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SMOOTHNESS OF THE DIFFUSION COEFFICIENTS FOR PARTICLE SYSTEMS IN CONTINUOUS SPACE

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ABSTRACT. For a class of particle systems in continuous space with local interactions, we show that the asymptotic diffusion matrix is an infinitely differentiable function of the density of particles. Our method allows us to identify relatively explicit descriptions of the derivatives of the diffusion matrix in terms of the corrector.

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KEYWORDS: interacting particle system, hydrodynamic limit, bulk diffusion matrix.

1. INTRODUCTION

We study a class of interacting particle systems with local interactions in continuous space. The models we consider are reversible with respect to the Poisson measures with constant density, uniformly elliptic, and of non-gradient type. The large-scale behavior of each model is captured by a diffusion equation governed by the *bulk diffusion matrix*. The purpose of this work is to show that this matrix is an infinitely differentiable function of the density of particles. That the bulk diffusion matrix is sufficiently regular as a function of the density of particles is a necessary ingredient in the proof of the hydrodynamic limit of the model, see for instance [10].

Similar results on the smoothness of the effective diffusion matrix have already been derived for a number of other models of particle systems [13, 7, 14, 6, 22, 19, 20, 21]. Those works all rely on the approach introduced in [13] to show the regularity of the self-diffusion matrix of a tagged particle in the symmetric simple exclusion process on \mathbb{Z}^d . This approach relies on certain duality properties of the process under consideration.

The approach we employ here seems different and more direct. In particular, we end up with relatively explicit expressions for the derivatives of the bulk diffusion matrix expressed in terms of the corrector, a natural object that already appears in the description of the bulk diffusion matrix itself.

Our method takes inspiration from works on the homogenization of elliptic equations with random coefficients [2, 1, 18, 8]. One can for instance consider a setting in which the random coefficients of the equation are a local function of a Poisson point process with constant density, and ask whether the homogenized matrix depends smoothly on the density of the point process. Perhaps surprisingly, this case has in fact not yet been addressed in the literature. Indeed, the analysis in [18] takes place in a discrete setting, while the results of [8] require that the perturbative point process has a uniformly bounded number of points in a given bounded region of space, a property that does not hold for Poisson point processes. We believe that the method used here could be adapted to the case of elliptic equations and yield the smoothness of the homogenized matrix in this case, without having to rely on fine quantitative estimates as suggested in [8, Remark 2.7]. Outside of the present paper, we are also

unaware of results concerning interacting particle systems for which the number of particles in a bounded region of space is not uniformly bounded.

Other settings in which similar problems were investigated include the $\nabla\phi$ model (a Gibbs measure modeling a fluctuating interface) [5], and non-linear elliptic equations with random coefficients [4, 3, 9]. In these contexts, the goal is to show that the homogenized coefficients depend smoothly on the slope of the limit homogenized solution. This is not a situation in which the varying parameter can be nicely encoded by random fields with short-range correlations. As a consequence, a different, more quantitative approach is then mandatory.

2. PRECISE STATEMENT OF THE MAIN RESULTS

We start by introducing some notation. We view a cloud of particles in \mathbb{R}^d as an element of $\mathcal{M}_\delta(\mathbb{R}^d)$, the space of σ -finite measures that are sums of Dirac masses on \mathbb{R}^d . The dynamics of the particles is encoded by a mapping $\mathbf{a}_\circ : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$ taking values in the space of symmetric d -by- d matrices. We assume that this mapping satisfies the following properties.

- *Uniform ellipticity*: there exists $\Lambda < \infty$ such that for every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$,

$$(2.1) \quad \text{Id} \leq \mathbf{a}_\circ(\mu) \leq \Lambda \text{Id}.$$

- *Finite range of dependence*: for every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$, we have that

$$(2.2) \quad \mathbf{a}_\circ(\mu) = \mathbf{a}_\circ(\mu \llcorner B_{1/2}),$$

where $B_{1/2}$ denotes the Euclidean ball of unit diameter centered at the origin, and \llcorner is the restriction operator defined in (3.1).

In (2.1) and throughout the paper, whenever a and b are symmetric matrices, we write $a \leq b$ to mean that $b - a$ is a positive semidefinite matrix.

Roughly speaking, we want a particle sitting at the origin and surrounded by a cloud of particles μ to undergo an instantaneous diffusion driven by the matrix $\mathbf{a}_\circ(\mu)$. We extend the mapping \mathbf{a}_\circ by stationarity by setting, for every $x \in \mathbb{R}^d$ and $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$,

$$\mathbf{a}(\mu, x) := \mathbf{a}_\circ(\tau_{-x}\mu),$$

where $\tau_{-x}\mu$ is the measure μ translated by the vector $-x$; in other words, for every Borel set U , we have $\tau_{-x}\mu(U) = \mu(x + U)$. For every $\rho_0 \geq 0$, we denote by \mathbb{P}_{ρ_0} the law of a Poisson point process over \mathbb{R}^d with constant intensity ρ_0 . We denote by \mathbb{E}_{ρ_0} the associated expectation, and use μ for the canonical random variable on this probability space. The interacting particle system we aim to study is associated with the formal Dirichlet form

$$f \mapsto \mathbb{E}_{\rho_0} \left[\int_{\mathbb{R}^d} \nabla f \cdot \mathbf{a} \nabla f \, d\mu \right].$$

We refer to (3.3) below for the definition of the gradient of a sufficiently smooth function defined on $\mathcal{M}_\delta(\mathbb{R}^d)$, and [12] for a rigorous construction of the stochastic process.

We expect the evolution of this particle system to be described by a “homogenized” or “hydrodynamic” equation over large scales. Indeed, this has been shown for discrete models similar to the continuous one studied here, see in particular [10]. In order to justify this rigorously, it is very useful to know about the regularity of the homogenized matrix, usually called the *bulk diffusion matrix*, that enters into the equation. The aim of the present work is to show that this matrix is indeed an infinitely differentiable function of the particle density.

