in Q_\varepsilon} R_i, \quad x \in Q_\varepsilon, \tag{3.7}$$

and notice that assumptions (H1) and (H5) imply:

$$0 \leq \mu_\varepsilon \leq C_0^2, \tag{3.8}$$

whereas (H4) yields:

$$\int_Q \mu_\varepsilon(x)\, dx \geq \frac{1}{C_0} \tag{3.9}$$

Theorem 3.2. *Consider a distribution of particles satisfying (H1)-(H5). Let us denote as $G(x,y)$ the unique solution of the problem*

$$\begin{aligned} -\Delta G(\cdot, y) &= \delta(\cdot - y) \qquad && \text{in } \mathcal{U}_\varepsilon\ ,\ y \in \mathcal{U}_\varepsilon \\ G(x,y) &= 0\ , && x \in \partial B_i \end{aligned}$$

which satisfies for each y that $G(x,y) \to 0$ as $|x| \to \infty$. Then there exist positive constants ε_0 and γ such that, for any $\varepsilon \le \varepsilon_0$:

$$G(x,y) \le \frac{1}{4\pi} \frac{e^{-\gamma|x-y|}}{|x-y|}\ , \qquad x, y \in \mathcal{U}_\varepsilon. \tag{3.10}$$

The proof of Theorem 3.2 is a consequence of the following Lemma.

Lemma 3.3. *Suppose that Q is a cube of volume 1 in $\mathbb{R}^3$. Assume that the particles in Q satisfy (H1)-(H5). Let us consider a solution of the boundary value problem*

$$\begin{aligned} \Delta\varphi_\varepsilon &= 0 \qquad && \text{in } Q \cap \mathcal{U}_\varepsilon \\ \varphi_\varepsilon &= 1 && \text{on } \partial Q \cap \overline{Q \cap \mathcal{U}_\varepsilon}, \\ \varphi_\varepsilon &= 0 && \text{on } \partial B_i \cap Q,\ \ \text{if } \overline{B_i} \subset Q. \end{aligned}$$

Then, there exists $\nu_0 > 0$ and $\varepsilon_0 > 0$ such that for $0 < \varepsilon \le \varepsilon_0$:

$$\varphi_\varepsilon(x_0) \le 1 - \nu_0$$

where x_0 is the center of Q.

Proof. We assume in the following that the functions φ_ε, as well as other functions which satisfy a constant Dirichlet condition on ∂B_i, are extended by the respective constant in the particles.

For the proof we argue by contradiction. Suppose that there are sequences of particles $\{(x_{i,\varepsilon}, R_{i,\varepsilon})\}$ satisfying (H1)-(H5) and

$$\limsup_{\varepsilon \to 0} \varphi_\varepsilon(x_0) = 1 \tag{3.11}$$

We claim that under the assumptions of Lemma 3.3 there exist subsequences such that (with μ_ε as in (3.7)):

$$\mu_\varepsilon \rightharpoonup \mu \ \text{ in } L^2(Q), \tag{3.12}$$

$$\varphi_\varepsilon \rightharpoonup \varphi \ \text{ in } H^1(Q), \tag{3.13}$$

where φ is a weak solution of

$$-\Delta\varphi + 4\pi\mu\varphi = 0 \ \text{ in } Q, \tag{3.14}$$

$$\varphi = 1 \ \text{ on } \partial Q \tag{3.15}$$

Assume for the moment that (3.12)-(3.15) hold true and let us continue. By (3.8) and (3.9) it holds $0 \le \mu \le C_0^2$ and $\int_Q \mu\, dy \ge 1/C_0$. Then it follows that $\mu \ge \frac{1}{2C_0} > 0$ in a set of positive measure, whence by the maximum principle we obtain $\varphi(x_0) < 1$. Furthermore, by the maximum principle we can assume that there are no particles in $\frac{1}{4}Q$. Then the functions φ_ε are harmonic in $\frac{1}{4}Q$. Using classical regularity theory for elliptic equations as well as (3.13) we obtain

$\varphi_\varepsilon \to \varphi$ uniformly in $\frac{1}{8}Q$. Then $\lim_{\varepsilon\to 0}\varphi_\varepsilon(x_0) = \varphi(x_0) < 1$ in contradiction with (3.11), whence the proof of Lemma 3.3 follows.

