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Ostwald ripening: The screening length revisited

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Abstract. We are interested in the coarsening of a spatial distribution of two phases, driven by the reduction of interfacial energy and limited by diffusion, as described by the Mullins–Sekerka model. We address the regime where one phase covers only a small fraction of the total volume and consists of many disconnected components ("particles"). In this situation, the energetically more advantageous large particles grow at the expense of the small ones, a phenomenon called Ostwald ripening. Lifshitz, Slyozov and Wagner formally derived an evolution for the distribution of particle radii. We extend their derivation by taking into account that only particles within a certain distance, the screening length, communicate. Our arguments are rigorous and are based on a homogenization within a gradient flow structure.

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1 Introduction

1.1 The Cahn–Hilliard model

Ostwald ripening may for instance occur in phase segregation of a two–component mixture, as described by the Cahn–Hilliard model. The Cahn–Hilliard model describes the state of the system at a time t by the spatially dependent relative concentration $c = c(t, x)$ of, say, the first component. We are interested in the case where the initial c is spatially uniform with value c_0 and unstable. The latter means that the free energy E favors two phases, each of a characteristic value for c (the two equilibrium concentrations $c_-^* < c_0 < c_+^*$), separated by an interfacial layer of characteristic width and of minimal area. The dynamics reduce the free energy E while preserving the spatial average of the relative concentration c. More precisely, the dynamics are driven by the negative gradient $-\nabla u$ of the chemical potential u (which mathematically speaking is the functional derivative of E with respect to c) and limited by the diffusion of each component.

Numerical simulations show that the system evolves as follows: After an initial stage, two phases form. In each of the two phases, c reaches its respective equilibrium value; the phases are separated by an interfacial layer of the characteristic thickness, which is much smaller than the typical lengthscale of the phase distribution. Subsequently, the system reduces E by reducing the area of the interfacial layer. This is reflected in an increase of the typical lengthscale of the phase distribution, which is called coarsening. Numerical simulations and heuristic arguments show that this lengthscale increases with time t like $t^{1/3}$.

1.2 The Mullins–Sekerka model

Coarsening in the Cahn–Hilliard model is well–described by the Mullins–Sekerka model [14, 1]. The Mullins–Sekerka model is a sharp–interface model: It describes the position of the interfacial layer by the boundary ∂G of a region $G \subset \mathbb{R}^3$ (the region where $c \approx c_+^*$). It is based on the assumption that the diffusion field, which is given by the negative gradient $-\nabla u$ of the chemical potential, is in quasistationary equilibrium given the normal velocity v of the interface ∂G. In dimensionless variables this reads

$$\triangle u = 0 \quad \text{in the bulk } \mathbb{R}^3 \backslash \partial G, \tag{1}$$

$$[\nabla u \cdot \vec{n}] = v \quad \text{at the interface } \partial G. \tag{2}$$

Here $\vec{n}$ denotes the normal to the interface, $[\nabla u \cdot \vec{n}]$ the jump of the normal component of the gradient $\nabla u \cdot \vec{n}$ across the interface. On the other hand, u is the functional derivative of E, which in the interfacial regime is proportional to the area of ∂G. As well–known, the first variation of the area of ∂G is given by its mean curvature κ. Hence in dimensionless variables, one obtains the so–called Gibbs–Thomson law:

$$u \;=\; \kappa \quad \text{at the interface } \partial G. \tag{3}$$

Since at a given time t, u is uniquely determined by ∂G via (1) &(3), (2),(1) & (3) indeed formally defines an evolution of G. This interfacial motion reduces the area of ∂G while preserving the volume of G.

1.3 Small volume fraction

We are interested in the regime where the volume fraction covered by G is very small. Numerical simulations of the Cahn–Hilliard model in this regime indicate that once the interfacial regime emerges, G consists of many disconnected components ("particles"), which quickly become approximately radially symmetric, and whose centers approximately do not move. Subsequently, the large particles grow at the expense of small particles, which eventually vanish. This particular form of coarsening is called Ostwald ripening. As the state of the system is described by the radii $\{R_i\}_i$ of the particles, it is tempting to try to identify the evolution law for $\{R_i\}_i$ from the Mullins–Sekerka model. By formal arguments, Lifshitz, Slyozov and Wagner [7,20] have done this and found that this evolution reduces to an evolution of the *distribution* ν of the $\{R_i\}_i$ — a tremendous reduction. We now have a closer look at the formal argument of LSW, in order to identify more clearly its crucial assumptions.

1.4 The LSW argument

We introduce the following notation:

- $\frac{1}{d^3}$ denotes particle number density, so that d is the typical particle distance,
- $\frac{4\pi}{3}\mathcal{R}^3$ denotes the average particle volume, so that $\mathcal{R}$ is the typical particle radius.

Small volume fraction means that

$$\mathcal{R} \ll d. \tag{4}$$

According to (1), the chemical potential u is a harmonic function outside the particles. Thanks to the separation of the particles expressed in (4), there exists a function $\bar{u}$ such that

- $\bar{u}$ is "slowly varying" in the sense that the length scale of variations of $\bar{u}$ is much larger than d,
- $\bar{u} \approx u$ "away from the particles" in the sense that the functions agree at distances from the particles which are much larger than $\mathcal{R}$.

This function $\bar{u}$ is called the mean field. Consider now u in the neighborhood of a fixed particle of center X_i and radius R_i. We have

$$u \left\{ \begin{array}{lll} \text{is harmonic} & \text{for } R_i \neq |x - X_i| \ll d & \text{according to (1),} \\ = \frac{1}{R_i} & \text{for } R_i = |x - X_i| & \text{according to (3),} \\ \approx \bar{u} & \text{for } R_i \ll |x - X_i| \ll d & \end{array} \right\}$$

Since $\bar{u}$ is approximately constant for $|x - X_i| \ll d$, this implies that

$$u \left\{ \begin{array}{ll} = \frac{1}{R_i} & \text{for } R_i \geq |x - X_i|, \\ \approx (1 - R_i\,\bar{u})\,\frac{1}{|x-X_i|} + \bar{u} & \text{for } R_i \leq |x - X_i| \ll d, \end{array} \right\}$$

and thus according to (2)

$$\dot{R}_i \;=\; [\nabla u \cdot \vec{n}] \;\approx\; \frac{1}{R_i^2}\,(R_i\,\bar{u} - 1). \tag{5}$$

In order to understand over which length scale the mean field $\bar{u}$ varies, we have to understand two lengths, the screening length and the correlation length.

1.5 The screening length

The screening length ξ_{scr} is defined as the maximal size of a box such that the average value of u, and hence $\bar{u}$, within the box is still dominated by the boundary values from the particles outside the box. We will argue that ξ_{scr} scales with the mean particle radius $\mathcal{R}$ and the average particle distance d as

$$\xi_{scr} \approx \left(\frac{d^3}{\mathcal{R}}\right)^{1/2}. \tag{6}$$

This has already been done e.g. in [6,8], but for the convenience of the reader we now present the heuristic argument in our language. We ask the following simplified question. Consider the solution U of

$$\begin{aligned} -\Delta U &= 0 && \text{outside the particles,} \\ U &= 1 && \text{inside the particles,} \\ U &= 0 && \text{on the boundary of the box } [0,\xi]^3. \end{aligned} \tag{7}$$

The boundary condition (7) mimicks the influence of the particles outside the box. Obviously, if ξ is small, U is dominated by (7), which for instance can be expressed as

$$\frac{1}{\xi^3}\int_{[0,\xi]^3} U^2 \ll 1. \tag{8}$$

For sufficiently large ξ, inequality (8) will become false. The cross-over value is the sought-after ξ_{scr}. By the Poincaré inequality on $[0,\xi]^3$, inequality (8) is a consequence of

$$\frac{1}{\xi}\int_{[0,\xi]^3} |\nabla U|^2 \ll 1.$$

Now $\int |\nabla U|^2$ is just the electrostatic capacity (see e.g. [5]) of the union of all particles within $[0,\xi]^3$. Since the particle diameter $\mathcal{R}$ is much smaller than the particle distance d (4), the capacity of a finite union of particles is approximately the sum of the capacity of the individual particles, which for radially symmetric particles is proportional to the radius and hence scales like $\mathcal{R}$. Within the box $[0,\xi]^3$ we have of the order of $\frac{\xi^3}{d^3}$ particles. This number might be so large that the above mentioned additivity fo the capacity breaks down, in which case the capacity of the conglomerate behaves like that of a single particle of diameter ξ. Hence

$$\frac{1}{\xi}\int_{[0,\xi]^3} |\nabla U|^2 = \frac{1}{\xi}\begin{cases} \frac{\xi^3}{d^3}\mathcal{R} & : \quad \text{for small } \xi \\ \xi & : \quad \text{for large } \xi \end{cases}$$
$$= \begin{cases} \frac{\xi^2}{d^3}\mathcal{R} & : \quad \text{for } \xi \ll \left(\frac{d^3}{\mathcal{R}}\right)^{1/2} \\ 1 & : \quad \text{for } \xi \gg \left(\frac{d^3}{\mathcal{R}}\right)^{1/2} \end{cases}$$

This is our argument in favor of (6).

1.6 The correlation length

A second length scale is important for the variations of $\bar{u}$: the correlation length ξ_{cor}. The correlation length is the minimal size of a box such that the distribution of the particle radii within this box is a good approximation to the distribution of all radii. As a very crude but convenient approximation to this subtle statistic motion, we think of ξ_{cor} as the size of a box with respect to which the particle arrangement is periodic. On one hand, u and hence $\bar{u}$ inherits this periodicity with period ξ_{cor}. On the other hand, u cannot vary significantly on length scales less than ξ_{scr} according to Subsect. 1.5. Hence the regime

$$\xi_{cor} \ll \xi_{scr}$$

is particularly simple:

$$\bar{u} \text{ is approximately constant in space.}$$

The value of $\bar{u}$ is determined by (5) and the a priori known conservation of the volume fraction, that is

$$\frac{d}{dt}\sum_i R_i^3 = 0,$$

where the sum $\sum_i$ extends over all particles within the periodic box $[0,\xi_{cor}]^3$ (For convenience of later notation, we include in this sum even those particles which may have already vanished, that is, $R_i = 0$). Indeed, one obtains

$$\bar{u} \;=\; \frac{\sum_{i:R_i\neq 0} 1}{\sum_i R_i} \;=\; \frac{1}{\text{average radius of non–vanished particles}}. \tag{9}$$

The closed system (5) and (9) is just the classical LSW-law.

The obvious but crucial observation is that (5) and (9) reduces to an evolution of the radii distribution $\nu(t,r)$, that is

$$\int_{r_1}^{r_2} \nu(t,r)\,dr \;=\; \left\{\begin{array}{l}\text{number of particles with radius in } (r_1,r_2)\\ \text{and center in the periodic box } [0,\xi_{cor}]^3.\end{array}\right\}$$

Indeed, the system of ordinary differential equations (5) translates into the kinetic equation

$$\partial_t\nu + \partial_r\left(\frac{1}{r^2}\,(r\,\bar{u}-1)\,\nu\right) \;=\; 0, \tag{10}$$

and (9) can be written as

$$\bar{u} \;=\; \frac{\int \nu\,dr}{\int r\,\nu\,dr}. \tag{11}$$

The derivation of (10) & (11) in the regime $\mathcal{R} \ll d$ and $\xi_{cor} \ll \xi_{scr}$ has been made rigorous by the first author [10].