For our purposes, it will be convenient to identify the bulk diffusion matrix as a limit of finite-volume approximations. In finite volume, there are in fact two natural approximations to the bulk diffusion matrix, based on the following subadditive quantities: for every bounded domain U , $p, q \in \mathbb{R}^d$, and $\rho_0 > 0$, we define

$$(2.3) \quad \begin{aligned} \nu(U, p, \rho_0) &:= \inf_{v \in \mathcal{H}_0^1(U)} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |U|} \int_U \frac{1}{2} (p + \nabla v) \cdot \mathbf{a}(p + \nabla v) \, d\mu \right], \\ \nu_*(U, q, \rho_0) &:= \sup_{u \in \mathcal{H}^1(U)} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |U|} \int_U \left(-\frac{1}{2} \nabla u \cdot \mathbf{a} \nabla u + q \cdot \nabla u \right) \, d\mu \right], \end{aligned}$$

where $|U|$ denotes the Lebesgue measure of U . Recall that μ is a sum of Dirac masses; for any function F , the integral $\int_U F \, d\mu = \int_U F(z) \, d\mu(z)$ therefore stands for the summation of $F(z)$ over every point z in the intersection of U and the support of μ . The precise definitions of the function spaces $\mathcal{H}^1(U)$ and $\mathcal{H}_0^1(U)$ are given in Section 3 below. Informally, the functions in $\mathcal{H}^1(U)$ are those whose squared gradient have finite integral over U ; the functions in $\mathcal{H}_0^1(U)$ must in addition respond continuously to the exit from U or the entrance into U of a particle. One can check (see [11, Proposition 4.1] or Subsection 3.3 below) that there exist symmetric d -by- d matrices $\bar{\mathbf{a}}(U, \rho_0), \bar{\mathbf{a}}_*(U, \rho_0)$ that satisfy the bound (2.1) and such that, for every $p, q \in \mathbb{R}^d$,

$$(2.4) \quad \nu(U, p, \rho_0) = \frac{1}{2} p \cdot \bar{\mathbf{a}}(U, \rho_0) p \quad \text{and} \quad \nu_*(U, q, \rho_0) = \frac{1}{2} q \cdot \bar{\mathbf{a}}_*^{-1}(U, \rho_0) q.$$

For every $m \in \mathbb{N}$, we denote by $\square_m := (-3^m/2, 3^m/2)^d$ the cube of side-length 3^m centered at the origin. We also have that the sequence $(\bar{\mathbf{a}}(\square_m, \rho_0))_{m \in \mathbb{N}}$ is decreasing, and the sequence $(\bar{\mathbf{a}}_*(\square_m, \rho_0))_{m \in \mathbb{N}}$ is increasing. We define the bulk diffusion matrix as the limit of the latter sequence:

$$(2.5) \quad \bar{\mathbf{a}}(\rho_0) := \lim_{m \rightarrow \infty} \bar{\mathbf{a}}_*(\square_m, \rho_0).$$

It was shown in [11] that the sequence $(\bar{\mathbf{a}}(\square_m, \rho_0))_{m \in \mathbb{N}}$ converges to the same limit, and moreover, that there exists an exponent $\alpha > 0$ and a constant $C < \infty$ such that for every $m \geq 1$,

$$(2.6) \quad |\bar{\mathbf{a}}(\square_m, \rho_0) - \bar{\mathbf{a}}(\rho_0)| + |\bar{\mathbf{a}}_*(\square_m, \rho_0) - \bar{\mathbf{a}}(\rho_0)| \leq C 3^{-\alpha m}.$$

The results of the present paper do not rely on this quantitative information. Indeed, to show our main results, we only appeal to (2.5) as the definition of the limit diffusion matrix. This definition coincides with the more classical one based on full-space stationary correctors, as explained in [11, Appendix B].

Throughout the paper, we fix $q \in \mathbb{R}^d$, and denote by $\psi_m \in \mathcal{H}^1(\square_m)$ the optimizer in the definition of $\nu_*(\square_m, q, \rho_0)$, see (2.3). The optimizer for $\nu_*(\square_m, q, \rho_0)$ is unique provided that we impose the condition in (3.9) (the formulas derived throughout the paper only involve gradients of ψ_m , and are therefore insensitive to the precise way we “fix the constants”).

For reasons that will be clarified below, we prefer to work with ψ_m , which optimizes some ν_* quantity, rather than with the corresponding optimizer for ν . One consequence of this choice is that we have easier access to information about the smoothness of the mapping $\rho \mapsto \bar{\mathbf{a}}^{-1}(\rho)$ than of the mapping $\rho \mapsto \bar{\mathbf{a}}(\rho)$. Of course, since these matrices are uniformly elliptic in the sense of (2.1), discussing the smoothness of one or the other is equivalent (and from a physical perspective, it is no less natural to focus on “fixing the average flux at q ” than to focus on “fixing the average gradient at p ”).

For clarity of exposition, we will first present a proof that the mapping $\rho \mapsto \bar{\mathbf{a}}^{-1}(\rho)$ is $C^{1,1}$. The precise statement is as follows.

Theorem 2.1 ($C^{1,1}$ regularity). *The following limit is well-defined and finite*

$$(2.7) \quad c_1(\rho_0) := \lim_{m \rightarrow \infty} \int_{\mathbb{R}^d} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\{1\}} d\mu \right] dx_1,$$

where we write $\mathbf{a}^{\{1\}}(\mu, z, x_1) := \mathbf{a}(\mu + \delta_{x_1}, z)$ and $\nabla \psi_m^{\{1\}}(\mu, z, x_1) := \nabla \psi_m(\mu + \delta_{x_1}, z)$. Moreover, as $\rho \in \mathbb{R}$ tends to zero, we have

$$(2.8) \quad q \cdot \bar{\mathbf{a}}^{-1}(\rho_0 + \rho)q = q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q + \rho c_1(\rho_0) + O(\rho^2).$$

The term $O(\rho^2)$ hides a multiplicative constant that depends only on d , Λ and $|q|$ (but not on ρ_0).

Remark 2.2. Theorem 2.1 yields that $q \cdot \bar{\mathbf{a}}^{-1}(\cdot)q$ is $C^{1,1}$. Indeed, an immediate consequence of expansion (2.8) is that $c_1(\cdot)$ is the derivative of $q \cdot \bar{\mathbf{a}}^{-1}(\cdot)q$. Moreover, using (2.8) around ρ_0 and $\rho_0 + \rho$, we see that $c_1(\rho_0 + \rho) = c_1(\rho_0) + O(\rho)$, i.e. that c_1 is Lipschitz continuous.

A more explicit writing of the right side of (2.7) is:

$$\int_{\mathbb{R}^d} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m(\mu, z) \cdot (\mathbf{a}(\mu, z) - \mathbf{a}(\mu + \delta_{x_1}, z)) \nabla \psi_m(\mu + \delta_{x_1}, z) d\mu(z) \right] dx_1.$$

In general, we use superscripts to indicate changes in the “measure” argument of the function under consideration: for instance, the quantity $\mathbf{a}^{\{1\}}$ is obtained from \mathbf{a} by replacing the argument μ with $\mu + \delta_{x_1}$.