Therefore, in order to conclude, it only remains to show (3.12)-(3.15). The proof is well-known for regular distributions of particles (see e.g. [3] for a periodic array). However, for less regular distributions as considered in this paper, only abstract results exist.

Before we start the proof we notice that we can assume without loss of generality that

$$\text{all particles are at a distance larger than } d_\varepsilon/2 \text{ from } \partial Q_\varepsilon. \tag{3.16}$$

Otherwise we define a new family of domains $\hat{Q}_\varepsilon$ by

$$\begin{aligned} \hat{Q}_\varepsilon^* &= \Big(Q_\varepsilon \cup \bigcup_{\{x_i\in Q_\varepsilon\}} B_{\frac{1}{2}d_\varepsilon}(x_i)\Big)\,, \\ \hat{Q}_\varepsilon &= \hat{Q}_\varepsilon^* \setminus \Big(\bigcup_{\hat{Q}_{\varepsilon'}\neq\hat{Q}_\varepsilon} \hat{Q}_{\varepsilon'}\Big) \end{aligned}$$

That is, we enlarge the cubes Q_ε adding balls of radii $\frac{1}{2}d_\varepsilon$ centered at the particles that are close enough to the boundaries of the cubes Q_ε and then subtract the portions that belong to other domains obtained in the same manner. Taking into account assumption (H2) it follows that the domains $\hat{Q}_\varepsilon$ cover completely the original cube Q and the intersection of two different domains $\hat{Q}_\varepsilon$ is empty. The we could work with $\hat{Q}_\varepsilon$ instead of Q_ε in the following.

Thus, let us assume that (3.16) holds. We proceed – similarly as in [3] – by testing the equation for φ_ε with a suitable test function which in the present case is just the capacity potential in the cubes Q_ε. More precisely, we define a family of continuous functions w_ε piecewise in Q_ε by

$$-\Delta w_\varepsilon = 0 \text{ in } Q_\varepsilon \setminus \bigcup_i B_i \tag{3.17}$$

$$w_\varepsilon = 1 \text{ on } \partial B_i \tag{3.18}$$

$$w_\varepsilon = 0 \text{ on } \partial Q_\varepsilon. \tag{3.19}$$

We first prove

$$\Big|\int_{Q_\varepsilon} |\nabla w_\varepsilon|^2 dx - \frac{4\pi}{N_\varepsilon}\sum_{x_i\in Q_\varepsilon} R_i\Big| \le C\Big(\delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon}\Big)\int_{Q_\varepsilon} |\nabla w_\varepsilon|^2 dx\,. \tag{3.20}$$

To this end, we integrate by parts and use (3.17)-(3.19) to find

$$\begin{aligned}
\int_{Q_\varepsilon} |\nabla w_\varepsilon|^2 dx &= - \sum_{x_i \in Q_\varepsilon} \int_{\partial B_i} \frac{\partial w_\varepsilon}{\partial n}\, dS \\
&= - \sum_{x_i \in Q_\varepsilon} \int_{\partial B_i} \frac{\partial w_\varepsilon}{\partial n} \frac{R_i}{N_\varepsilon |x - x_i|}\, dS \\
&= - \sum_{x_i \in Q_\varepsilon} \int_{Q_\varepsilon} \nabla w_\varepsilon \cdot \nabla \Big(\frac{R_i}{N_\varepsilon |x - x_i|} \Big)\, dx \\
&\quad + \sum_{x_i \in Q_\varepsilon} \sum_{j \neq i} \int_{\partial B_j} \frac{\partial w_\varepsilon}{\partial n} \frac{R_j}{N_\varepsilon |x - x_i|}\, dS \\
&\quad - \int_{\partial Q_\varepsilon} \frac{\partial w_\varepsilon}{\partial n} \sum_{x_i \in Q_\varepsilon} \frac{R_i}{N_\varepsilon |x - x_i|}\, dS.
\end{aligned}$$