1.7 The modification of LSW in our regime

Marder [6,8] argues that correlations are induced by screening effects so that it is relevant to understand the regime

$$\xi_{cor} \approx \xi_{scr},$$

which is the goal of this paper. As we will show, in this regime the evolution for $\{R_i\}_i$ reduces only to an evolution of the joint distribution of particle radii and particle center $\nu(t,x,r)$, that is

$$\int_\omega\int_{r_1}^{r_2} \nu(t,x,r)\,dr\,dx \;=\; \left\{\begin{array}{l}\text{number of particles with radius in } (r_1,r_2)\\ \text{and center in the set } \omega \text{ in } [0,\xi_{cor}]^3\end{array}\right\},$$

since (9) generalizes to

$$-\Delta\bar{u} \,+\, 4\pi\left(\bar{u}\int r\,\nu\,dr \,-\, \int \nu\,dr\right) \;=\; 0. \tag{12}$$

The kinetic equation

$$\partial_t \nu + \partial_r \left(\frac{1}{r^2} (r\,\bar{u} - 1)\,\nu \right) = 0 \tag{13}$$

now has x as a parameter. The rigorous derivation of the evolution (13) & (12) from the Mullins–Sekerka evolution (restricted to radially symmetric particles) is the content of this paper, the result is formulated in Theorem 3.1.

If all radii are identical, it would immediately follows from the classical homogenization result by Cioranescu and Murat [4] that u solving (1) & (3) converges to $\bar{u}$ solving (12). Their argument can be extended to treat the case of non–identical radii. But in order to obtain (12) with this limit, one roughly speaking would need to know the corrector in this convergence.

Our analysis takes a different venue: We use the fact that the Mullins–Sekerka evolution (and thus its homogenization) has the structure of a gradient flow in a physically natural way. The gradient flow perspective has been successful in analyzing diverse problems as e.g. the porous medium equation [12] or the lubrication approximation equation [13]. Here, it allows to exploit the Rayleigh principle, which characterizes a solution of a gradient flow as a minimum of a quadratic functional. Hence, the analysis reduces to identifying the Γ–limit of this variational problem. Roughly speaking, this amounts to homogenizing the Neumann problem (1) & (2) rather than the Dirichlet problem (1) & (3).

The outline of the paper is as follows. In Sect. 2, we introduce the Rayleigh principle for a gradient flow, argue that Mullins–Sekerka has the structure of a gradient flow, and use this structure to restrict the evolution to spherical particles (see [2,17] for a justification of this simplification). In Sect. 3, we introduce the precise assumptions, the appropriate scaling and state our main result. In Sect. 4, we establish several preliminary results on the convergence of the distribution functions. In Sect. 5, we identify the Γ-limit of the functional corresponding to Rayleigh's principle. In Sect. 6, we translate the limiting Rayleigh principle into (13) and (12).

1.8 Outlook

The second part of the classical LSW-theory predicts the long-time behavior of the radii distribution ν_t. More precisely, by a formal analysis of (5) & (9) LSW predict that ν_t, independently of the initial distribution, approaches a specific self–similar solution of (5) & (9). This allows them to conclude that the average radius $\frac{1}{\bar{u}(t)}$ grows like $(\frac{4}{9}t)^{1/3}$. In [11], Pego and the first author however show that the long time behavior is not universal. In fact, for particle distributions with compact support the asymptotics depend sensitively on the behavior of the initial distribution near the end of its support. Qualitatively similar results to [11] but with different methods are obtained in [3] for a simplified LSW model. In [16] a Fokker–Planck approximation of the LSW conservation law is studied.

Even though the self similar nature can often be observed in experiments, none of the profiles and rate constants possible for the LSW model can be validated. One reason for these deviations is certainly that in the LSW theory all particles of the same size evolve according to the same law and thus direct interactions between particles are entirely neglected. For an overview we refer the interested reader to the survey articles [6, 18, 19] and the references therein.

2 The structure and the microscopic problem

Our analysis will be guided by the gradient flow structure of the evolution. In this chapter, we start by introducing the general framework. Then we will show that the Mullins–Sekerka free boundary problem fits into this framework. We will use this structure to "restrict" Mullins–Sekerka to radially symmetric particles and finally we argue that also the limit evolution can be interpreted as a gradient flow.

2.1 The abstract gradient flow structure and the Rayleigh principle

A vector field f on a differentiable manifold $\mathcal{M}$ (a vector field attaches a tangent vector $f(x) \in T_x\mathcal{M}$ to every point $x \in \mathcal{M}$) defines the dynamical system $\dot{x} = f(x)$. A gradient flow is a dynamical system where f is the negative gradient $-\mathrm{grad}E$ of a function E on $\mathcal{M}$. The notion of a gradient requires a Riemannian structure, that is, a metric tensor g on $\mathcal{M}$ (a metric tensor endows the tangent space $T_x\mathcal{M}$ with the scalar or inner product g_x). Indeed, the differential of a function E on $\mathcal{M}$ attaches the linear form or cotangent vector $\mathrm{diff}E_x$ to each point $x \in \mathcal{M}$. Only the scalar product g_x converts the cotangent vector $\mathrm{diff}E_x$ into the tangent vector $\mathrm{grad}E_x$ via

$$g_x(\mathrm{grad}E_x, v) \;=\; \langle \mathrm{diff}E_x, v\rangle \quad \text{for all } v \in T_x\mathcal{M}.$$

Hence the extended version of $\dot{x} = -\mathrm{grad}E_x$ is

$$g_{x(t)}(\dot{x}(t), v) + \langle \mathrm{diff}E_{x(t)}, v\rangle = 0 \quad \text{for all } v \in T_{x(t)}\mathcal{M} \text{ and } t. \tag{14}$$

It is immediate from (14) that the value of E decreases along trajectories:

$$\frac{d}{dt}E(x(t)) \;=\; -g_{x(t)}(\dot{x}(t), \dot{x}(t)). \tag{15}$$

Indeed, the intuitive understanding of a gradient flow is that of a steepest descent in an energy landscape. The geometry of the base space $\mathcal{M}$ is given by g whereas the height is determined by E. The integrated version of (15), that is,

$$E(x(T)) + \int_0^T g_{x(t)}(\dot{x}(t), \dot{x}(t))\, dt \;=\; E(x(0)) \tag{16}$$

will be the starting point for all our a priori estimates. For our analysis, it will be important that (14) can be reformulated as a variational problem

$$\begin{aligned} &\text{For all t, } \dot{x}(t) \text{ is the minimizer of} \\ &\qquad \frac{1}{2}\, g_{x(t)}(v, v) + \langle \operatorname{diff} E_{x(t)}, v\rangle \\ &\text{among all } v \in T_{x(t)}\mathcal{M}, \end{aligned} \tag{17}$$

which is also referred to as Rayleigh principle in the applied literature. It will be convenient to have (17) in the more robust time integrated version

$$\begin{aligned} &\text{For all nonnegative functions } \beta \text{ of } t,\ \dot{x} \text{ minimizes} \\ &\qquad \int_0^\infty \beta(t) \left(\frac{1}{2}\, g_{x(t)}(v(t), v(t)) + \langle \operatorname{diff} E_{x(t)}, v(t)\rangle \right) dt \\ &\text{among all vector fields } v \text{ along the curve } x. \end{aligned} \tag{18}$$

Finally, we observe that a gradient flow — as opposed to a general dynamical system — can be naturally restricted to a lower dimensional submanifold $\mathcal{N} \subset \mathcal{M}$. Indeed, both ingredients E and g restrict canonically to $\mathcal{N}$. We will use this in Subsect. 2.3.

2.2 Mullins–Sekerka as a gradient flow

We now argue that the Mullins–Sekerka free boundary problem formally fits into the gradient flow framework: $\mathcal{M}$ has to be chosen as the manifold of all sets $G \subset \mathbb{R}^3$ (the distribution of one of the two phases), which are periodic with period ξ_{cor}, that is,

$$G + \xi_{cor}\, \mathbf{n} \;=\; G \quad \text{for all } \mathbf{n} \in \mathbb{Z}^3,$$

and have a fixed volume in this periodic box $(0, \xi_{cor})^3$, that is

$$\mathcal{L}^3(G \cap (0, \xi_{cor})^3) \;=\; const.$$

The tangent space $T_G\mathcal{M}$ in a $G \in \mathcal{M}$ is conveniently described by all kinematically admissible normal velocities of ∂G, that is,

$$T_G\mathcal{M} \;=\; \left\{ v\colon \partial G \to \mathbb{R} \mid v \text{ is } \xi_{cor}\text{–periodic}, \int_{\partial G \cap [0,\xi_{cor})^3} v\, d\mathcal{H}^2 \;=\; 0 \right\}.$$

The metric tensor has to be chosen as

$$g_G(v^1,v^2) \;=\; \int_{(0,\xi_{cor})^3} \nabla u^1 \cdot \nabla u^2 \, d\mathcal{L}^3, \tag{19}$$

where u^α in view of (1) & (2) solves the elliptic problem

$$\begin{aligned} -\Delta u^\alpha \;&=\; 0 \;\text{ in } \mathbb{R}^3\backslash\partial G, \\ [\nabla u^\alpha \cdot \vec{n}] &= v^\alpha \text{ on } \partial G. \end{aligned}$$

An integration by part yields the representation

$$g_G(v^1,v^2) \;=\; -\int_{\partial G\cap[0,\xi_{cor})^3} u^1\, v^2 \, d\mathcal{H}^2. \tag{20}$$

The functional E is just the total interfacial area (within a periodic box)

$$E(G) \;=\; \mathcal{H}^2(\partial G \cap [0,\xi_{cor})^3).$$

It is well–known that the first variation of surface area is the mean curvature

$$\langle \mathrm{diff} E_G, \tilde{v}\rangle \;=\; \int_{\partial G\cap[0,\xi_{cor})^3} \kappa\, \tilde{v}\, d\mathcal{H}^2$$

for all $\tilde{v} \in T_G\mathcal{M}$. Therefore we have according to (20)

$$g_G(v,\tilde{v}) + \langle \mathrm{diff} E_G, \tilde{v}\rangle \;=\; \int_{\partial G\cap[0,\xi_{cor})^3} (\kappa - u)\, \tilde{v}\, d\mathcal{H}^2$$

so that the Gibbs–Thomson law (3) (up to an irrelevant additive constant) is indeed equivalent to the gradient flow formulation (14). We observe that the metric tensor can also be written as

$$g_G(v^1,v^2) \;=\; \langle v^1\, d\mathcal{H}^2|\partial G, v^2\, d\mathcal{H}^2|\partial G\rangle_{H^{-1}}$$

where $\langle\cdot,\cdot\rangle_{H^{-1}}$ is the homogeneous part of the H^{-1}–scalar product on the space of periodic distributions with mean value zero, that is

$$\langle f^1, f^2\rangle_{H^{-1}} \;=\; \int_{(0,\xi_{cor})^3} \nabla u^1 \cdot \nabla u^2 \, d\mathcal{L}^3, \tag{21}$$

where u^α solves the elliptic problem

$$-\triangle u^\alpha \;=\; f^\alpha \quad \text{in } \mathbb{R}^3$$

and is periodic with period ξ_{cor}. Hence, loosely speaking, the Mullins–Sekerka free boundary problem is the gradient flow of the surface area w. r. t. H^{-1}, a fact well known to the experts.