In order to describe higher-order derivatives, we need to generalize this notation to arbitrary subsets of indices. For every finite subset $E \subseteq \mathbb{N}_+$ and f an arbitrary function of the measure μ , we define

$$(2.9) \quad f^E : (\mu, (x_i)_{i \in E}) \mapsto f(\mu + \sum_{i \in E} \delta_{x_i}).$$

For every $i \in \mathbb{N}_+$, we also write

$$(2.10) \quad D_i f := f^{\{i\}} - f.$$

Notice that for every $i \neq j \in \mathbb{N}_+$, we have

$$D_i D_j f = (f^{\{j\}} - f)^{\{i\}} - (f^{\{i\}} - f) = f^{\{i,j\}} - f^{\{i\}} - f^{\{j\}} + f.$$

In particular, the operators D_i and D_j commute. We can therefore define, for every $E = \{i_1, \dots, i_p\} \subseteq \mathbb{N}_+$, the quantity

$$(2.11) \quad D_E f := D_{i_1} \cdots D_{i_p} f.$$

Finally, we need at times to apply these operators to more complex expressions such as $f + g$, where f and g are two functions of the measure μ , with the understanding that the operator applies only to f and not to g . We use the superscript $\#$ to indicate the functions on which these operators are meant to be applied, keeping the others “frozen”. That is, we write for instance

$$(f^\# + g)^E = f^E + g, \quad (f^\# g)^E = f^E g,$$

and similarly with more complex expressions. We also have

$$D_E(f^\# + g) = \begin{cases} f + g, & \text{if } E = \emptyset, \\ D_E f, & \text{if } E \neq \emptyset, \end{cases} \quad D_E(f^\# g) = (D_E f)g.$$

We use the notation $[[1, k]] := \{1, 2, \dots, k\}$. Here is our main result.

Theorem 2.3 (Smoothness). *For each $k \in \mathbb{N}_+$, the limit*

$$(2.12) \quad c_k(\rho_0) := \lim_{m \rightarrow \infty} \int_{(\mathbb{R}^d)^k} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_{[[1,k]]} ((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) d\mu \right] dx_1 \cdots dx_k,$$

is well-defined and finite. Moreover, as $\rho \in \mathbb{R}$ tends to zero, we have

$$(2.13) \quad q \cdot \bar{\mathbf{a}}^{-1}(\rho_0 + \rho)q = q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q + \sum_{\ell=1}^k c_\ell(\rho_0) \frac{\rho^\ell}{\ell!} + O(\rho^{k+1}).$$

The term $O(\rho^{k+1})$ hides a multiplicative constant that depends only on d , Λ , k , and $|q|$ (but not on ρ_0). In particular, the mapping $\rho_0 \mapsto q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q$ is infinitely differentiable, with ℓ -th derivative given by $c_\ell(\rho_0)$ for every $\ell \in \mathbb{N}_+$.

Note that due to the local nature of the term $(\mathbf{a} - \mathbf{a}^\#)$, see (2.2), the integrals in (2.7) and (2.12) are in fact finite-volume quantities, as the outermost integrals may be replaced by, for instance, $\int_{\square_{m+1}}$ and $\int_{(\square_{m+1})^k}$, respectively.

We also remark that the proof in fact shows that uniformly over ρ_0 , the derivatives $c_k(\rho_0)$ are bounded by some constant $C_k(\Lambda, d)$ depending only on Λ and the dimension, and a careful inspection of the proof yields that $C_k \lesssim (k!)^2$ (see in particular Subsection 5.5 for more on this matter). Finally, we also show in Section 6 that the convergence in (2.12) is locally uniform in ρ_0 . We do not know how to show that $\bar{\mathbf{a}}$ is an analytic function of the density of particles.

We now comment on the reason why we choose to work with quantities derived from ν_* rather than ν . Recall that the function ψ_m is the optimizer in the definition (2.3) of $\nu_*(\square_m, q, \rho_0)$. This object may seem to depend upon the choice of the particle density ρ_0 . However, it is in fact not the case. Indeed, the optimization problem for ν_* can be split into a sum of unrelated optimization problems, one for each fixed number of particles in \square_m . The optimizer for ν_* is thus a superposition of these optimizers, irrespectively of the underlying density of the measure. We refer to Section 3 below for a more detailed discussion of this property. The fact that we can view the same object ψ_m as the optimizer of $\nu_*(\square_m, q, \rho_0)$ for arbitrary values of ρ_0 would not be valid were we to work with the optimizers of $\nu(\square_m, p, \rho_0)$.

The remainder of the paper is organized as follows. We discuss function spaces more precisely in Section 3, and prove a technically useful lemma stating that the quantity ν_* does not change if the particles become distinguishable. We then show Theorem 2.1 in Section 4. The more general Theorem 2.3 is then proved in Section 5. Finally, in Section 6, we show that the mappings $\rho_0 \mapsto \bar{\mathbf{a}}(\square_m, \rho_0)$ and $\rho_0 \mapsto \bar{\mathbf{a}}_*(\square_m, \rho_0)$ converge to $\rho_0 \mapsto \bar{\mathbf{a}}(\rho_0)$ locally uniformly, and that this is also the case for the convergence in (2.12) towards the higher-order derivatives of $\bar{\mathbf{a}}(\rho_0)$.

3. SETTING AND FUNCTIONAL FRAMEWORK

In this section, we rigorously introduce the notation and functional framework that we use in this paper. In particular, we define the function spaces $\mathcal{H}^1(\square_m)$ and $\mathcal{H}_0^1(\square_m)$ that appear in the optimization problems ν and ν_* in (2.3). This will also allow us to justify why, as mentioned in the previous section, we will prove the main results of this paper by mainly working with the quantity ν_* instead of ν .

3.1. Configuration space. We denote by \mathbb{R}^d the standard Euclidean space, by $Q_s := (-s/2, s/2)^d$ the open hypercube of side length $s > 0$, and we write $\square_m := Q_{3^m}$ for $m \in \mathbb{N}$. We also use \square as a shorthand notation for the unit cube \square_0 .

We recall that $\mathcal{M}_\delta(\mathbb{R}^d)$ is the space of σ -finite measures that are sums of Dirac masses on \mathbb{R}^d , which we think of as the configuration space of particles, and that \mathbb{P}_{ρ_0} corresponds to the probability measure for the Poisson point process having constant density $\rho_0 > 0$. We write \mathbb{E}_{ρ_0} for the expectation with respect to \mathbb{P}_{ρ_0} . For a Borel set $U \subseteq \mathbb{R}^d$, we denote by \mathcal{F}_U the σ -algebra generated by the mappings $\mu \mapsto \mu(V)$, for all Borel sets $V \subseteq U$, completed with all the \mathbb{P}_{ρ_0} -null sets. We use the notation \mathcal{F} for $\mathcal{F}_{\mathbb{R}^d}$. With this construction, assumption (2.2) yields that the random matrix $\mathbf{a}_\circ : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$ is an $\mathcal{F}_{B_{1/2}}$ -measurable mapping.