Since

$$\begin{aligned}
\sum_{x_i \in Q_\varepsilon} \int_{Q_\varepsilon} \nabla w_\varepsilon \cdot \nabla \Big(\frac{R_i}{N_\varepsilon |x - x_i|} \Big) dx &= - \sum_{x_i \in Q_\varepsilon} \int_{\partial B_i} \frac{\partial}{\partial n} \left(\frac{R_i}{N_\varepsilon |x - x_i|} \right) dS \\
&= \frac{4\pi}{N_\varepsilon} \sum_{x_i \in Q_\varepsilon} R_i
\end{aligned}$$

we find

$$\begin{aligned}
\Big| \int_{Q_\varepsilon} |\nabla w_\varepsilon|^2 dx - \frac{4\pi}{N_\varepsilon} \sum_{x_i \in Q_\varepsilon} R_i \Big| = \Big| &\sum_{X_i \in Q_\varepsilon} \sum_{j \neq i} \int_{\partial B_j} \frac{\partial w_\varepsilon}{\partial n} \frac{R_j}{N_\varepsilon |x - x_i|}\, dS \\
&- \int_{\partial Q_\varepsilon} \frac{\partial w_\varepsilon}{\partial n} \sum_{x_i \in Q_\varepsilon} \frac{R_i}{N_\varepsilon |x - x_i|}\, dS \Big|.
\end{aligned} \tag{3.21}$$

For $x \in \partial Q_\varepsilon$ let x_j be such that $|x - x_j| = \min_i |x - x_i|$. Then $|x - x_i| \geq \frac{1}{2}|x_j - x_i|$ for all $i \neq j$ and we find with (3.16), recalling $N_\varepsilon = 1/r_\varepsilon$,

$$\frac{1}{N_\varepsilon} \sum_{x_i \in Q_\varepsilon} \frac{1}{|x - x_i|} \leq \frac{2}{N_\varepsilon d_\varepsilon} + \frac{2}{N_\varepsilon} \sum_{\substack{x_i \in Q_\varepsilon \\ i \neq j}} \frac{1}{|x_i - x_j|} \leq 2 \Big(\frac{r_\varepsilon}{d_\varepsilon} + \delta_\varepsilon \Big). \tag{3.22}$$

Consequently, since $-\frac{\partial w_\varepsilon}{\partial n} \geq 0$, we find

$$\begin{aligned}
\sum_{x_i \in Q_\varepsilon} \int_{\partial Q_\varepsilon} \Big(- \frac{\partial w_\varepsilon}{\partial n} \Big) \frac{R_i}{N_\varepsilon |x - x_i|}\, dS &\leq C \Big(\delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon} \Big) \int_{\partial Q_\varepsilon} \Big(- \frac{\partial w_\varepsilon}{\partial n} \Big) dS \\
&= C \Big(\delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon} \Big) \int_{Q_\varepsilon} |\nabla w_\varepsilon|^2\, dS.
\end{aligned} \tag{3.23}$$

On the other hand, using again (H3) and (H5) it follows that

$$\begin{aligned}\sum_{x_i\in Q_\varepsilon}\sum_{j\neq i}\int_{\partial B_j}\frac{\partial w_\varepsilon}{\partial n}\frac{R_j}{N_\varepsilon|x-x_j|}\,dS &\le C\delta_\varepsilon\sum_{x_j\in Q_\varepsilon}\int_{\partial B_j}\Big(-\frac{\partial w_\varepsilon}{\partial n}\Big)\,dS\\ &= C\delta_\varepsilon\int_{Q_\varepsilon}|\nabla w_\varepsilon|^2\,dS.\end{aligned}\tag{3.24}$$

Thus using (3.22)-(3.24) in (3.21) we obtain (3.20). Combining (3.20), (H1) and (H5) we find

$$\int_Q|\nabla w_\varepsilon|^2dx\le\frac{C}{N_\varepsilon}\sum_{x_i\in Q}R_i\le C\tag{3.25}$$

Finally, using Poincare's inequality in each domain Q_ε and adding the different contributions, we easily obtain the bound

$$\int_Q|w_\varepsilon|^2dx\le Cl_\varepsilon^2\int_Q|\nabla w_\varepsilon|^2\,dx\to 0\tag{3.26}$$

as $\varepsilon\to 0$. By comparison, estimate (3.25) also implies for φ_ε that

$$\int_Q|\nabla\varphi_\varepsilon|^2\;dx\le\int_Q|\nabla\left(1-w_\varepsilon\right)|^2\;dx\le C\tag{3.27}$$