2.3 The restriction of Mullins–Sekerka to radial particles

We now want to restrict this dynamical system to the submanifold $\mathcal{N} \subset \mathcal{M}$ of all sets G which are the union of disjoint balls

$$G \;=\; \cup_i B_{R_i}(X_i),$$

where the centers $\{X_i\}_i$ are given and the radii $\{R_i\}_i$ are variable. Hence $\mathcal{N}$ can be identified with an open subspace of the hypersurface $\{\mathbf{R} = \{R_i\}_i | \sum_i R_i^3 = const\}$ in $\mathbb{R}^N$, where N is the number and $i = 1, \cdots, N$ an enumeration of particles with centers in the periodic box $[0, \xi_{cor})$. Therefore, the tangent space can be identified with the hyperplane

$$T_R\mathcal{N} \;=\; \left\{ \mathbf{V} \;=\; \{V_i\}_i | \sum_i R_i^2 V_i \;=\; 0 \right\} \;\subset\; \mathbb{R}^N.$$

It is obvious that the restriction of the metric tensor is

$$g_{\mathbf{R}}(\mathbf{V}^1, \mathbf{V}^2) \;=\; \int_{(0,\xi_{cor})^3} \nabla u^1 \cdot \nabla u^2 \, d\mathcal{L}^3, \qquad (22)$$

where u^α solves

$$\begin{aligned} -\Delta u^\alpha \;&=\; 0 \;\; \text{in } \mathbb{R}^3 \setminus \cup_i \partial B_{R_i}(X_i), \\ [\nabla u^\alpha \cdot \vec{n}] &= V_i^\alpha \text{ on } \partial B_{R_i}(X_i). \end{aligned}$$

The restriction of the functional is simply

$$E(\mathbf{R}) \;=\; 2\pi \sum_i R_i^2 \qquad (23)$$

so that

$$\langle \mathrm{diff} E_R, \tilde{\mathbf{V}} \rangle \;=\; 4\pi \sum_i R_i \, \tilde{V}_i.$$

Hence the dynamical system we will investigate is the gradient flow of the functional (23) w. r. t. the metric tensor (22) on $\mathcal{N}$. Existence and uniqueness for the initial value problem of this dynamical system is not standard since the dynamical system is not smooth at the boundary of $\mathcal{N}$, that is, when one of the radii goes to zero (which occurs generically) and when two of the balls touch (which can be ruled out for the regime of small volume fraction, see (31)). Our topic is not the existence or uniqueness, but the asymptotic behavior for small volume fraction — hence we will always assume that a weak solution in the sense of (18) exists.

2.4 The gradient flow structure of the limit

Our analysis can be characterized as a homogenization of the above gradient flow structure. Let us point out here in which sense the homogenized limit (13), (12) is a gradient flow. $\mathcal{M}$ is the manifold of all distributions $\nu = \nu(x,r)$ such that

$$\int_{(0,\xi_{cor})^3} \int_0^\infty r^3 \nu \, dr \, dx = 1$$

and the tangent space is described by

$$T_\nu \mathcal{M} = \left\{ v = v(x,r) \; : \; \int_{(0,\xi_{cor})^3} \int_0^\infty r^2 \, v \, \nu \, dr \, dx = 0 \right\}.$$

The energy is

$$E(\nu) \;=\; 2\pi \int_{(0,\xi_{cor})^3} \int_0^\infty r^2 \, \nu \, dr \, dx$$

and the metric tensor turns out to be

$$g_\nu(v,v) = \int_{(0,\xi_{cor})^3} |\nabla u|^2 \, dx \;+\; 4\pi \int_{(0,\xi_{cor})^3} \int_0^\infty |v|^2 r^3 \, \nu \, dr \, dx \qquad (24)$$

where

$$-\Delta u \;+\; 4\pi \int r^2 \, v \, \nu \, dr = 0 \qquad \text{in } (0,\xi_{cor})^3.$$

Indeed, the main part of our analysis will be to show, that (24) is the limit functional of (19) in an appropriate homogenization setting (cf. chapter 5).

Finally, we remark that the classical LSW–model is a gradient flow in the above setting if one neglects the inhomogeneous term $\int |\nabla u|^2 \, dx$ in (24).

3 The scaling and the homogenization result

As explained in Subsect. 2.3, we consider a periodic arrangement of particles with period ξ_{cor}, described by the fixed particle centers $\mathbf{X} = \{X_i \in \mathbb{R}^3\}_{i=1,\cdots,N}$ and time–dependent radii $\mathbf{R} = \{R_i \in [0,\infty)\}_{i=1,\cdots,N}$, which evolve according to the gradient flow with metric tensor (22) and energy (23). Note that we allow R_i to be zero, accounting for particles which vanish over time.

3.1 Definition of d, $\mathcal{R}$ and ξ_{scr}

Following Subsect. 1.4, the number density $\frac{1}{d^3}$ of particles is defined by

$$d^3 \sum_i 1 = \xi_{cor}^3 \tag{25}$$

and the average volume $\frac{4\pi}{3}\mathcal{R}^3$ by

$$\sum_i R_i(t)^3 = \mathcal{R}^3 \sum_i 1. \tag{26}$$

As in Subsect. 1.6, the sum $\sum_i$ extends over all particles in a box of length ξ_{cor}, even those which may have already vanished. Observe that the evolution preserves the l. h. s. of (26), so that $\mathcal{R}$ is indeed well–defined. As motivated in Subsect. 1.5, we introduce the screening length

$$\xi_{scr} = \left(\frac{d^3}{\mathcal{R}}\right)^{1/2}.$$

Our aim is to identify the evolution in the limit of vanishing volume fraction of particles. More precisely, we consider a sequence of systems characterized by the parameter

$$\varepsilon := \frac{d}{\xi_{scr}} = \left(\frac{\mathcal{R}}{d}\right)^{1/2} \tag{27}$$

in the limit $\varepsilon \to 0$.

3.2 Three assumptions on the particle arrangement

We have to assume that particle centers are well separated in the sense that there exists a $\lambda > 0$ such that

$$\{B_{\lambda\, d}(X_i)\}_i \quad \text{are disjoint for all } \varepsilon > 0. \tag{28}$$

We have to require that *initially*, the particles much larger than $\mathcal{R}$ do not carry too much of the total mass, that is

$$d^3 \sum_{i:\frac{R_i(0)}{\mathcal{R}} \geq M} \left(\frac{R_i(0)}{\mathcal{R}}\right)^3 \to 0 \quad \text{as } M \to \infty \quad \text{uniformly in } \varepsilon \to 0. \tag{29}$$

We want to assume that the correlation length (see Subsect. 1.6) is of order of the screening length in the limit $\varepsilon \to 0$; for simplicity

$$\xi_{cor} = \xi_{scr}. \tag{30}$$

As a consequence of (30) and the definitions (25), (26) and (27), we have

$$\begin{aligned} R_i(t) \;&\le\; \Big(\sum_i R_i(t)^3\Big)^{1/3} \;\le\; \frac{\mathcal{R}\xi_{scr}}{d} \;\le\; (\mathcal{R}\, d)^{1/2} \\ &=\; \varepsilon\, d \quad \text{for all } i \text{ and } t\in[0,\infty). \end{aligned} \tag{31}$$

It now follows from (28) that for sufficiently small ε,

$$\{B_{R_i(t)}(X_i)\}_i \text{ are disjoint for all } t\in[0,\infty).$$

3.3 The joint distribution of centers and radii

It is canonical to measure

$$\begin{aligned} &\text{particle centers } x \text{ in units of } \xi_{scr}, \\ &\text{particle radii } r \text{ in units of } \mathcal{R}. \end{aligned} \tag{32}$$

The LSW argument (5) suggests to measure

$$\text{time } t \text{ in units of } \mathcal{R}^3. \tag{33}$$

Hence we define the joint distribution ν_t^ε of particle centers and radii at a given time t by

$$\int \zeta\, d\nu_t^\varepsilon \;=\; \left(\frac{d}{\xi_{scr}}\right)^3 \sum_i \zeta\left(\frac{X_i}{\xi_{scr}}, \frac{R_i(t/\mathcal{R}^3)}{\mathcal{R}}\right) \quad \text{for } \zeta\in C_p^0, \tag{34}$$

where C_p^0 stands for the space of continuous functions on $\zeta=\zeta(x,r)$ which

- are periodic in x w. r. t. the unit box $\Omega=(0,1)^3$,
- have compact support in $r\in(0,\infty)$.

Note that since $\zeta(x,r)=0$ for $r=0$, particles which have vanished do not enter the distribution. Hence the natural space for ν_t^ε and its limit ν_t is the space $(C_p^0)^*$ of Borel measures on $\Omega\times(0,\infty)$, that is, the product of the torus and the positive half axis. The natural space for potentials of diffusion fields is H_p^1, the space of functions $u=u(x)$ which

- are periodic in x w. r. t. the box Ω,
- are square integrable with square integrable gradient.

Furthermore we will denote by $\overset{\circ}{H}{}_p^1$ the subspace of H_p^1 of functions with mean value zero.

3.4 The result

Theorem 3.1. *There exist a subsequence, again denoted by* $\varepsilon \to 0$*, and a weakly continuous map* $[0,\infty) \ni t \mapsto \nu_t \in (C_p^0)^*$ *with*

$$\int \zeta \, d\nu_t^\varepsilon \ \to \int \zeta \, d\nu_t \quad \text{locally uniformly in } t \in [0,\infty) \quad \text{for all } \zeta \in C_p^0.$$

This limit is non trivial, indeed

$$\int r^3 \, d\nu_t \ = \ 1.$$

Furthermore, there exists a measurable map $(0,\infty) \ni t \mapsto \bar{u}(t) \in H_p^1$ *such that (13) and (12) hold in the following weak sense*

$$\frac{d}{dt} \int \zeta \, d\nu_t \ = \ \int \partial_r \zeta \, \frac{1}{r^2} \, (r\,\bar{u}(t) - 1) \, d\nu_t$$

$$\text{distributionally on } (0,\infty) \text{ for all } \zeta \in C_p^0 \text{ with } \partial_r \zeta \in C_p^0$$

resp.

$$\int_\Omega \nabla \bar{u}(t) \cdot \nabla \zeta \, dx \ + \ 4\pi \int \zeta \, \bar{u}(t) \, r \, d\nu_t \ = \ 4\pi \int \zeta \, d\nu_t$$

$$\text{for all } \zeta \in H_p^1 \quad \text{and a. e. } \ t \in (0,\infty).$$

4 Weak compactness

In this chapter we do everything which can be done by soft arguments.

4.1 Rescaling

For the ease of presentation, we will rescale the spatial variables by ξ_{scr} such that

$$\xi_{scr} \ = \ \xi_{cor} \ = \ 1 \quad \text{and hence} \quad d \ = \ \varepsilon, \ \mathcal{R} \ = \ \varepsilon^3.$$

We also rescale r and t as indicated in (32), resp. (33). In the rescaled variables the submanifold $\mathcal{N}$ from Sect. 2 is given by

$$\mathcal{N}^\varepsilon = \left\{ \mathbf{R}^\varepsilon = \{R_i\}_i \,|\, \varepsilon^3 \sum_i R_i^3 = 1 \right\}$$

and the tangent space by

$$T_{\mathbf{R}^\varepsilon}\mathcal{N}^\varepsilon = \left\{ \tilde{\mathbf{V}}^\varepsilon = \{\tilde{V}_i\}_i \mid \sum_i R_i^2 \tilde{V}_i = 0 \right\}.$$

In the following we will always denote $\mathbf{V}^\varepsilon = \{V_i\}_i$ with $V_i = \frac{d}{dt} R_i$, whereas $\tilde{\mathbf{V}}^\varepsilon$ will be an arbitrary element of the tangent space. Furthermore we use the abbreviation $B_i := B_{\varepsilon^3 R_i}(X_i)$. The metric tensor for $\tilde{\mathbf{V}}^\varepsilon \in T_{\mathbf{R}^\varepsilon}\mathcal{N}^\varepsilon$ is computed via

$$g_{\mathbf{R}^\varepsilon}\left(\tilde{\mathbf{V}}^\varepsilon, \tilde{\mathbf{V}}^\varepsilon\right) = \int_\Omega |\nabla \tilde{u}^\varepsilon|^2, \tag{35}$$

where $\tilde{u}^\varepsilon \in \overset{\circ}{H}{}^1_p$ solves

$$\int_\Omega \nabla \tilde{u}^\varepsilon \cdot \nabla \zeta \; + \sum_{i:R_i>0} \int_{\partial B_i} \frac{1}{\varepsilon^3} \tilde{V}_i \, \zeta = 0 \tag{36}$$

for all $\zeta \in \overset{\circ}{H}{}^1_p$. With the energy

$$E(\mathbf{R}^\varepsilon) := 2\pi\, \varepsilon^3 \sum_i R_i^2$$

the energy estimate (16) reads

$$\int_0^T \int_\Omega |\nabla u^\varepsilon|^2 \, dx \, dt \; + \; 4\pi\varepsilon^3 \sum_i R_i^2(T) \; = \; 4\pi\varepsilon^3 \sum_i R_i^2(0) \tag{37}$$

for all $T > 0$. Note that by (25) and (26) the right hand side is uniformly bounded by 4π. We observe that in the rescaled variables, the non negative Borel measure $\nu_t^\varepsilon \in (C_p^0)^*$ is given by

$$\int \zeta \, d\nu_t^\varepsilon \; = \; \varepsilon^3 \sum_i \zeta\left(X_i, R_i(t)\right) \quad \text{for } \zeta \in C_p^0.$$