3.2. Function spaces. We now introduce several function spaces on $\mathcal{M}_\delta(\mathbb{R}^d)$ that will be used in this paper. In particular, we will give the rigorous definition of $\mathcal{H}^1(U)$ and $\mathcal{H}_0^1(U)$.

We start with basic considerations concerning \mathcal{F} -measurable functions on $\mathcal{M}_\delta(\mathbb{R}^d)$. Given a Borel set $U \subseteq \mathbb{R}^d$, it is often useful to decompose an \mathcal{F} -measurable function into a series of Borel-measurable functions on Euclidean spaces, conditioned on the number of particles in U and the configuration outside U . More precisely, we denote by \mathcal{B}_U the set of Borel subsets of U . For every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$, we denote by $\mu \llcorner U \in \mathcal{M}_\delta(\mathbb{R}^d)$ the measure such that, for every Borel set $V \subseteq \mathbb{R}^d$,

$$(3.1) \quad (\mu \llcorner U)(V) = \mu(U \cap V).$$

Then for $f : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$ which is \mathcal{F} -measurable, we define

$$(3.2) \quad f_n(\cdot, \mu \llcorner U^c) : \begin{cases} U^n & \rightarrow \mathbb{R} \\ (x_1, \dots, x_n) & \mapsto f(\sum_{i=1}^n \delta_{x_i} + \mu \llcorner U^c). \end{cases}$$

The function f_n is $\mathcal{B}_U^{\otimes n} \otimes \mathcal{F}_{U^c}$ -measurable. Reciprocally, given a series of permutation-invariant functions with such measurability properties, we can reconstruct an \mathcal{F} -measurable function f by specifying that, on the event $\mu \llcorner U = \sum_{i=1}^n \delta_{x_i}$, we have $f(\mu) := f_n(x_1, \dots, x_n, \mu \llcorner U^c)$. We call the mapping $f \mapsto (f_n)_{n \in \mathbb{N}}$ the “canonical projection”, and refer to [11, Lemmas 2.2 and A.1] for more details.

We now explain the notion of derivatives for functions defined on $\mathcal{M}_\delta(\mathbb{R}^d)$. For every sufficiently smooth function $f : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$, $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$, and $x \in \text{supp } \mu$, the gradient $\nabla f(\mu, x)$ is such that, for every $k \in \{1, \dots, d\}$,

$$(3.3) \quad \mathbf{e}_k \cdot \nabla f(\mu, x) = \lim_{h \rightarrow 0} \frac{f(\mu - \delta_x + \delta_{x+h\mathbf{e}_k}) - f(\mu)}{h},$$

where $(\mathbf{e}_1, \dots, \mathbf{e}_d)$ is the canonical basis of \mathbb{R}^d . While we wish to emphasize that the function $\nabla f(\mu, \cdot)$ is naturally defined only on $\text{supp } \mu$, we extend it for convenience as

$$(3.4) \quad \text{for every } x \notin \text{supp } \mu, \quad \nabla f(\mu, x) := 0.$$

To clarify the notion of smooth functions appearing in the previous paragraph, we can appeal to the canonical projections discussed above. For every bounded open set $U \subseteq \mathbb{R}^d$, we define the sets of smooth functions $\mathcal{C}^\infty(U)$ and $\mathcal{C}_c^\infty(U)$ in the following way. We have that $f \in \mathcal{C}^\infty(U)$ if and only if f is an \mathcal{F} -measurable function, and for every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$ and $n \in \mathbb{N}$, the function $f_n(\cdot, \mu \llcorner U^c)$ appearing in (3.2) is infinitely differentiable on U^n . The space $\mathcal{C}_c^\infty(U)$ is the subspace of $\mathcal{C}^\infty(U)$ of functions that are \mathcal{F}_K -measurable for some compact set $K \subseteq U$.

We define \mathcal{L}^2 to be the space of \mathcal{F} -measurable functions f such that $\mathbb{E}_{\rho_0}[f^2]$ is finite. As usual, elements in this function space that coincide \mathbb{P}_{ρ_0} -almost surely are identified. We now define $\mathcal{H}^1(U)$ as the infinite-dimensional analogue of the classical Sobolev space H^1 : for every $f \in \mathcal{C}^\infty(U)$, we introduce the norm

$$(3.5) \quad \|f\|_{\mathcal{H}^1(U)} = \left(\mathbb{E}_{\rho_0}[f^2(\mu)] + \mathbb{E}_{\rho_0} \left[\int_U |\nabla f(\mu, x)|^2 d\mu(x) \right] \right)^{\frac{1}{2}},$$

and set

$$(3.6) \quad \begin{aligned} \mathcal{H}^1(U) &:= \overline{\{f \in \mathcal{C}^\infty(U) : \|f\|_{\mathcal{H}^1(U)} < +\infty\}}^{\|\cdot\|_{\mathcal{H}^1(U)}}, \\ \mathcal{H}_0^1(U) &:= \overline{\{f \in \mathcal{C}_c^\infty(U) : \|f\|_{\mathcal{H}^1(U)} < +\infty\}}^{\|\cdot\|_{\mathcal{H}^1(U)}}, \end{aligned}$$

namely the completion, under $\|\cdot\|_{\mathcal{H}^1(U)}$, of the sets of functions in $\mathcal{C}^\infty(U)$ or $\mathcal{C}_c^\infty(U)$ that have finite norm $\|\cdot\|_{\mathcal{H}^1(U)}$. As for classical Sobolev spaces, for every $f \in \mathcal{H}^1(U)$, we can interpret $\nabla f(\mu, x)$ when $x \in U \cap \text{supp } \mu$ in a weak sense. This may be understood via the canonical projection in (3.2).

The two spaces $\mathcal{H}^1(U)$ and $\mathcal{H}_0^1(U)$ share many similarities as well as some fundamental differences. The latter ones, in turn, derive from the differences between $\mathcal{C}^\infty(U)$ and $\mathcal{C}_c^\infty(U)$: On the one hand, functions in $\mathcal{C}^\infty(U)$ do depend on $\mu \ll U^c$ and the number of particles $\mu(U)$ in a relatively arbitrary (measurable) way. On the other hand, functions in the subset $\mathcal{C}_c^\infty(U)$ are \mathcal{F}_U -measurable as they do not depend on particles that cross the boundary ∂U .