On the other hand by the maximum principle $0\le\varphi_\varepsilon\le 1$. A standard compactness argument shows that, for suitable subsequences (3.12), (3.13) hold, where φ satisfies (3.15). It only remains to check that (3.14) is satisfied. To this end we multiply the equation for φ_ε by the test function $\eta\left(1-w_\varepsilon\right)$ where $\eta\in C_0^\infty\left(Q\right)$. Then

$$\int_Q\left(1-w_\varepsilon\right)\nabla\varphi_\varepsilon\cdot\nabla\eta\,dx-\int_Q\nabla\varphi_\varepsilon\cdot\nabla w_\varepsilon\eta\,dx=0\tag{3.28}$$

Using (3.13) and (3.26) we easily obtain:

$$\int_Q\left(1-w_\varepsilon\right)\nabla\varphi_\varepsilon\cdot\nabla\eta\,dx\to\int_Q\nabla\varphi\cdot\nabla\eta\,dx\ \text{ as }\varepsilon\to 0.\tag{3.29}$$

The second term in (3.28) equals after an integration by parts

$$\int_Q\varphi_\varepsilon\nabla w_\varepsilon\cdot\nabla\eta\,dx\;-\sum_{Q_\varepsilon}\int_{\partial Q_\varepsilon}\varphi_\varepsilon\eta\frac{\partial w_\varepsilon}{\partial n}\,dS.\tag{3.30}$$

Due to (3.13), (3.26) the first term in (3.30) vanishes as $\varepsilon\to 0$. For the following we denote by $\overline{\varphi_\varepsilon\eta}$ the average of $\varphi_\varepsilon\eta$ over ∂Q_ε. We find

$$\begin{aligned}&-\sum_{Q_\varepsilon}\int_{\partial Q_\varepsilon}\varphi_\varepsilon\eta\,\frac{\partial w_\varepsilon}{\partial n}\,dS\\ &\qquad=\sum_{Q_\varepsilon}\overline{\varphi_\varepsilon\eta}\int_{\partial Q_\varepsilon}\Big(-\frac{\partial w_\varepsilon}{\partial n}\Big)\;+\sum_{Q_\varepsilon}\int_{\partial Q_\varepsilon}(\varphi_\varepsilon\eta-\overline{\varphi_\varepsilon\eta})\Big(-\frac{\partial w_\varepsilon}{\partial n}\Big)\,dS.\end{aligned}\tag{3.31}$$

Now we use (3.7), (3.12), (3.13) and (3.20) to obtain

$$\begin{aligned}\sum_{Q_\varepsilon} \overline{\varphi_\varepsilon \eta} \int_{\partial Q_\varepsilon} -\frac{\partial w_\varepsilon}{\partial n}\, dS &= 4\pi \int_Q \varphi_\varepsilon \eta \mu_\varepsilon \, dx + o(1) \\ &\to 4\pi \int_Q \varphi \eta \mu \, dx \qquad \text{as } \varepsilon \to 0.\end{aligned} \tag{3.32}$$

Furthermore (3.20), (H1) and (H5) imply that

$$\int_{\partial Q_\varepsilon} -\frac{\partial w_\varepsilon}{\partial n}\, dS = \int_{Q_\varepsilon} |\nabla w_\varepsilon|^2 \, dx \le C|Q_\varepsilon| \tag{3.33}$$

Using then (3.33) as well as the boundedness of μ_ε it follows that:

$$\Big| \int_{\partial Q_\varepsilon} (\varphi_\varepsilon \eta - \overline{\varphi_\varepsilon \eta}) \cdot \Big(-\frac{\partial w_\varepsilon}{\partial n} \Big)\, dS \Big| \le C \|\varphi_\varepsilon \eta - \overline{\varphi_\varepsilon \eta}\|_{L^\infty(\partial Q_\varepsilon)} |Q_\varepsilon| \tag{3.34}$$