The definitions (25) and (26) translate into the normalizations

$$\int d\nu_t^\varepsilon \leq 1 \quad \text{for all } t \in [0, \infty), \tag{38}$$

$$\int r^3 \, d\nu_t^\varepsilon = 1 \quad \text{for all } t \in [0, \infty). \tag{39}$$

Next to ν_t^ε, we introduce $\mu_t^\varepsilon \in (C_p^0)^*$, a signed Borel measure on $\Omega \times (0, \infty)$ via

$$\int \zeta \, d\mu_t^\varepsilon \; = \; \varepsilon^3 \sum_i \zeta(X_i, R_i(t)) \, V_i(t) \quad \text{for } \zeta \in C_p^0.$$

$\{\mu_t^\varepsilon\}_t$ is just constructed such that

$$\int_0^\infty \left(\partial_t \beta(t) \int \zeta \, d\nu_t^\varepsilon + \beta(t) \int \partial_r \zeta \, d\mu_t^\varepsilon \right) dt \;=\; 0 \tag{40}$$
$$\text{for all } \zeta \in C_p^0 \cap C^\infty \text{ and } \beta \in C^\infty((0,\infty))$$

As will be shown in the proof of Lemma 5.3 in chapter 5, the energy dissipation rate $\int_0^\infty \int_\Omega |\nabla u^\varepsilon|^2$ controls

$$\mathcal{D}^\varepsilon \;:=\; \int_0^\infty \varepsilon^3 \sum_{i:R_i>0} R_i^3 \, V_i^2 \, dt$$

which yields

$$\mathcal{D} \;:=\; \liminf_{\varepsilon \to 0} \mathcal{D}^\varepsilon \;<\; \infty. \tag{41}$$

This indeed translates into the following control of $\{\mu_t^\varepsilon\}_t$

$$\int_0^\infty \left| \int \zeta(t) \, d\mu_t^\varepsilon \right|^2 dt \le \mathcal{D}^\varepsilon \sup_t \int |\zeta(t)|^2 \, \frac{1}{r^3} \, d\nu_t^\varepsilon, \tag{42}$$

$$\left| \int_0^\infty \int \zeta(t) \, d\mu_t^\varepsilon \, dt \right| \le \left(\mathcal{D}^\varepsilon \int_0^\infty \int |\zeta(t)|^2 \, \frac{1}{r^3} \, d\nu_t^\varepsilon \, dt \right)^{1/2}, \tag{43}$$

where $\zeta = \{t \mapsto \zeta(t)\} \in C_0^0((0,\infty); C_p^0)$. Together with (40), (42) yields the following weak regularity in t of $\{\nu_t^\varepsilon\}_t$:

$$\begin{aligned} \left| \int \zeta \, d\nu_{t_1}^\varepsilon \; - \; \int \zeta \, d\nu_{t_2}^\varepsilon \right| &\le |t_1 - t_2|^{1/2} \left(\int_0^\infty \left| \frac{d}{dt} \int \zeta \, d\nu_t^\varepsilon \right|^2 dt \right)^{1/2} \\ &\le \; |t_1 - t_2|^{1/2} \left(\mathcal{D}^\varepsilon \sup_t \int |\partial_r \zeta|^2 \, \frac{1}{r^3} \, d\nu_t^\varepsilon \right)^{1/2} \end{aligned} \tag{44}$$

for $\zeta \in C_p^0 \cap C^\infty$.

4.2 Weak limits

By Arzela–Ascoli, the uniform control of $\{\nu_t^\varepsilon\}_t$ encoded in (38) and (44) is enough to ensure the existence of a weakly continuous familiy $\{\nu_t\}_t$ of nonnegative Borel measures on $\Omega \times (0,\infty)$ such that for a subsequence

$$\int \zeta \, d\nu_t^\varepsilon \;\to\; \int \zeta \, d\nu_t \quad \text{locally uniformly in } t \in [0,\infty) \tag{45}$$

for ζ in a countable subset of $C^0_p \cap C^\infty$. Again by (38), we see that we actually can extend the locally uniform convergence in (45) to all $\zeta \in C^0_p$. Of course, the normalizations (38) and (39) are conserved in a one–sided way

$$\int d\nu_t \leq 1 \quad \text{for all } t \in [0,\infty), \tag{46}$$

$$\int r^3\, d\nu_t \leq 1 \quad \text{for all } t \in [0,\infty). \tag{47}$$

By Riesz, the uniform control of $\{\mu_t^\varepsilon\}_t$ expressed in (43) ensures the existence of a $v \in L^2(r^3\, d\nu_t\, dt)$ with

$$\int_0^\infty \int |v(t)|^2\, r^3\, d\nu_t\, dt \;\leq\; \mathcal{D}, \tag{48}$$

such that for a subsequence

$$\int_0^\infty \beta(t) \int \zeta\, d\mu_t^\varepsilon\, dt \;\to\; \int_0^\infty \beta(t) \int \zeta\, v(t)\, d\nu_t\, dt \tag{49}$$
$$\text{for all } \beta \in C^0_0((0,\infty)) \text{ and } \zeta \in C^0_p.$$

Of course, (40) is preserved in the limit

$$\int_0^\infty \left(\partial_t\beta(t) \int \zeta\, d\nu_t + \beta(t) \int \partial_r\zeta\, v(t)\, d\nu_t \right) dt \;=\; 0 \tag{50}$$
$$\text{for all } \zeta \in C^0_p \cap C^\infty \text{ and } \beta \in C^\infty_0((0,\infty)).$$

4.3 Volume conservation

The infinitesimal version of volume conservation on the ε–level is

$$\int r^2\, d\mu_t^\varepsilon \;=\; 0 \quad \text{for a. a. } t \in (0,\infty). \tag{51}$$

This is preserved in the limit. Indeed, the control (43) together with the normalizations (38) und (39) yields for fixed $T < \infty$

$$\int_0^T \int r^{\frac{3}{2}} d|\mu_t^\varepsilon|\, dt \;\leq\; (T\,\mathcal{D}^\varepsilon)^{1/2},$$
$$\int_0^T \int r^3 d|\mu_t^\varepsilon|\, dt \;\leq\; (T\,\mathcal{D}^\varepsilon)^{1/2}.$$

Hence (49) improves to

$$\int_0^\infty \beta(t) \int r^2 \, d\mu_t^\varepsilon \, dt \to \int_0^\infty \beta(t) \int r^2 \, v(t) \, d\nu_t \, dt \quad \text{for all } \beta \in C_0^0((0,\infty)). \tag{52}$$

In particular, (51) turns into infinitesimal volume conservation at the limit level

$$\int r^2 \, v(t) \, d\nu_t \; = \; 0 \quad \text{for a. a. } t \in (0,\infty). \tag{53}$$

At time $t = 0$, none of the unit volume (39) can escape to infinity thanks to the tightness assumption (29). Indeed, in the rescaled setting, (29) turns into

$$\int_{\{r>R\}} r^3 \, d\nu_0^\varepsilon \; \to \; 0 \quad \text{for } R \to \infty \qquad \text{uniformly for } \varepsilon \to 0.$$

Together with (38), which implies

$$\int_{\{r<\delta\}} r^3 \, d\nu_0^\varepsilon \; \to \; 0 \quad \text{for } \delta \to 0 \qquad \text{uniformly for } \varepsilon \to 0,$$

we see that (39) is at least preserved for $t = 0$

$$\int r^3 \, d\nu_0 \; = \; 1. \tag{54}$$

We now argue on the limit level that infinitesimal volume preservation (53) and initial unit volume (54) ensure unit volume for all t. Since according to (45), $t \mapsto \int \zeta \, d\nu_t$ is continuous, we obtain from (50) for arbitrary but fixed T

$$\int \zeta \, d\nu_T \; = \; \int \zeta \, d\nu_0 + \int_0^T \int \partial_r \zeta \, v(t) \, d\nu_t \, dt \quad \text{for all } \zeta \in C_p^0 \cap C^\infty. \tag{55}$$

We now approximate r^3 by $\{\zeta_n = \zeta_n(r)\}_n \subset C_p^0 \cap C^\infty$ in the sense of

$$\zeta_n(r) \; \uparrow \; r^3 \quad \text{pointwise} \quad \text{and} \quad \frac{\partial_r \zeta_n - 3\, r^2}{r^{\frac{3}{2}} + r^3} \; \to \; 0 \quad \text{uniformly.}$$

By monotone convergence, we then may pass to the limit $n \to \infty$ in the first two terms of (55). For the last term, we observe that

$$\left| \int_0^T \int (\partial_r \zeta_n - 3\, r^2) \, v(t) \, d\nu_t \, dt \right| \le \sup_r \left| \frac{\partial_r \zeta_n - 3\, r^2}{r^{\frac{3}{2}} + r^3} \right| \int_0^T \int (r^{\frac{3}{2}} + r^3) \, |v(t)| \, d\nu_t \, dt$$

and

$$\begin{aligned}
&\int_0^T \int (r^{\frac{3}{2}} + r^3)\, |v(t)|\, d\nu_t\, dt \\
&\quad \le \left(\int_0^T \int |v(t)|^2\, r^3\, d\nu_t\, dt \;\; T\, \sup_t \int d\nu_t \right)^{1/2} \\
&\quad + \left(\int_0^T \int |v(t)|^2\, r^3\, d\nu_t\, dt \;\; T\, \sup_t \int r^3\, d\nu_t \right)^{1/2} \\
&\quad \overset{(48,46,47)}{\le} \;\; 2\, (T\, \mathcal{D})^{1/2}.
\end{aligned}$$

Hence (55) turns into

$$\int r^3\, d\nu_T \;=\; \int r^3\, d\nu_0 + \int_0^T \int 3\, r^2\, v(t)\, d\nu_t\, dt.$$

Together with (53) and (54), we obtain as desired

$$\int r^3\, d\nu_T \;=\; 1 \quad \text{for all } T \in [0, \infty). \tag{56}$$

4.4 Lebesgue density in x

In one respect, the limit measure ν_t is nicer than the ν_t^ε: Its marginal w. r. t. x has a bounded Lebesgue density, that is, there exists a constant $C < \infty$ such that

$$\int \zeta\, d\nu_t \;\le\; C \int_\Omega \zeta\, dx$$
$$\text{for all nonnegative, } \Omega\text{–periodic } \zeta \in C^0(\mathbb{R}^3) \text{ and } t \in [0, \infty). \tag{57}$$

Indeed, fix a periodic $\zeta \in C^1(\mathbb{R}^3)$ and compute

$$\zeta(X_i) \;\le\; C\, \frac{\int_{B_{\lambda\varepsilon}(X_i)} \zeta\, dx}{\int_{B_{\lambda\varepsilon}(X_i)} 1\, dx} \;\le\; \frac{C}{\lambda^3\, \varepsilon^3} \int_{B_{\lambda\varepsilon}(X_i)} \zeta\, dx \quad \text{for all } i,$$

where λ is as in (28). Hence

$$\int \zeta\, d\nu_t^\varepsilon \;=\; \varepsilon^3 \sum_i \zeta(X_i) \;\le\; \frac{C}{\lambda^3} \sum_i \int_{B_{\lambda\varepsilon}(X_i)} \zeta\, dx \;\overset{(28)}{\le}\; \frac{C}{\lambda^3} \int_\Omega \zeta\, dx. \tag{58}$$

This inequality is preserved under the convergence (45) and follows for general ζ by approximation.