When managing elements in $\mathcal{H}^1(U)$ or $\mathcal{H}_0^1(U)$, it is at times useful to think about them in terms of their canonical projection defined in (3.2): Let $f \in \mathcal{H}^1(U)$ and let $(f_n)_{n \in \mathbb{N}}$ be the associated canonical projection. Then for \mathbb{P}_{ρ_0} -almost every $\mu \ll U^c$ and every $n \in \mathbb{N}$, we have that

- The function $f_n(\cdot, \mu \ll U^c)$ belongs to the (standard) Sobolev space $H^1(U^n)$;
- The function $f_n(\cdot, \mu \ll U^c)$ is invariant under permutations: if S_n denotes the set of permutations of $\llbracket 1, n \rrbracket$ and we write $(x_1, \dots, x_n) \in U^n$, then for every $\sigma \in S_n$ it holds

$$(3.7) \quad f_n(x_1, \dots, x_n, \mu \ll U^c) = f_n(x_{\sigma(1)}, \dots, x_{\sigma(n)}, \mu \ll U^c) \quad \text{almost everywhere in } U^n.$$

If $f \in \mathcal{H}_0^1(U)$, then the canonical partition needs to satisfy the following additional “compatibility condition”: for every $n \in \mathbb{N}_+$ and on the set $\{(x_1, \dots, x_n) \in U^n : x_1 \in \partial U\}$, it holds

$$(3.8) \quad f_n(x_1, \dots, x_n, \mu \ll U^c) = f_{n-1}(x_2, \dots, x_n, \mu \ll U^c),$$

where the identity is to be understood in the sense of traces. Note that, by the invariance under permutations, the above property also holds if x_1 is replaced by any other coordinate x_i , $i = 2, \dots, n$. Moreover, for every $f \in \mathcal{H}_0^1(U)$ and $n \in \mathbb{N}$, we have that $f_n(\cdot, \mu \ll U^c)$ in fact does not depend on $\mu \ll U^c$.

We summarize the previous remarks in Table 3.1.

3.3. Elementary properties of optimizers. As seen in the previous subsection, the spaces \mathcal{H}^1 and \mathcal{H}_0^1 differ in important ways, and this will translate into differences for the optimizers of ν and ν_* . In fact, except in part of Section 6, we will only rely on quantities derived from ν_* . In this subsection, we present some key properties of optimizers of this quantity, and highlight those that would not be shared by the optimizers of ν .

Function space	H^1 -regularity for particles in U	Compatibility condition when particles cross ∂U	\mathcal{F}_U -measurable	For every open set $V \subseteq U$
$\mathcal{H}^1(U)$	Yes	No	No	$\mathcal{H}^1(U) \subseteq \mathcal{H}^1(V)$
$\mathcal{H}_0^1(U)$	Yes	Yes	Yes	$\mathcal{H}_0^1(V) \subseteq \mathcal{H}_0^1(U)$

TABLE 3.1. Differences between $\mathcal{H}^1(U)$ and $\mathcal{H}_0^1(U)$.

For U a Lipschitz domain and $q \in \mathbb{R}^d$, we denote by $\psi_{U,q} \in \mathcal{H}^1(U)$ the maximizer in the definition of $\nu_*(U, q, \rho_0)$. By [11, Proposition 4.1] (see also Lemma 3.1 below), this optimizer exists, and is unique provided we also impose that

$$(3.9) \quad \mathbb{E}[\psi_{U,q} \mid \mu(U), \mu \llcorner U^c] = 0.$$

This optimizer is $\mathcal{F}_{B_{1/2}(U)}$ -measurable, with $B_{1/2}(U) = \{x \in \mathbb{R}^d : \text{dist}(x, U) < \frac{1}{2}\}$. Since $q \mapsto \psi_{U,q}$ is a linear mapping, there exists a matrix $\bar{\mathbf{a}}_*(U, \rho_0)$ such that

$$\nu_*(U, q, \rho_0) = \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|U|} \int_U \left(-\frac{1}{2} \nabla \psi_{U,q} \cdot \mathbf{a} \nabla \psi_{U,q} + q \cdot \nabla \psi_{U,q} \right) d\mu \right] = \frac{1}{2} q \cdot \bar{\mathbf{a}}_*^{-1}(U, \rho_0) q.$$

The uniform ellipticity assumption (2.1) readily implies that $\text{Id} \leq \bar{\mathbf{a}}_*(U, \rho_0) \leq \Lambda \text{Id}$. By the first variation, we have for every $u \in \mathcal{H}^1(U)$ that

$$(3.10) \quad \mathbb{E}_{\rho_0} \left[\int_U (-\nabla \psi_{U,q} \cdot \mathbf{a} \nabla u + q \cdot \nabla u) d\mu \right] = 0.$$

Using this with $u = \psi_{U,q}$, we get that

$$(3.11) \quad \begin{aligned} q \cdot \bar{\mathbf{a}}_*^{-1}(U, \rho_0) q &= \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|U|} \int_U \nabla \psi_{U,q} \cdot \mathbf{a} \nabla \psi_{U,q} d\mu \right] \\ &= \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|U|} \int_U q \cdot \nabla \psi_{U,q} d\mu \right]. \end{aligned}$$

In particular, using the uniform ellipticity assumption once more, we obtain the basic Dirichlet energy estimate

$$(3.12) \quad \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|U|} \int_U |\nabla \psi_{U,q}|^2 d\mu \right] \leq |q|^2.$$

Similar properties are also valid for optimizers of ν , and we refer to [11, Proposition 4.1] for details. Optimizers of ν_* differ however in one crucial aspect: denoting by $(\psi_{U,q,n})_{n \in \mathbb{N}}$ the canonical projection of $\psi_{U,q}$, see (3.2), we can identify each $\psi_{U,q,n}(\cdot, \mu \llcorner U^c)$ as the solution to an elliptic equation. In particular, the function $\psi_{U,q}$, which was defined as the optimizer in the definition of $\nu_*(U, q, \rho_0)$, *in fact does not depend on ρ_0* . This property would not be valid for optimizers of ν .

In order to clarify this, we introduce the following notation: for each $n \in \mathbb{N}$, $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$, and $u \in H^1(U^n)$, we write

$$(3.13) \quad \begin{aligned} &\mathcal{J}_n(u, U, q, \mu \llcorner U^c) \\ &:= \frac{1}{\rho_0|U|} \int_{U^n} \sum_{i=1}^n \left(-\frac{1}{2} \nabla_{x_i} u \cdot \mathbf{a} \left(\sum_{i=1}^n \delta_{x_i} + \mu \llcorner U^c, x_i \right) \nabla_{x_i} u + q \cdot \nabla_{x_i} u \right) dx_1 \cdots dx_n. \end{aligned}$$

This quantity corresponds to the functional that is optimized in the definition of ν_* , see (2.3), but where we have conditioned on $\mu(U) = n$ and $\mu \llcorner U^c$; and where moreover,

we substituted an arbitrary $u \in H^1(U^n)$ in place of the canonical projection u_n of some function $u \in \mathcal{H}^1(U)$. We thus have

$$(3.14) \quad \begin{aligned} \nu_*(U, q, \rho_0) &= \sup_{u \in \mathcal{H}^1(U)} \mathbb{E}_{\rho_0} \left[\sum_{n \in \mathbb{N}} \mathbb{P}_{\rho_0} [\mu(U) = n] \mathcal{J}_n(u_n(\cdot, \mu \llcorner U^c), U, q, \mu \llcorner U^c) \right] \\ &\leq \mathbb{E}_{\rho_0} \left[\sum_{n \in \mathbb{N}} \mathbb{P}_{\rho_0} [\mu(U) = n] \sup_{u \in H^1(U^n)} \mathcal{J}_n(u, U, q, \mu \llcorner U^c) \right]. \end{aligned}$$

The next lemma implies that the inequality above is in fact an equality. Recall that we denote by $(\psi_{U,q,n})_{n \in \mathbb{N}}$ the canonical projection of $\psi_{U,q}$, the optimizer of $\nu_*(U, q, \rho_0)$.