It only remains to estimate the oscillation of $\varphi_\varepsilon \eta$ on each ∂Q_ε. Due to the presence of the cutoff η it is enough to restrict our attention to cubes Q_ε in the interior of Q. Given Q_ε we can take a cube with size L times larger and concentric with it and denote it by $\tilde{Q}_\varepsilon$. We can assume that $\tilde{Q}_\varepsilon \subset Q$ due to the cutoff η. By the maximum principle $0 \le \varphi_\varepsilon \le 1$, in particular also on $\partial \tilde{Q}_\varepsilon$. We construct a harmonic function ψ in $\tilde{Q}_\varepsilon$ which has as boundary data the same values as $\varphi_\varepsilon \eta$. Furthermore let ζ be a harmonic function in $\tilde{Q}_\varepsilon \backslash \cup_i B_i$ taking the value 1 at the boundaries of all the holes in $\tilde{Q}_\varepsilon$. Using the maximum principle we immediately obtain the inequalities: $\psi - \zeta \le \varphi_\varepsilon \eta \le \psi$. Assumption (H3) and (3.16) imply that $|\zeta| \le C(L^3 \delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon})$ on ∂Q_ε. In particular, due to (3.2), this contribution approaches zero as $\varepsilon \to 0$. Then, if we denote as osc_Ω the difference between the maximum and the minimum of a function in a given set Ω, we easily obtain: $\mathrm{osc}_{\partial Q_\varepsilon} \varphi_\varepsilon \eta \le \mathrm{osc}_{\partial Q_\varepsilon} \psi + C(L^3 \delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon})$. The Classical Harnack inequality for Laplace equation implies $\mathrm{osc}_{\partial Q_\varepsilon} \varphi_\varepsilon \eta \le \frac{C}{L} + C(L^3 \delta_\varepsilon + \frac{r_\varepsilon}{d_\varepsilon})$. Taking then the limits $\varepsilon \to 0$, $L \to \infty$, we easily obtain that $\lim_{\varepsilon \to 0} \mathrm{osc}_{\partial Q_\varepsilon} \eta \varphi_\varepsilon = 0$. Therefore (3.28)-(3.34) imply

$$\Big| \int_{\partial Q_\varepsilon} (\varphi_\varepsilon \eta - \overline{\varphi_\varepsilon \eta}) \cdot \frac{\partial w_\varepsilon}{\partial n}\, dS \Big| \ll |Q_\varepsilon|$$

as $\varepsilon \to 0$, and also:

$$\int_{Q_\varepsilon} \nabla \varphi_\varepsilon \cdot \nabla w_\varepsilon \, dx = -4\pi \int_{Q_\varepsilon} \mu_\varepsilon \varphi_\varepsilon \eta \, dx + o(|Q_\varepsilon|) \ \text{ as } \ \varepsilon \to 0.$$

Combining this expression with (3.12), (3.13), (3.28), (3.29) we finally obtain:

$$\int_Q \nabla \varphi \cdot \nabla \eta \, dx \; + \; 4\pi \int_Q \eta \mu \varphi \, dx = 0,$$

which proves (3.14) and thus concludes the proof of Lemma 3.3. $\square$

Using Lemma 3.3 we can easily prove Theorem 3.2.

Proof of Theorem 3.2. Comparison with the Green's function for the Laplace equation in $\mathbb{R}^3$ yields:

$$G(x,y) \leq \frac{1}{4\pi|x-y|} \tag{3.35}$$

In particular (3.35) implies $G(x,y) \leq \frac{1}{4\pi}$ for $|x-y| \geq 1$. Covering $B_{3/2} \backslash B_1(x)$ with suitable unit cubes and using Lemma 3.3 implies $G(x,y) \leq \frac{1}{4\pi}(1-\nu_0)$ for $|x-y| \geq \frac{5}{4}$. Iterating the argument we obtain:

$$G(x,y) \leq \frac{1}{4\pi}(1-\nu_0)^n \quad \text{for} \quad |x-y| \geq \left(1+\frac{n}{4}\right)$$

and this implies (3.10) with $\gamma \sim -\ln(1-\nu_0)$.□

Remark 3.4. It is not very difficult to adapt the ideas of the proof of Theorem 3.2 to obtain the corresponding result for the Green's function with periodic boundary condition in a (before rescaling) bounded domain. The only change occurs in the proof of the a priori estimate (3.35), where instead of the fundamental solution one needs to compare with the Green's function of the Laplace operator with periodic boundary conditions. However, the construction and estimate of such a periodic Green's function is rather standard. We neglect the details here.