5 The variational formulation in the limit $\varepsilon \to 0$

This section comprises the heart of our analysis where we identify the Γ –limit of Rayleigh's variational principle. For the notion of Γ–convergence consult e.g. the monograph [9]. For the convenience of the reader we recall Rayleigh's principle: for all nonnegative $\beta = \beta(t) \in C_0^\infty([0,\infty))$, it holds for $\mathbf{V}^\varepsilon = \frac{d}{dt}\mathbf{R}^\varepsilon$ that

$$\int_0^\infty \beta \left(\tfrac{1}{2}\, g_{\mathbf{R}^\varepsilon}\big(\mathbf{V}^\varepsilon, \mathbf{V}^\varepsilon\big) \;+\; \big\langle \mathrm{diff} E(\mathbf{R}^\varepsilon), \mathbf{V}^\varepsilon \big\rangle \right) dt \;\le\; \int_0^\infty \beta \left(\tfrac{1}{2}\, g_{\mathbf{R}^\varepsilon}\big(\tilde{\mathbf{V}}^\varepsilon, \tilde{\mathbf{V}}^\varepsilon\big) \;+\; \big\langle \mathrm{diff} E(\mathbf{R}^\varepsilon), \tilde{\mathbf{V}}^\varepsilon \big\rangle \right) dt \tag{59}$$

for all $\tilde{\mathbf{V}}^\varepsilon$ such that $\tilde{\mathbf{V}}^\varepsilon \in T_{\mathbf{R}^\varepsilon}\mathcal{M}$.

Theorem 5.1. *For all nonnegative $\beta = \beta(t) \in C_0^\infty([0,\infty))$ it holds*

$$\int_0^\infty \beta \left(\tfrac{1}{2}\int_\Omega |\nabla u|^2\, dx \;+\; 4\pi \int \tfrac{1}{2}|v|^2\, r^3\, d\nu_t + \; 4\pi \int (v - \tilde{v})\, r\, d\nu_t \right) dt \le \int_0^\infty \beta \left(\tfrac{1}{2}\int_\Omega |\nabla \tilde{u}|^2\, dx \;+\; 4\pi \int \tfrac{1}{2}|\tilde{v}|^2\, r^3\, d\nu_t \right) dt \tag{60}$$

for all $\tilde{v} \in L^2(r^3\, d\nu)$ such that $\int r^2\, \tilde{v}\, d\nu_t = 0$ for almost all t and such that $(v - \tilde{v})(t, x, \cdot) = 0$ in a neighborhood of $r = 0$. Here $\tilde{u}(t,\cdot) \in \overset{\circ}{H}{}^1_p$ (and $u(t,\cdot)$ resp.) is determined for a.a. t via

$$\int_\Omega \nabla \tilde{u}(t) \cdot \nabla \zeta\, dx \;+\; 4\pi \int \zeta\, r^2\, \tilde{v}(t)\, d\nu_t \;=0 \tag{61}$$

for all $\zeta \in \overset{\circ}{H}{}^1_p$.

In the following we will for simplicity use the notation

$$d\nu :=\; d\nu_t\, dt.$$

Remark 5.2. We note that the functional

$$< L\,,\, \zeta >:= \int \zeta\, r^2\, \tilde{v}\, d\nu$$

is an element of $L^2((0,T); (\overset{\circ}{H}{}^1_p)^*) \cong L^2((0,T); H_p^{-1})$. This follows from $\int r^2\, \tilde{v}\, d\nu_t = 0$,

$$\int \zeta\; r^2\, \tilde{v}\, d\nu \le\; C\, \left(\int \tilde{v}^2\, r^3\, d\nu \right)^{1/2} \sup_t \left(\int r^3\, d\nu_t \right)^{1/6} \|\zeta\|_{L^2(L^3(\Omega))},$$

where we use (57), and the embedding from $L^2((0,T);\overset{\circ}{H}{}^1_p)$ into $L^2((0,T);L^3)$.

We first compute the limit of the metric tensor. For that we have to prove lower semicontinuity of the metric tensor for the mimimizing sequence $\mathbf{V}^\varepsilon$. The second step is to construct for an arbitrary $\tilde{v} \in L^2(r^3\,d\nu)$ an approximating sequence such that the metric tensor is upper semicontinuous for this sequence. These two ingredients for Γ–convergence are contained in the forthcoming two lemmas.

Lemma 5.3. *(Lower semicontinuity)*
It holds for all nonnegative $\beta = \beta(t) \in C_0^\infty([0,\infty))$ that

$$\begin{aligned} \liminf_{\varepsilon\to 0} \int_0^\infty \beta\, g_{\mathbf{R}^\varepsilon}\big(\mathbf{V}^\varepsilon, \mathbf{V}^\varepsilon\big)\, dt &= \liminf_{\varepsilon\to 0} \int_0^\infty \beta \int_\Omega |\nabla u^\varepsilon|^2\, dx\, dt \\ &\geq \int_0^\infty \beta \int_\Omega |\nabla u|^2\, dx\, dt \;+\; 4\pi \int \beta\, |v|^2\, r^3\, d\nu, \end{aligned} \tag{62}$$

where for almost all t the function $u(t,\cdot) \in \overset{\circ}{H}{}^1_p$ is determined as in (61).

Lemma 5.4. *(Construction)*
For any $\tilde{v} \in L^2(r^3\,d\nu)$ with $\int \tilde{v}\, r^2\, d\nu_t = 0$ for almost all t the following holds: there exists a sequence $\tilde{\mathbf{V}}^\varepsilon$ with $\tilde{\mathbf{V}}^\varepsilon \in T_{\mathbf{R}^\varepsilon}\mathcal{N}^\varepsilon$ such that

$$\begin{aligned} \limsup_{\varepsilon\to 0} \int_0^\infty \beta\, g_{\mathbf{R}^\varepsilon}\big(\tilde{\mathbf{V}}^\varepsilon, \tilde{\mathbf{V}}^\varepsilon\big)\, dt \;&= \limsup_{\varepsilon\to 0} \int_0^\infty \beta \int_\Omega |\nabla \tilde{u}^\varepsilon|^2\, dx\, dt \\ &\leq \;\int_0^\infty \beta \int_\Omega |\nabla \tilde{u}|^2\, dx\, dt \;+\; 4\pi \int \beta\, |\tilde{v}|^2\, r^3\, d\nu \end{aligned} \tag{63}$$

for all nonnegative $\beta = \beta(t) \in C_0^\infty([0,\infty))$ and with $\tilde{u}$ determined as in (61).

Our strategy will be to split $\int_\Omega |\nabla \tilde{u}^\varepsilon|^2\, dx$ into the part where $\nabla \tilde{u}^\varepsilon$ concentrates, that is the neighborhood of the particles, and the rest where $\tilde{u}^\varepsilon$ is slowly varying. In the proof Lemma 5.3 we consider balls $B_{l_i}(X_i)$ with $l_i = \gamma\varepsilon^3 R_i$ and let first ε tend to zero and then γ to ∞. To prove Lemma 5.4 we choose $l_i \equiv l = \gamma\varepsilon$ and let first ε and then γ tend to zero.

Proof of Lemma 5.3:

Step 1: A lower bound for $\int_\Omega |\nabla u^\varepsilon|^2$

Denote $B_{l_i} := B_{l_i}(X_i)$ with $l_i = \gamma\varepsilon^3 R_i$ and note that B_{l_i} are disjoint due to (31). We are going to show

$$\int_{B_{l_i}} |\nabla u^\varepsilon|^2\, dx \geq 4\pi\varepsilon^3\, R_i^3\, V_i^2 \left(1 - \frac{1}{\gamma}\right). \tag{64}$$

For that purpose observe that

$$\int_{B_{l_i}} |\nabla u^\varepsilon|^2 \, dx \;\geq\; \inf_{\xi} \int_{B_{l_i}} |\xi|^2 \, dx \,, \tag{65}$$

where the infimum is taken over all $\xi \in L^2(B_{l_i})$ which satisfy

$$\int_{B_{l_i}} \xi \cdot \nabla\zeta \, dx \;+\; \int_{\partial B_i} \frac{1}{\varepsilon^3} \, V_i \, \zeta = 0$$

for all $\zeta \in C_0^\infty(B_{l_i})$. Indeed, the minimizer $\hat{\xi}$ of (65) satisfies

$$\int_{B_{l_i}} \hat{\xi} \cdot y \, dx \;=\; 0$$

for all smooth divergence–free y. Hence $\hat{\xi} = \nabla\phi$ and $\phi = const.$ on ∂B_{l_i}, where $-\Delta\phi = 0$ in $(B_{l_i}\backslash\overline{B_i})\cup B_i$ and $[\nabla\phi\cdot\vec{n}] = \frac{1}{\varepsilon^3} V_i$ on ∂B_i. The solution is given by

$$\hat{\xi} = \begin{cases} \varepsilon^3 \, R_i^2 \, V_i \, \frac{(x-x_i)}{|x-x_i|^3} & : \quad x \in B_{l_i}\backslash\overline{B_i} \\ 0 & : \quad x \in B_i \end{cases} \tag{66}$$

and we compute

$$\begin{aligned} \int_{B_{l_i}} |\hat{\xi}|^2 \, dx = \int_{B_{l_i}\backslash B_i} |\hat{\xi}|^2 \, dx &= \varepsilon^6 \, R_i^4 \, V_i^2 \int_{B_{l_i}\backslash B_i} \frac{1}{|x-x_i|^4} \, dx \\ &= \varepsilon^6 \, R_i^4 \, V_i^2 \, 4\pi \int_{\varepsilon^3 R_i}^{l_i} \frac{1}{r^4} \, r^2 \, dr \\ &= 4\pi \, \varepsilon^6 \, R_i^4 \, V_i^2 \Big(\frac{1}{\varepsilon^3 R_i} - \frac{1}{l_i} \Big) \\ &= 4\pi\varepsilon^3 \, R_i^3 \, V_i^2 \Big(1 - \frac{\varepsilon^3 R_i}{l_i} \Big) \\ &= 4\pi \, \varepsilon^3 \, R_i^3 \, V_i^2 \, \Big(1 - \frac{1}{\gamma} \Big) \end{aligned}$$

which proves (64). We obtain a uniform bound for $\mathcal{D}^\varepsilon = \int_0^\infty \varepsilon^3 \sum_i R_i^3 V_i^2 \, dt$ and thus (41) if we choose $\gamma = 2$, sum over all particles, integrate over t and use (37).

Step 2: Identify the weak limit of u^ε
We recall that the potential u^ε solves (36) and observe that for all Ω–periodic $\zeta \in C^\infty(\mathbb{R}^3)$

$$\int_0^\infty \beta \Big| \sum_{i:R_i>0} \int_{\partial B_i} \frac{1}{\varepsilon^3} \, \zeta \, V_i \;-\; \sum_{i:R_i>0} 4\pi\varepsilon^3 \, \zeta(X_i) \, R_i^2 \, V_i \Big| \, dt \to 0.$$

We obtain with (52) that

$$\int_0^\infty \beta \sum_{i:R_i>0} \int_{\partial B_i} \frac{1}{\varepsilon^3} \zeta\, V_i\, dt \;\to\; 4\pi \int \beta\, \zeta\; r^2\, v\, d\nu \tag{67}$$

for all Ω–periodic $\zeta = \zeta(x) \in C^\infty(\mathbb{R}^3)$. By Remark 5.2 this also holds for $\zeta \in \mathring{H}^1_p$. Consequently ∇u^ε converges weakly in $L^2((0,\infty)\times\Omega)$ to ∇u.