Lemma 3.1. *For every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$ and $n \in \mathbb{N}$, let $u_{U,q,n}(\cdot, \mu \llcorner U^c) \in H^1(U^n)$ be the unique maximizer of the functional $\mathcal{J}_n(\cdot, U, q, \mu \llcorner U^c)$ subject to the constraint $\int_{U^n} u_{U,q,n}(\cdot, \mu \llcorner U^c) = 0$. For \mathbb{P}_{ρ_0} -almost every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$ and every $n \in \mathbb{N}$, we have*

$$(3.15) \quad u_{U,q,n}(\cdot, \mu \llcorner U^c) = \psi_{U,q,n}(\cdot, \mu \llcorner U^c).$$

Remark 3.2. The quantities $u_{U,q,n}(\cdot, \mu \llcorner U^c)$ and $\psi_{U,q,n}(\cdot, \mu \llcorner U^c)$ in fact only depend on the restriction of $\mu \llcorner U^c$ to the set of points that are at distance at most $1/2$ from U , by the finite-range dependence assumption (2.2). The statement that (3.15) holds for \mathbb{P}_{ρ_0} -almost every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$ therefore does not depend on $\rho_0 > 0$. We are forced to state (3.15) only for \mathbb{P}_{ρ_0} -almost every μ since a priori we only know that $\psi_{U,q,n}(\cdot, \mu \llcorner U^c)$ is well-defined for \mathbb{P}_{ρ_0} -almost every μ ; but the lemma itself provides us with a straightforward way to extend the definition to every $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$. In the proof below, we observe that there exists a function $u_{U,q} \in \mathcal{H}^1(U)$ whose canonical projection is $(u_{U,q,n})_{n \in \mathbb{N}}$, and then show that $u_{U,q} = \psi_{U,q}$.

Proof of Lemma 3.1. We first observe that, for each $\mu \in \mathcal{M}_\delta(\mathbb{R}^d)$, the function $u_{U,q,n}(\cdot, \mu \llcorner U^c)$ is invariant under permutation of its coordinates. This is immediate from the facts that $\mathcal{J}_n(\cdot, U, q, \mu \llcorner U^c)$ admits a unique mean-zero maximizer, and that this functional as well as the mean-zero constraint are invariant under permutations.

We now define the function $u_{U,q} : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$ in such a way that, on the event that $\mu \llcorner U = \sum_{i=1}^n \delta_{x_i}$, we have

$$u_{U,q}(\mu) := u_{U,q,n}(x_1, \dots, x_n, \mu \llcorner U^c).$$

This definition makes sense since we have verified that $u_{U,q,n}(\cdot, \mu \llcorner U^c)$ is invariant under permutation of its coordinates. It is also clear that the canonical projection of the function $u_{U,q}$ is the family of functions $(u_{U,q,n})_{n \in \mathbb{N}}$ (so the notation is sound).

We now argue that $u_{U,q} \in \mathcal{H}^1(\square_m)$, and by the uniqueness of the optimizer for ν_* and (3.14), this will imply that $u_{U,q} = \psi_{U,q}$, as desired. Let now $\mu \llcorner U^c$ be fixed. By construction, each function $u_{U,q,n}(\cdot, \mu \llcorner U^c)$ satisfies, for every $v \in H^1(U^n)$, the variational identity

$$\int_{U^n} \sum_{i=1}^n \left(\nabla_{x_i} u_{U,q,n}(\cdot, \mu \llcorner U^c) \cdot \mathbf{a} \left(\sum_{i=1}^n \delta_{x_i} + \mu \llcorner U^c, x_i \right) \nabla_{x_i} v - q \cdot \nabla_{x_i} v \right) dx_1 \cdots dx_n = 0.$$

Choosing $v = u_{U,q,n}(\cdot, \mu \llcorner U^c)$ and using (2.1) and Young's inequality, we infer that

$$(3.16) \quad \frac{1}{n} \sum_{i=1}^n \int_{U^n} |\nabla_{x_i} u_{U,q,n}(\cdot, \mu \llcorner U^c)|^2 \leq |q|^2.$$

Moreover, since $u_{U,q,n}(\cdot, \mu \llcorner U^c)$ has zero-average on U^n , we may apply Poincaré's inequality in the product domain U^n (see for instance [17] or [11, Proposition 3.1])

and obtain that there exists a constant $C(U) < +\infty$ such that

$$(3.17) \quad \int_{U^n} |u_{U,q,n}(\cdot, \mu \llcorner U^c)|^2 \leq C \sum_{i=1}^n \int_{U^n} |\nabla_{x_i} u_{U,q,n}(\cdot, \mu \llcorner U^c)|^2 \stackrel{(3.16)}{\leq} Cn|q|^2.$$

Estimates (3.16) and (3.17) and the definition of $\mathbb{E}_{\rho_0}[\cdot]$ immediately imply that $u_{u,q} \in \mathcal{H}^1(U)$. This concludes the proof of Lemma 3.1. \square

As announced, Lemma 3.1 demonstrates that the optimizer for $\nu_*(U, q, \rho_0)$ in fact does not depend on ρ_0 : regardless of the density, it is always the same $\psi_{U,q}$ whose canonical projections are described by this lemma. The only difference is that optimizers for $\nu_*(U, q, \cdot)$ at different densities receive point processes with different densities as their argument.

We also stress that another immediate consequence of Lemma 3.1, see also (3.16), is that each maximizer $\psi_{U,q}$ satisfies the following improved energy inequality:

$$(3.18) \quad \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|U|} \int_U |\nabla \psi_{U,q}|^2 d\mu \middle| \mu(U), \mu \llcorner U^c \right] \leq |q|^2 \frac{\mu(U)}{\rho_0|U|},$$

for every $\mu \llcorner U^c$ and number of particles $\mu(U) \in \mathbb{N}$ fixed. Note that this inequality implies (3.12).

In most of the paper, we keep the parameter q fixed, and work with the domain $U = \square_m$. We recall the notation $\psi_m := \psi_{\square_m, q}$.