Furthermore, one can easily obtain the corresponding result of Theorem 3.2 for the continuum limit; for details we refer to [10].

3.3 A counterexample

In order to further illustrate the importance of assumption (H3) we now construct particle configurations where (H3) fails and as a consequence the screening property is lost.

For that we introduce a new length $\hat{l}_\varepsilon$ such that $N_\varepsilon^{-1/3} \ll \hat{l}_\varepsilon \ll l_\varepsilon$. We recall that by assumption $\xi_\varepsilon = 1$. We place new cubes $\hat{Q}_\varepsilon$ of size $\hat{l}_\varepsilon$ at the centers of the cubes Q_ε and assume that all particles of Q_ε are in $\hat{Q}_\varepsilon$, and sit, say, on a periodic lattice. Then, the number of particles in $\hat{Q}_\varepsilon$ is $N_\varepsilon l_\varepsilon^3$ and the distance between particles is $d_\varepsilon = \frac{\hat{l}_\varepsilon}{l_\varepsilon N_\varepsilon^{1/3}}$. We choose the ansatz $d_\varepsilon = N_\varepsilon^{-1+\alpha}$ and $l_\varepsilon = N_\varepsilon^{-1/3+\beta}$ for some positive constants α, β. To ensure that $d_\varepsilon \ll N_\varepsilon^{-1/3}$ we need $\alpha < 2/3$ and to ensure that $l_\varepsilon \ll 1$ we need $\beta < 1/3$.

We are now going to argue that Lemma 3.3 does not hold if we choose $\alpha < 2\beta$. In fact, we can construct a subsolution $\underline{\varphi_\varepsilon}$ to the auxiliary potential φ_ε as defined in Lemma 3.3, which satisfies $\underline{\varphi_\varepsilon} \to 1$ as $\varepsilon \to 0$. The function $\underline{\varphi_\varepsilon}$ is just defined to be zero in $\bigcup \hat{Q}_\varepsilon$, to be one on ∂Q and harmonic in $Q \backslash \bigcup \hat{Q}_\varepsilon$. The capacity of each $\hat{Q}_\varepsilon$ in Q is of order $\hat{l}_\varepsilon$ such that the total capacity of $\bigcup \hat{Q}_\varepsilon$ in Q is estimated by $\hat{l}_\varepsilon l_\varepsilon^{-3} = N_\varepsilon^{1/3} d_\varepsilon l_\varepsilon^{-2} = N_\varepsilon^{\alpha-2\beta} \to 0$. Thus, arguing as in the proof of Lemma 3.3 we find $\underline{\varphi_\varepsilon} \to 1$ as $\varepsilon \to 0$ and the conclusion of Lemma 3.3 fails. With similar arguments we can also conclude that Theorem 3.2 fails to hold for the above particle configuration. We omit details here.

Let us now investigate, when (H3) for such a particle configuration holds. In fact, for $x_i \in Q_\varepsilon$ we find

$$\sum_{\substack{x_j \in Q_\varepsilon \\ j \neq i}} \frac{1}{|x_i - x_j| N_\varepsilon} \sim \frac{1}{N_\varepsilon d_\varepsilon^3} \int_{Q_\varepsilon} \frac{1}{|x-y|}\, dy \sim \frac{\hat{l}_\varepsilon^2}{N_\varepsilon d_\varepsilon^3} \sim N_\varepsilon^{4/3+2\beta-3\alpha}.$$

Hence, (H3) is satisfied if $2\beta - 3\alpha < -4/3$. But if $\alpha < 2\beta$, this would require $\alpha > 2/3$ which is not possible.

3.4 The case of two space dimensions

Our result can be easily extended to the case of two space dimension. This is often of interest in applications, for example if one studies the coarsening of thin droplets on a substrate, and has attracted also some mathematical interest [2, 9]. Typically, the two-dimensional case is considered to be technically slightly more difficult, due to the logarithmic divergence of the Green's function.

However, as we will point out now, our result transfers with no further difficulties to two dimensions. First, we recall (cf. e.g. [9]) that the screening length in two dimensions is given by $\xi_\varepsilon \sim \frac{1}{N_\varepsilon} \ln\left(\frac{1}{\sqrt{N_\varepsilon} r_\varepsilon}\right)$.