Step 3: Lower semicontinuity
We have for almost all t that

$$\begin{aligned}\int_\Omega |\nabla u^\varepsilon|^2\, dx &= \int_{\Omega\setminus\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx \;+\; \int_{\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx \\ &\overset{(64)}{\geq} \int_{\Omega\setminus\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx \;+\; 4\pi\varepsilon^3 \sum_{i:R_i>0} R_i^3\, V_i^2 \Big(1 - \frac{1}{\gamma}\Big) \\ &= \int_{\Omega\setminus\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx \;+\; 4\pi\Big(1-\frac{1}{\gamma}\Big)\,\varepsilon^3 \sum_{i:R_i>0} R_i^3\, V_i^2.\end{aligned}$$

Multiplying with β and integrating over t we obtain

$$\begin{aligned}\int_0^\infty \beta \int_\Omega |\nabla u^\varepsilon|^2\, dx\, dt \geq{}& \int_0^\infty \beta \int_{\Omega\setminus\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx\, dt \\ &+\; 4\pi\Big(1-\frac{1}{\gamma}\Big) \int_0^\infty \beta\, \varepsilon^3 \sum_{i:R_i>0} R_i^3\, V_i^2\, dt.\end{aligned}$$

Arguing as in chapter 4 one finds that

$$\liminf_{\varepsilon\to 0} \int_0^\infty \beta\, \varepsilon^3 \sum_{i:R_i>0} R_i^3\, V_i^2\, dt \geq \int_0^\infty \beta\, |v|^2\, r^3\, d\nu.$$

Furthermore we claim that

$$\int_0^\infty \beta \int_\Omega |\nabla u|^2\, dx\, dt \;\leq\; \liminf_{\varepsilon\to 0} \int_0^\infty \beta \int_{\Omega\setminus\cup B_{l_i}} |\nabla u^\varepsilon|^2\, dx\, dt$$

with $l_i = \gamma\varepsilon^3 R_i$. This is a consequence of the fact that

$$|\cup B_{l_i}| \leq C\,\varepsilon^6\,\gamma^3 \int r^3\, d\nu_t^\varepsilon \to 0$$

as $\varepsilon \to 0$ and Lemma 5.5. For $\gamma \to \infty$ we recover the assertion of the lemma.

Lemma 5.5. *Let $E_n \subset \Omega \subset \mathbb{R}^n$ be a sequence of sets such that $|E_n| \to 0$ as $n \to \infty$. If z_n converges weakly in $L^2(\Omega)$ to a function z then it holds*

$$\|z\|_{L^2(\Omega)} \leq \liminf_{n\to\infty} \|z_n\|_{L^2(\Omega\setminus E_n)}.$$

Proof: We have

$$\int_\Omega z_n z = \int_{E_n} z_n z + \int_{\Omega\setminus E_n} z_n z \\ \leq \|z_n\|_{L^2(\Omega)}\|z\|_{L^2(E_n)} + \|z_n\|_{L^2(\Omega\setminus E_n)}\|z\|_{L^2(\Omega)}$$

and the lemma follows for $n \to \infty$.

Proof of Lemma 5.4:

Step 1: Proof for smooth $\tilde{v}$

Assume first that $\tilde{v} \in C_0^\infty([0,\infty);(C_p^0 \cap C^\infty))$ with $\int r^2\,\tilde{v}\,d\nu_t = 0$ for all t. Our first idea to define $\tilde{\mathbf{V}}^\varepsilon := (\tilde{V}_i)_i$ is $\tilde{V}_i := \tilde{v}(t, X_i, R_i)$. But then $\tilde{\mathbf{V}}_\varepsilon$ is in general not in the tangent space of $\mathcal{N}^\varepsilon$. For that reason we make the ansatz

$$\tilde{V}_i := \tilde{v}(t, X_i, R_i) \,+\, f^\varepsilon(t)\,\eta(R_i),$$

where $f^\varepsilon(t)$ is chosen such that $\tilde{\mathbf{V}}_\varepsilon \in T_{\mathbf{R}^\varepsilon}\mathcal{N}^\varepsilon$. This requires

$$f^\varepsilon(t) \int \eta\, r^2\, d\nu_t^\varepsilon = -\int \tilde{v}\, r^2\, d\nu_t^\varepsilon.$$

We observe that there is $\eta = \eta(r) \in C_0^0((0,\infty))$ such that

$$t \mapsto \int \eta\, r^2\, d\nu_t \qquad \text{is continuous and positive in } [0,\infty).$$

Indeed, let $\eta_n \subset C_0^0((0,\infty))$ be a sequence converging to 1 in the sense that

$$\sup_{r\in(0,\infty)} \frac{|\eta_n(r)-1|\, r^2}{1+r^3} \to 0 \qquad \text{as } n \to \infty.$$

Since by (46) and (47) we control $\int(1+r^3)\,d\nu_t$ uniformly in t, we have

$$\int \eta_n\, r^2\, d\nu_t \to \int r^2\, d\nu_t \qquad \text{uniformly in } t \in (0,\infty).$$

By volume conservation (56) we have

$$\int r^2\, d\nu_t > 0 \qquad \text{for all } t \in [0,\infty)$$

and according to (45)

$$t \mapsto \int \eta_n\, r^2\, d\nu_t \qquad \text{is continuous for fixed } n.$$

With (44) and the properties of $\tilde{v}$ we find that f^ε converges uniformly in $[0,T]$ to 0.

The corresponding potential $\tilde{u}^\varepsilon$ to $\tilde{\mathbf{V}}^\varepsilon$ solves for a. a. t

$$\int_\Omega \tfrac{1}{2}|\nabla \tilde{u}^\varepsilon|^2\,dx \;=\; \inf_\xi \Big\{ \int_\Omega \tfrac{1}{2}|\xi|^2\,dx \;:\; \int_\Omega \xi\cdot\nabla\zeta\,dx + \sum_{i:R_i>0} \int_{\partial B_i} \frac{1}{\varepsilon^3}\,\tilde{V}_i\,\zeta \;=0\,;\; \zeta\in \mathring{H}^1_p \Big\}.$$

As a comparison function we choose for $l=\gamma\varepsilon, \gamma<\lambda$,

$$\xi = \left\{ \begin{array}{ccc} R_i^2\,\tilde{V}_i\,\varepsilon^3\,\frac{x-X_i}{|x-X_i|^3} & : & \varepsilon^3 R_i < |x-X_i| < l \\ 0 & : & \text{elsewhere} \end{array} \right\} + \nabla\bar{u}^\varepsilon,$$

where $\nabla\bar{u}^\varepsilon$ is such that ξ is admissible. Since

$$\begin{aligned} \int_\Omega \xi\cdot\nabla\zeta\,dx &= \int_\Omega \nabla\bar{u}^\varepsilon\cdot\nabla\zeta\,dx + \int_\Omega (\xi-\nabla\bar{u}^\varepsilon)\cdot\nabla\zeta\,dx \\ &= \int_\Omega \nabla\bar{u}^\varepsilon\cdot\nabla\zeta\,dx - \sum_{i:R_i>0}\int_{\partial B_i}\frac{1}{\varepsilon^3}\,\tilde{V}_i\,\zeta + \int_{\partial B_l}\frac{\varepsilon^3}{l^2}\,R_i^2\,\tilde{V}_i\,\zeta, \end{aligned}$$

this requires

$$\int_\Omega \nabla\bar{u}^\varepsilon\cdot\nabla\zeta + \sum_{i:R_i>0}\int_{\partial B_l}\frac{\varepsilon^3}{l^2}\,R_i^2\,\tilde{V}_i\,\zeta \;=\; 0 \tag{68}$$

for all $\zeta\in\mathring{H}^1_p$. Then it holds for small $\alpha>0$

$$\begin{aligned} \tfrac{1}{2}\int_\Omega|\xi|^2\,dx &\le \sum_{i:R_i>0}\tfrac{1}{2}\int_{B_l\setminus B_i}|\varepsilon^3\,R_i^2\,\tilde{V}_i\,\frac{1}{|x-X_i|^2}|^2dx \\ &\quad + \sum_{i:R_i>0}\int_{B_l\setminus B_i}\varepsilon^3\,R_i^2\,\tilde{V}_i\,\frac{(x-X_i)}{|x-X_i|^3}\cdot\nabla\bar{u}^\varepsilon\,dx + \tfrac{1}{2}\int_\Omega|\nabla\bar{u}^\varepsilon|^2\,dx \\ &\le (1+\alpha)\sum_{i:R_i>0}\tfrac{1}{2}\int_{B_l\setminus B_i}|\varepsilon^3\,R_i^2\,\tilde{V}_i\,\frac{1}{|x-X_i|^2}|^2\,dx \\ &\quad +\frac{1}{\alpha}\sum_{i:R_i>0}\tfrac{1}{2}\int_{B_l}|\nabla\bar{u}^\varepsilon|^2\,dx + \tfrac{1}{2}\int_\Omega|\nabla\bar{u}^\varepsilon|^2\,dx. \end{aligned}$$

We observe that

$$\begin{aligned} &\tfrac{1}{2}\int_{B_l\setminus B_i}|\varepsilon^3\,R_i^2\,\tilde{V}_i\,\frac{1}{|x-X_i|^2}|^2\,dx \\ &\quad = 4\pi\,R_i^4\,\tilde{V}_i^2\,\varepsilon^6\,\tfrac{1}{2}\int_{\varepsilon^3 R_i}^{l}\frac{1}{r^2}\,dr \le 4\pi\varepsilon^3\,R_i^3\,\tfrac{1}{2}\tilde{V}_i^2 \end{aligned}$$

and conclude that

$$\tfrac{1}{2}\int_\Omega |\xi|^2\,dx \;\le\; (1+\alpha)\,4\pi\,\varepsilon^3 \sum_{i:R_i>0} R_i^3\,\tfrac{1}{2}\tilde{V}_i^2 \\ + \frac{1}{\alpha}\,\omega_\varepsilon(\,C\gamma^3)\;+\;\tfrac{1}{2}\int_\Omega |\nabla \bar{u}^\varepsilon|^2\,dx,$$

where

$$\omega_\varepsilon(z) := \sup_E \left\{ \int_E \tfrac{1}{2}|\nabla \bar{u}^\varepsilon|^2\,dx \;:\; |E|\le z \right\}.$$

Remember that $\tilde{V}_i = \tilde{v}(R_i) + f^\varepsilon(t)\,\eta(R_i)$, with $\tilde{v},\eta \in C_p^0$ and that f^ε converges uniformly to 0. This gives

$$\int \beta\,\varepsilon^3 \sum_{i:R_i>0} \tilde{V}_i^2\,R_i^3\,dt \to \int \beta\,\tilde{v}^2\,r^3\,d\nu.$$

In the next step we will prove that $\nabla\bar{u}^\varepsilon$ converges strongly to $\nabla\tilde{u}$. This leads to

$$\limsup_{\varepsilon\to 0} \int_0^\infty \beta\,\tfrac{1}{2}\int_\Omega |\nabla\tilde{u}^\varepsilon|^2\,dx\,dt \le (1+\alpha)\,4\pi \int \beta\,\tfrac{1}{2}v^2\,r^3\,d\nu \\ QQ + \frac{1}{\alpha}\,\omega(\,C\gamma^3\,)\;+\;\int_0^\infty \beta\,\tfrac{1}{2}\int_\Omega |\nabla\tilde{u}|^2\,dx\,dt,$$

where

$$\omega(z) := \sup_E \left\{ \int_E |\nabla\tilde{u}|^2\,dx \;:\; |E|\le z \right\}.$$

Finally, let first γ and then α converge to 0 to obtain the assertion of the lemma for smooth $\tilde{v}$ with compact support in the r –variable.