3.4. Coupling of point processes. When studying the regularity of the bulk diffusion matrix, it is useful to introduce a coupling between different densities. Recall that we keep $\rho_0 \in (0, \infty)$ fixed, and let $\mu \sim \text{Poisson}(\rho_0)$ be the “reference” Poisson point process, with constant density ρ_0 . For $\rho \geq 0$, we define another independent Poisson point process $\mu_\rho \sim \text{Poisson}(\rho)$, which we think of as a small perturbation. Then we denote by $\mathbb{P} = \mathbb{P}_{\rho_0} \otimes \mathbb{P}_\rho$ the joint probability measure, with associated expectation \mathbb{E} , and we observe that $\mu + \mu_\rho \sim \text{Poisson}(\rho_0 + \rho)$, by the superposition property for independent Poisson point processes.

Notice that the definition of the space \mathcal{H}^1 actually depends on the density of particles, although this was kept implicit in the notation. When we want to resolve the ambiguity, we write $\mathcal{H}^1(U, \mu)$ for the space as defined in (3.5), and we write $\mathcal{H}^1(U, \mu + \mu_\rho)$ for the same space but with density $(\rho_0 + \rho)$. In line with the notation introduced in (2.9), we use a superscript ρ to indicate when the measure argument of a function is taken to be $\mu + \mu_\rho$. For instance, when we write \mathbf{a}^ρ in some expression, we always understand that it is evaluated as $\mathbf{a}(\mu + \mu_\rho, \cdot)$; the notation \mathbf{a} is understood to be evaluated at μ instead. The same convention applies as well to ψ_m and ψ_m^ρ : the former represents $\psi_m(\mu)$ and the latter $\psi_m(\mu + \mu_\rho)$. As discussed in the previous subsection, the function ψ_m^ρ can be interpreted as the optimizer of $\nu_*(\square_m, q, \rho_0 + \rho)$. This notation allows us to write, for instance,

$$\nu_*(\square_m, q, \rho_0 + \rho) = \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} \left(-\frac{1}{2} \nabla \psi_m^\rho \cdot \mathbf{a}^\rho \nabla \psi_m^\rho + q \cdot \nabla \psi_m^\rho \right) d(\mu + \mu_\rho) \right].$$

We can also define a quantity ν_* perturbed by adding a finite number of particles uniformly. We denote by $E \subseteq \mathbb{N}_+$ the index set, and write $\mu_E := \sum_{i \in E} \delta_{x_i}$. Throughout the paper we use the following compact notation for the integration with respect to the particles in E :

$$(3.19) \quad \int_{U^E} (\cdots) := \int_{U^{|E|}} (\cdots) \prod_{i \in E} dx_i, \quad \int_{U^E} (\cdots) := \frac{1}{|U|^{|E|}} \int_{U^{|E|}} (\cdots) \prod_{i \in E} dx_i,$$

with the understanding that, if $E = \emptyset$, then $f_{U\emptyset}(\cdots) = (\cdots)$.

We define the function space $\mathcal{H}^1(U, \mu + \mu_E)$ as the completion in $\mathcal{H}^1(U, \mu + \mu_E)$ of the space of functions in $\mathcal{C}^\infty(U)$ such that the norm

$$\|f\|_{\mathcal{H}^1(U, \mu + \mu_E)}^2 := \int_{U^E} \left(\mathbb{E}_{\rho_0} [f^2(\mu + \mu_E)] + \mathbb{E}_{\rho_0} \left[\int_U |\nabla f(\mu + \mu_E, x)|^2 d(\mu + \mu_E)(x) \right] \right),$$

is finite. Similarly to the notation \mathbf{a}^ρ discussed above, we use the shorthand notation \mathbf{a}^E to denote the function $\mathbf{a}(\mu + \mu_E, \cdot)$. The dual problem $\nu_*^E(\square_m, q, \rho_0)$ is defined as

$$(3.20) \quad \nu_*^E(\square_m, q, \rho_0) := \sup_{u \in \mathcal{H}^1(\square_m, \mu + \mu_E)} \int_{(\square_m)^E} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(-\frac{1}{2} \nabla u \cdot \mathbf{a}^E \nabla u + q \cdot \nabla u \right) d(\mu + \mu_E) \right],$$

and we denote its optimizer by ψ_m^E . Similarly to what was discussed for ψ_m^ρ in the previous subsection, we have that ψ_m^E coincides with the function $\psi_m(\mu + \mu_E)$, and we can always think of the superscript E as indicating the operation of adding μ_E to the argument of the function, see (2.9).

We have built the configuration space in order to capture the notion of indistinguishable particles: if we exchange the positions of two particles, the measure does not change. However, when perturbing the measure μ with the addition of μ_ρ (or μ_E), the setting naturally introduces some amount of distinguishability between particles, as some come from the measure μ and some from the measure μ_ρ (or μ_E). Lemma 3.1 has clarified in particular that “nothing is gained” in the optimization problem if we allow the particles to be distinguishable. We now “project” this statement into a form in which, roughly speaking, we can only distinguish from which measure (such as μ , μ_ρ or μ_E) a particle “comes”.

Proposition 3.3. *For all finite sets $E, F \subseteq \mathbb{N}_+$, we have that*

$$(3.21) \quad \int_{(\square_{m+1})^{E \cup F}} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d\mu \right] = 0,$$

$$(3.22) \quad \int_{(\square_{m+1})^{E \cup F}} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^F \cdot \mathbf{a}^{\rho, E} \nabla \psi_m^{\rho, E} - \nabla \psi_m^F \cdot q) d\mu \right] = 0.$$

Before turning to the proof, we point out some possibly surprising features of this result. First, as pointed out above, these relations differ from (3.10) in that the test functions can distinguish between different types of particles: for instance, the function ψ_m^F depends only on $\mu + \mu^F$, and cannot be thought of as a function of $\mu + \mu^\rho + \mu^E$, as one might hope at first. Second, the integration of the additional particles indexed by $E \cup F$ is carried over the larger domain \square_{m+1} , instead of the domain \square_m that one might expect. And finally, we integrate over μ only, while one might at first expect (3.21) and (3.22) to be integrated against $\mu + \mu^E$ and $\mu + \mu^\rho + \mu^E$ respectively. The proof below will need to address each of these aspects. The particular form of (3.21) and (3.22) we have chosen here will turn out to be the most convenient later on: for instance, we will often need to study linear combinations of ψ_m^E 's for different sets E , and it is most convenient that the measure against which we integrate does not depend on E . Similarly, when we study the effect of a change in the density, some additional particles that fall in a layer around \square_m will need to be taken into account, and it is more convenient that (3.21) and (3.22) take such perturbations into account.