Then, after rescaling with respect to ξ_ε, the appropriate definition of μ_ε in (3.7) is $\mu_\varepsilon(x) = \frac{1}{N_\varepsilon l_\varepsilon^2} \sum_{x_i \in Q_\varepsilon} 1$ for $x \in Q_\varepsilon$, whereas (H1), (H3) and (H4) change to

(H1-2d)

$$n(Q_\varepsilon) \le C_0 l_\varepsilon^2 N_\varepsilon.$$

(H3-2d)

$$\max_{Q_\varepsilon} \max_{x_i \in Q_\varepsilon} \sum_{x_j \in Q_\varepsilon,\, j \neq i} \ln\left(\frac{1}{\sqrt{N}_\varepsilon |x - x_i|}\right) \frac{1}{N_\varepsilon} \le \delta_\varepsilon.$$

(H4-2d)

$$\frac{1}{N_\varepsilon} \sum_{x_i \in Q} 1 \ge \frac{1}{C_0}.$$

With these adapted assumptions the proofs of Lemma 3.3 and Theorem 3.2 transfer apart from obvious changes.

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References

[1] N. Alikakos and G. Fusco. Ostwald ripening for dilute systems under quasistationary dynamics. *Comm. Math. Phys.*, 238/3: 429-470, 2003.

[2] N. Alikakos, G. Fusco and G. Karali. Ostwald ripening in two dimensions. Preprint

[3] D. Cioranescu and F. Murat. A strange term coming from nowhere. *Topics in the Mathematical Modelling of Composite Materials.* A. Cherkaev and R. V. Kohn ed., Birkhäuser, 45-94, 1997.

[4] R. Figari, G. Papanicolaou and J. Rubinstein. The point interaction approximation for diffusion in regions with many small holes. *Stochastic methods in biology (Nagoya, 1985).* Lecture notes in Biomath., 70, Springer, Berlin: 75-86, 1987.

[5] E. Giusti, Minimal surfaces and functions of bounded variation, Birkhäuser, 1984.

[6] P.E. Jabin and F. Otto. Control on the distribution function of particles in a Stokes flow. *Comm. Math. Phys.*, to appear

[7] I. M. Lifshitz and V. V. Slyozov. The kinetics of precipitation from supersaturated solid solutions. *J. Phys. Chem. Solids*, 19:35–50, 1961.

[8] B. Niethammer and F. Otto. Ostwald Ripening: The screening length revisited. *Calc. Var. and PDE*, 13, 1:33-68, 2001.

[9] B. Niethammer and F. Otto. Domain coarsening in thin films *Comm. Pure Appl. Math.*, 54:361-384, 2001.

[10] B. Niethammer and J.J.L. Velázquez. Global well-posedness for an inhomogeneous LSW model in unbounded domains. Preprint.

[11] B. Niethammer and J.J.L. Velázquez. Homogenization in coarsening systems I: deterministic case. Preprint.

[12] B. Niethammer and J.J.L. Velázquez. Homogenization in coarsening systems II: stochastic case. Preprint.

[13] J. A. Marqusee and J. Ross. Theory of Ostwald ripening: Competitive growth and its dependence on volume fraction. *J. Chem. Phys.*, 80:536–543, 1984.

[14] S. Ozawa, On an elaboration of M. Kac's theorem concerning eigenvalues of the Laplacian in a region with randomly distributed small obstacles. *Comm. Math. Phys.*, 22 1/2:337-358, 1997.

[15] J. Rauch and M. Taylor, Electrostatic screening, *J. Math. Phys.*, 16:284-288, 1976.

[16] J. Rauch and M. Taylor, Potential and scattering theory on wildly perturbed domains. *J. Funct. Anal.* , 18: 27-59, 1975.

[17] J.J.L. Velázquez. On the effect of stochastic fluctuations in the dynamics of the Lifshitz–Slyozov–Wagner model. *J. Stat. Phys.*, 99:57-113, 2000.

[18] C. Wagner. Theorie der Alterung von Niederschlägen durch Umlösen. *Z. Elektrochemie*, 65:581–594, 1961.