Step 2: Strong convergence of $\nabla\bar{u}^\varepsilon$
Our goal is to show that $\nabla\bar{u}^\varepsilon$ as defined in (68) converges for any $T>0$ strongly in $L^2((0,T)\times\Omega)$ provided $l=\gamma\varepsilon$ for some $\gamma<\lambda$. Without loss of generality let $T>0$ be so large such that $\beta(t)=0$ for all $t>T$ and introduce the functionals

$$< L_\varepsilon\,,\,\zeta > := \int_0^\infty \beta \sum_{i:R_i>0} \int_{\partial B_l} \frac{\varepsilon^3}{l^2}\,R_i^2\,\tilde{V}_i\,\zeta\,dt \\ = \int_0^\infty \beta \sum_{i:R_i>0} \frac{l}{\gamma^3} \int_{\partial B_l} R_i^2\,\tilde{V}_i\,\zeta\,dt, \\ < \tilde{L}_\varepsilon\,,\,\zeta > := \int_0^\infty \beta \sum_{i:R_i>0} \frac{3}{\gamma^3} \int_{B_l} R_i^2\,\tilde{V}_i\,\zeta\,dx\,dt, \\ < L\,,\,\zeta > := 4\pi \int \beta\,\zeta\;r^2\,\tilde{v}\,d\nu,$$

for $\zeta \in L^2((0,T); \overset{\circ}{H}{}^1_p)$. We will prove

a) $L_\varepsilon - \tilde{L}_\varepsilon \to 0$ in $L^2((0,T); H_p^{-1})$,
b) $\tilde{L}_\varepsilon - L \to 0$ weakly in $C_0^0([0,T]; C_p^0)^*$,
c) $\tilde{L}_\varepsilon$ is relatively compact in $C^0([0,T]; H_p^{-1})$.

To prove $a)$ we modify an idea used in [4], Lemma 2.3. We consider the auxiliary function

$$\psi(t,x) = \begin{cases} \frac{1}{\gamma^3} R_i^2 \tilde{V}_i \frac{1}{2}(l^2 - |x - X_i|^2) & : \quad |x - X_i| < l \\ 0 & : \quad \text{elsewhere} \end{cases}$$

such that ψ is continuous,

$$\nabla\psi(t,x) = \begin{cases} -\frac{1}{\gamma^3} R_i^2 \tilde{V}_i (x - X_i) & : \quad |x - X_i| < l \\ 0 & : \quad \text{elsewhere} \end{cases}$$

and

$$-\Delta\psi = \frac{3}{\gamma^3} R_i^2 \tilde{V}_i, \qquad |x - X_i| < l,$$
$$\nabla\psi \cdot \vec{n} = -\frac{l}{\gamma^3} R_i^2 \tilde{V}_i, \qquad |x - X_i| = l.$$

With this construction it holds

$$\left\langle \tilde{L}_\varepsilon - L_\varepsilon, \zeta \right\rangle = \int_0^T \beta \int_\Omega \nabla\psi \cdot \nabla\zeta \, dx \, dt$$

and

$$\begin{aligned} \|\tilde{L}_\varepsilon - L_\varepsilon\|^2_{L^2(H_p^{-1})} &\leq C \int_0^T \int_\Omega |\nabla\psi|^2 \, dx \, dt \\ &\leq C \int_0^T \sum_{i:R_i>0} \frac{1}{\gamma^6} R_i^4 \tilde{V}_i^2 \int_{B_l} |x - X_i|^2 \, dt \\ &\leq C \int_0^T \sum_{i:R_i>0} R_i^4 \tilde{V}_i^2 \frac{4\pi}{5} \frac{l^5}{\gamma^6} \\ &\leq C \sup \left(|\tilde{v}^2 r^4| + |f^\varepsilon \eta|^2 \right) \frac{\varepsilon^2}{\gamma} \to 0 \qquad \text{as } \varepsilon \to 0. \end{aligned}$$

To prove part $b)$ observe that for $\zeta \in C_0^0([0,\infty); C_p^0)$

$$\begin{aligned}
&\int_0^\infty \beta \sum_{i:R_i>0} \zeta(t,X_i)\,\frac{3}{\gamma^3}\,|B_l|\,R_i^2\,\tilde V_i\,dt \\
&\quad = \int_0^\infty \beta\,4\pi \sum_{i:R_i>0} \zeta(t,X_i)\,\frac{l^3}{\gamma^3}\,R_i^2\,\big(\tilde v(R_i) + f^\varepsilon(t)\,\eta(R_i)\big)\,dt \\
&\quad = 4\pi \int \beta\,\zeta\, r^2\,(\tilde v + f^\varepsilon \eta)\,d\nu_t^\varepsilon\,dt \\
&\quad \to 4\pi \int \beta\,\zeta\, r^2\,\tilde v\,d\nu,
\end{aligned}$$

and

$$\begin{aligned}
&\int_0^\infty \beta(t) \sum_{i:R_i>0} \frac{3}{\gamma^3} \int_{B_l} R_i^2\,|\tilde V_i|\,|\zeta(t,x)-\zeta(t,X_i)|\,dx\,dt \\
&\qquad\qquad \le C_\zeta \int_0^T \sum_{i:R_i>0} \frac{3}{\gamma^3}\,R_i^2\,|\tilde v(R_i) + f^\varepsilon\,\eta(R_i)|\,l^4\,dt \\
&\qquad\qquad \le C_\zeta\,\sup|r^2(\tilde v + f^\varepsilon\eta)|\,\frac{l^4}{\varepsilon^3\gamma^3} \\
&\qquad\qquad \le C_\zeta\,\sup|R_i^2(\tilde v + f^\varepsilon\eta)|\,\gamma\,\varepsilon \to 0.
\end{aligned}$$

which implies statement $b)$.

To prove part c) we show for $\tilde L_\varepsilon(t)$ defined via

$$\Big\langle \tilde L_\varepsilon(t)\,,\,\zeta \Big\rangle = \sum_{i:R_i>0} \frac{3}{\gamma^3} \int_{B_l} R_i^2\,\tilde V_i\,\zeta\,dx \qquad \text{for } \zeta = \zeta(x) \in L^2(\Omega)$$

the following:

i) $\sup_{t\in(0,T)} \|\tilde L_\varepsilon(t)\|_{L^2(\Omega)} \le C.$
ii) $\|\tilde L_\varepsilon(t_1) - \tilde L_\varepsilon(t_2)\|_{L^2(\Omega)} \le C|t_1-t_2|^{1/2}$ for all $t_1, t_2 \in (0,T)$.

Then the desired result follows from the compact embedding of $\overset{\circ}{H}{}_p^1$ into $L^2(\Omega)$ and the generalized Arzela–Ascoli Theorem (cf. e.g. [15], chapter 2).

Indeed, $i)$ follows from

$$\begin{aligned}
\Big\langle \tilde L_\varepsilon(t),\zeta \Big\rangle &\le \sup\big(|r^2\,\tilde v| + |f^\varepsilon\,\eta\,r^2|\big) \sum_{i:R_i>0} \int_{B_l} |\zeta|\,dx \\
&\le C\,\|\zeta\|_{L^1(\Omega)} \le C\,\|\zeta\|_{L^2(\Omega)}.
\end{aligned}$$

The equicontinuity $ii)$ follows similarly as (44) via

$$\begin{aligned}
&\left\langle \tilde{L}_\varepsilon(t_1) \,-\, \tilde{L}_\varepsilon(t_2), \zeta \right\rangle \le |t_1 - t_2|^{1/2} \\
&\quad \times \left(\int_0^T \Big| \frac{d}{dt} \sum_{i:R_i>0} \frac{3}{\gamma^3} R_i^2 \tilde{V}_i \int_{B_l} \zeta \, dx \Big|^2 dt \right)^{1/2} \\
&\quad \le\; C\,|t_1 - t_2|^{1/2} \\
&\quad \times \left(\int_0^T \Big| \sum_{i:R_i>0} \big(R_i V_i \tilde{V}_i +\, R_i^2\, \partial_t \tilde{V}_i\big) \int_{B_l} |\zeta|\, dx \Big|^2 dt \right)^{1/2} \\
&\quad \le\; C\,|t_1 - t_2|^{1/2} \\
&\quad \times \left(\int_0^T \sum_{i:R_i>0} \varepsilon^3 \Big| R_i V_i \tilde{V}_i \,+\, R_i^2\, \partial_t \tilde{V}_i \Big|^2 \sum_i \int_{B_l} |\zeta|^2 \, dx\, dt \right)^{1/2} \\
&\quad \le\; C\,|t_1 - t_2|^{1/2} \\
&\quad \times \left(\int_0^T \int |r\, v\, \tilde{v} \,+\, r^2\, \partial_t(\tilde{v} \,+\, f^\varepsilon \eta)|^2 \, d\nu_t^\varepsilon \, dt \right)^{1/2} \|\zeta\|_{L^2(\Omega)} \\
&\overset{(38)}{\le}\; C\,|t_1 - t_2|^{1/2}\, \|\zeta\|_{L^2(\Omega)} \\
&\quad \times \left(\mathcal{D}^\varepsilon \sup \frac{|\tilde{v}|^2}{r} \,+\, T \,\sup |r^2\, \partial_t \tilde{v}|^2 + \,\sup |r^2 \eta|^2 \int_0^T |\partial_t f^\varepsilon|^2 \, dt \right)^{1/2}.
\end{aligned}$$

The desired result follows if we show that $\partial_t f^\varepsilon$ is uniformly bounded in $L^2(0,T)$. But this follows from

$$\begin{aligned}
\partial_t f^\varepsilon \;=\; \frac{1}{\int \eta\, r^2\, d\nu_t^\varepsilon} \Bigg(\int \partial_t \tilde{v}\, r^2\, d\nu_t^\varepsilon \;-& \\
\int \partial_r (\tilde{v}\, r^2)\, d\mu_t^\varepsilon \,+\, f^\varepsilon \int \partial_t (\eta\, r^2)\, d\mu_t^\varepsilon &\Bigg)
\end{aligned}$$

the properties of $\tilde{v}$ and (41).

Step 3: Approximate general $\tilde{v}$ by continuous functions
In order to prove the lemma for $\tilde{v} \in L^2(r^3\, d\nu)$ we have to show that we can approximate $\tilde{v}$ in the $L^2(r^3\, d\nu)$ –norm by smooth functions v_n with compact support such that

$$\begin{aligned}
&\int_0^\infty \beta \int_\Omega |\nabla u_n|^2 \, dx\, dt \,+\, 4\pi \int \beta\, |v_n|^2\, r^3\, d\nu \\
&\quad \to \int_0^\infty \beta \int_\Omega |\nabla \tilde{u}|^2 \, dx\, dt \,+\, 4\pi \int \beta\, \tilde{v}^2\, r^3\, d\nu
\end{aligned}$$

as $n \to \infty$ where u_n is defined according to (61). But this follows from Remark 5.2 which finishes the proof of Lemma 5.4.

Since we computed the Γ–limit of the metric tensor we are ready to finish the proof of Theorem 5.1.

Proof of Theorem 5.1. The main part of the theorem has been proved in Lemmas 5.3 and 5.4 which give Γ–convergence of the metric tensor. The seemingly easy linear part of our functional

$$\int_0^\infty \beta \left\langle \text{diff } E(\mathbf{R}^\varepsilon), \mathbf{V}^\varepsilon \right\rangle dt \tag{69}$$

involves some technicalities since we do not have an estimate which guarantees that $4\pi \int r\, v \; d\nu$ is well-defined. For that reason we take $\beta \in C_0^\infty((0, \infty))$, integrate the term in (69) by parts and obtain

$$\begin{aligned}\int_0^\infty \beta \left\langle \text{diff } E(\mathbf{R}^\varepsilon), \mathbf{V}^\varepsilon \right\rangle dt &= -\int_0^\infty \partial_t \beta\, E(\mathbf{R}^\varepsilon(t))\, dt \\ &= -4\pi \int \partial_t \beta\, \tfrac{1}{2} r^2 \, d\nu_t^\varepsilon \, dt\end{aligned}$$

Since we have uniform control of $\int (1 + r^3)\, d\nu_t^\varepsilon \, dt$ we can pass to the limit in this term.

As a comparison function we take first $\tilde{v}$ such that $\tilde{v}(t, x, \cdot)$ has compact support in $(0, \infty)$. With Lemmas 5.3 and 5.4 one gets

$$\begin{aligned}&\int_0^\infty \beta\, \tfrac{1}{2} \int_\Omega |\nabla u|^2 \, dx\, dt \;+\; 4\pi \int \beta\, \tfrac{1}{2} |v|^2\, r^3 \, d\nu \;-\; 4\pi \int \partial_t \beta\, \tfrac{1}{2}\, r^2 \, d\nu \\ &\quad \le \int_0^\infty \beta\, \tfrac{1}{2} \int_\Omega |\nabla \tilde{u}|^2 \, dx\, dt \;+\; 4\pi \int \beta\, \tfrac{1}{2} |\tilde{v}|^2\, r^3 \, d\nu \;+\; 4\pi \int \beta\, r\, \tilde{v} \; d\nu\end{aligned} \tag{70}$$

for all $\beta \in C_0^\infty((0, \infty))$ and $\tilde{v}$ with compact support in $(0, \infty)$.

For the proof of the theorem we want to approximate a general $\tilde{v}$ as in the statement of the theorem by $\tilde{v}_\delta$ with compact support. Define

$$\tilde{v}_\delta := \eta_\delta(\tilde{v} + f_\delta),$$

where $\eta_\delta = \eta_\delta(r) \in C_0^\infty((0, \infty))$, $0 \le \eta_\delta \le 1$, and η_δ approximates 1 such that

$$\sup_{r \in (0,\infty)} \frac{|1 - \eta_\delta|\, r^2}{1 + r^3} \to 0 \qquad \text{as } \delta \to 0.$$

The function f_δ is determined such that $\int r^2\, \tilde{v}_\delta \, d\nu_t = 0$ which requires

$$f_\delta(t) = \frac{\int (1 - \eta_\delta)\, r^2\, \tilde{v}\, d\nu_t}{\int \eta_\delta\, r^2\, d\nu_t}.$$

We conclude with similar arguments as in Step 1 of Lemma 5.4 that for sufficiently small δ the denominator is uniformly bounded in any finite time interval $[0,T]$. Hence

$$\begin{aligned}\int_0^T |f_\delta|^2\,dt &\le C_T \int_0^T \left(\int (1-\eta_\delta)\,r^2\,\tilde v\,d\nu_t\right)^2 dt\\ &\le C_T \int_0^T \left(\int \tilde v^2\,r^3\,d\nu_t \int |1-\eta_\delta|^2\,r\,d\nu_t\right) dt\\ &\le C_T\,\mathcal{D}\,\sup_r \frac{|1-\eta_\delta|\,r}{1+\,r^3}\,\sup_t \int (1+r^3)\,d\nu_t\\ &\to 0 \qquad \text{as } \delta\to 0.\end{aligned}$$

Since $\tilde v_\delta$ is admissible we have by (70)

$$\begin{aligned}&\int_0^\infty \beta\,\tfrac12 \int_\Omega |\nabla u|^2\,dx\,dt \;+\; 4\pi \int \beta\,\tfrac12 |v|^2\,r^3\,d\nu \;-\; 4\pi \int \partial_t\beta\,\tfrac12\,r^2\,d\nu\\ &\quad\le \int_0^\infty \beta\,\tfrac12 \int_\Omega |\nabla \tilde u_\delta|^2\,dx\,dt \;+\; 4\pi \int \beta\,\tfrac12 |\tilde v_\delta|^2\,r^3\,d\nu + 4\pi \int \beta\,r\,\tilde v_\delta\,d\nu.\end{aligned} \tag{71}$$

We first consider the difference of the energy terms. For that we define q_δ such that

$$q_\delta'(r) = \eta_\delta(r) r, \qquad q_\delta(0) = 0$$

and with the construction of η_δ it follows

$$\sup_{r\in(0,\infty)} \frac{|q_\delta - \frac12 r^2|}{1+r^3} \to 0 \qquad \text{as } \delta \to 0.$$

We observe

$$\begin{aligned}\left|\int \partial_t\beta\,(\tfrac12\,r^2 - q_\delta)\,d\nu\right| &\le \sup_r \frac{|\frac12\,r^2 - q_\delta|}{1+r^3} \int |\partial_t\beta|\,(1+r^3)\,d\nu\\ &\to 0 \qquad \text{as } \delta\to 0,\end{aligned} \tag{72}$$

and

$$\begin{aligned}\left|\int \beta\,f_\delta\,\eta_\delta\,r\,d\nu\right| &= \left|\int \beta(t) f_\delta(t) \int r\,\eta_\delta\,d\nu_t\,dt\right|\\ &\le C\,\sup_t \int (1+r^3)\,d\nu_t \int_0^T |f_\delta|\,dt \;\to\; 0 \qquad \text{as } \delta\to 0.\end{aligned} \tag{73}$$

Hence,

$$
\begin{aligned}
-\int \partial_t\beta\,\tfrac{1}{2}\,r^2\,d\nu - \int \beta\,r\,\tilde{v}_\delta\,d\nu &\overset{(72)}{=} -\int \partial_t\beta\,q_\delta\,d\nu \\
&\quad - \int \beta\,r\,\tilde{v}_\delta\,d\nu + o(1) \\
&\overset{(50)}{=} \int \beta\,q_\delta'\,v\,d\nu - \int \beta\,r\,\tilde{v}_\delta\,d\nu + o(1) \\
&\overset{(73)}{=} \int \beta\,\eta_\delta\,r\,(v-\tilde{v})\,d\nu + o(1) \\
&= \int \beta\,r\,(v-\tilde{v})\,d\nu + o(1).
\end{aligned}
$$

For the convergence of the metric tensor for $\tilde{v}_\delta$ observe

$$
\begin{aligned}
\int \beta\,|\tilde{v}_\delta - \tilde{v}|^2\,r^3\,d\nu &= \int \beta\,|(1-\eta_\delta)\,\tilde{v} + \eta_\delta\,f_\delta\,|^2\,r^3\,d\nu \\
&\le 2\int \beta\,(1-\eta_\delta)^2\,|\tilde{v}|^2\,r^3\,d\nu + 2\int \beta\,f_\delta^2\,r^3\,d\nu \\
&\to 0 \qquad \text{as } \delta \to 0.
\end{aligned}
$$

Furthermore we conclude

$$
\int_0^\infty \beta \int_\Omega |\nabla \tilde{u}_\delta|^2\,dx\,dt \to \int_0^\infty \beta \int_\Omega |\nabla \tilde{u}|^2\,dx\,dt
$$

with Remark 5.2. Thus, in the limit $\delta \to 0$ we obtain from (71) equation (60) which finishes the proof of the theorem.

6 From the variational principle to the equation

In this last section we derive the expression for v from the variational formulation of Theorem 5.1 which will finish the proof of Theorem 3.1.

In the following we fix an arbitrary time $T \in (0,\infty)$. For any $w \in L^2(r^3\,d\nu)$ with $\int r^2\,w\,d\nu_t = 0$ for a.a. t, $w = 0$ in a neighborhood of $r = 0$ we choose $\tilde{v} = v + \delta\,w$ in (60). For $\delta \to 0$ we obtain the first variation of (60)

$$
-\int \beta\,r^2\,u\,w\,d\nu + \int \beta\,v\,w\,r^3\,d\nu + \int \beta\,r\,w\,d\nu = 0 \tag{74}
$$

for all nonnegative $\beta \in C_0^\infty((0,\infty))$ and w as above.

For an arbitrary $w \in C_p^0$ we construct an admissible test function $\bar{w}$ for (74) via

$$
\bar{w}(x,r) := w(x,r) + f(t)\,\eta(r),
$$

where $\eta \in C_0^0((0,\infty))$ and f is determined such that $\int r^2\,\bar{w}\,d\nu_t = 0$ for all $t \in (0,\infty)$, that is

$$\int r^2\,w\,d\nu_t \;+\; f(t)\int r^2\,\eta\,d\nu_t = 0.$$

Since $w(x,\cdot)$ and η have compact support in $(0,\infty)$, (50) implies that both integrals are continuous in t. Furthermore $\int r^2\,\eta\,d\nu_t$ is positive in $[0,\infty)$ for an appropriate choice of η. Hence, f is bounded and continuous and thus, also $\bar{w}$ is bounded and continuous. Ergo we have equation (74) for $\bar{w}$ instead of w.

We want to obtain equation (74) pointwise in t. For that we observe that due to (46),(47), (48), Remark 5.2 and the embedding from $\mathring{H}^1_p$ into $L^2(\Omega)$ the mapping

$$t \mapsto \int (-r^2\,u(t) \;+\; r^3\,v(t) \;+\; r\,)\,\bar{w}\,d\nu_t$$

is in $L^2(0,T)$. Consequently there exists a set E_w of Lebesgue measure 0 such that

$$-\int r^2\,u\,\bar{w}\,d\nu_t \;+\; \int r^3\,v\,\bar{w}\,d\nu_t \;+\; \int r\,\bar{w}\,d\nu_t \;=\; 0$$

for all $t \notin E_w$. Equivalently it holds

$$-\int r^2\,u\,w\,d\nu_t \;+\; \int r^3\,v\,w\,d\nu_t + \int r\,w\,d\nu_t \;+\lambda(t)\int r^2\,w\,d\nu_t = 0 \tag{75}$$

for all $t \notin E_w$, where

$$\lambda(t) = \frac{1}{\int r^2\,\eta\,d\nu_t}\left(-\int r^2\,u\,\eta\,d\nu_t + \int r^3\,v\,\eta\,d\nu_t + \int r\,\eta\,d\nu_t\right).$$

So far the set E_w depends on w. We want to find a set E of measure zero such that (75) holds for all w as above for almost all $t \notin E$. This argument is standard: we select a countable set $\{w_i\}_i \subset C_p^0$ such that any function $w \in C_p^0$ can be approximated uniformly by a sequence $\{w_i(x,\cdot)\}_i$ such that the sequence has uniformly compact support in $(0,\infty)$. We set

$$E := \bigcup_i E_{w_i} \cup E_0,$$

where E_0 is such that

$$\int_\Omega |u(t,\cdot)|^2 dx < \infty \qquad \text{and} \qquad \int r^3 |v|^2\,d\nu_t < \infty$$

for all $t \notin E_0$ and obtain (75) for w_i. By approximation we finally obtain

$$\int \{-r^2\, u(t) \;+\; r^3\, v(t) \;+\; r \;+\; \lambda\, r^2\}\, w\, d\nu_t = 0$$

for all $w \in C_p^0$ and all $t \notin E$. This means

$$-\,r^2\, u(t) \;+\; r^3 v(t) \;+\; r \;+\; \lambda(t)\, r^2 = 0 \qquad \nu_t \text{ a.e. in } \Omega \text{ for all } t \notin E, \tag{76}$$

where

$$\int_\Omega \nabla u(t) \cdot \nabla\zeta\, dx \;+\; 4\pi \int \zeta\, r^2\, v(t)\, d\nu_t = 0.$$

If one plugs (76) into the second term one obtains

$$\int_\Omega \nabla u(t) \cdot \zeta\, dx \;+\; 4\pi \left(\int \zeta (u(t) - \lambda(t))\, r\, d\nu_t \;-\; \int \zeta\, d\nu_t \right) \;=\; 0$$

Since λ is constant in space we see that $\bar{u} := u \;-\; \lambda$ solves

$$\int_\Omega \nabla \bar{u}(t) \cdot \zeta\, dx \;+\; 4\pi \int \zeta\, \bar{u}(t)\, r\, d\nu_t = 4\pi \int \zeta\, d\nu_t$$

for almost all t which finishes the proof of Theorem 3.1.

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