Proof of Proposition 3.3. We first show (3.21). The proof can be divided into 4 steps.

Step 1: Decomposition. For $E, F \subseteq \mathbb{N}$ fixed, we split $E \cup F = E \sqcup (F \setminus E)$ and write $\mu_F = \mu_{F \cap E} + \mu_{F \setminus E}$. By Fubini's theorem we reorganize

$$(3.23) \quad \begin{aligned} & \int_{(\square_{m+1})^{E \cup F}} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d\mu \right] \\ &= \int_{(\square_{m+1})^{F \setminus E}} \mathbb{E} \left[\sum_{n \in \mathbb{N}} \mathbb{P}_{\rho_0}[\mu(\square_m) = n] A_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}) \right], \end{aligned}$$

where for every $n \in \mathbb{N}$ we defined

$$\begin{aligned} & A_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}) \\ &:= \int_{(\square_{m+1})^E} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d\mu \middle| \mu_\rho, \mu \llcorner (\square_m)^c, \mu(\square_m) = n \right]. \end{aligned}$$

We note that only $\psi_m^{\rho, F}$ depends on the realization of μ_ρ . Hence, the previous term can be rewritten as

$$\begin{aligned} & A_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}) \\ &= \int_{(\square_{m+1})^E} \mathbb{E}_{\rho_0} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d\mu \middle| \mu \llcorner (\square_m)^c, \mu(\square_m) = n \right], \end{aligned}$$

in which the measures μ_ρ and $\mu_{F \setminus E}$ in $\psi_m^{\rho, F}$ are fixed.

We now apply a further decomposition of A_n . Let $G \subseteq E$ be the set of particles in \square_m , then the integration becomes

$$\int_{(\square_{m+1})^E} = \sum_{G \subseteq E} \int_{(\square_{m+1} \setminus \square_m)^{E \setminus G}} \int_{(\square_m)^G},$$

and we can write

$$(3.24) \quad \begin{aligned} & A_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}) \\ &= \sum_{G \subseteq E} \int_{(\square_{m+1} \setminus \square_m)^{E \setminus G}} B_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}), \end{aligned}$$

where the quantity $B_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G})$ is defined as

$$\begin{aligned} & B_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) \\ &:= \int_{(\square_m)^G} \mathbb{E}_{\rho_0} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d\mu \middle| \mu \llcorner (\square_m)^c, \mu(\square_m) = n \right]. \end{aligned}$$

Step 2: Finding the associated variational problem. We now claim that, for each $G \subseteq E$ and every $\mu_{E \setminus G}$,

$$(3.25) \quad B_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) = 0.$$

To prove this, we begin by specifying where the functions ψ_m^E and \mathbf{a}^E are evaluated. Splitting $\mu_E = \mu_{E \cap G} + \mu_{E \setminus G}$ and recalling the definition (3.2) of the canonical projection for ψ_m , we note that the term ψ_m^E in the expectation corresponds to $\psi_{m, n+|G|}(\cdot, \mu \llcorner (\square_m)^c + \mu_{E \setminus G})$. By Lemma 3.1, this function is a maximizer for the functional $\mathcal{J}_{n+|G|}(\cdot, \square_m, q, \mu \llcorner (\square_m)^c + \mu_{E \setminus G})$. Moreover, we notice that the left-hand side of (3.25) is quite similar to the variational formulation for the optimization problem for $\mathcal{J}_{n+|G|}(\cdot, \square_m, q, \mu \llcorner (\square_m)^c + \mu_{E \setminus G})$ that is tested against the function $\psi_m^{\rho, F}$,

so we define

$$\begin{aligned} & \tilde{B}_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) \\ &:= \int_{(\square_m)^G} \mathbb{E}_{\rho_0} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d(\mu + \mu_G) \middle| \mu \llcorner (\square_m)^c, \mu(\square_m) = n \right]. \end{aligned}$$

In the following, we will

- verify that $\psi_m^{\rho, F}$ is an admissible test function for the optimization problem for $\mathcal{J}_{n+|G|}(\cdot, \square_m, q, \mu \llcorner (\square_m)^c + \mu_{E \setminus G})$, showing that $\tilde{B}_n = 0$;
- deduce from $\tilde{B}_n = 0$ the claim (3.25).

Step 3: The test function is admissible. Conditioned on $\mu(\square_m) = n$, we write $\mu \llcorner \square_m$ and μ_F as

$$\mu \llcorner \square_m = \sum_{i=1}^n \delta_{y_i}, \quad \mu_F = \sum_{i=1}^{|F \cap G|} \delta_{x_{\alpha_i}} + \sum_{j=1}^{|F \setminus G|} \delta_{x_{\beta_j}}.$$

Then conditioned on $\mu(\square_m) = n$, for \mathbb{P} -almost every realization of $\mu \llcorner (\square_m)^c, \mu_\rho$, and (Lebesgue-) almost every realization of $\mu_{F \setminus E}$, the function

$$(y_1, \dots, y_n, x_{\alpha_1}, \dots, x_{\alpha_{|F \cap G|}}) \mapsto \psi_m \left(\sum_{i=1}^n \delta_{y_i} + \sum_{i=1}^{|F \cap G|} \delta_{x_{\alpha_i}} + \mu_{F \setminus G} + \mu \llcorner (\square_m)^c + \mu_\rho \right),$$

belongs to $H^1((\square_m)^{n+|F \cap G|})$ thanks to (3.18). Thus it also belongs to $H^1((\square_m)^{n+|G|})$ with respect to the integration $(\mu + \mu_G)$, and it is an admissible function for the optimization problem for $\mathcal{J}_{n+|G|}(\cdot, \square_m, q, \mu \llcorner (\square_m)^c + \mu_{E \setminus G})$. This implies that for \mathbb{P} -almost every realization of $\mu \llcorner (\square_m)^c, \mu_\rho$, and Lebesgue-almost every realization of $\mu_{F \setminus E}$, we have

$$\tilde{B}_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) = 0.$$

Step 4: Passage from $\tilde{B}_n = 0$ to $B_n = 0$. We stress that from the gradient of $\psi_m^{\rho, F}$ in \tilde{B}_n , out of the $(n + |G|)$ particles in $(\mu + \mu_G)$ only those in the support of $(\mu + \mu_{F \cap G})$ contribute. Thus we can rewrite \tilde{B}_n as

$$\begin{aligned} & \tilde{B}_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) \\ &= \int_{(\square_m)^G} \mathbb{E}_{\rho_0} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d(\mu + \mu_{F \cap G}) \middle| \mu \llcorner (\square_m)^c, \mu(\square_m) = n \right]. \end{aligned}$$

Notice now that the integrals above give the same contribution for every particle in $(\mu + \mu_{F \cap G})$, because $\psi_m^{\rho, F}, \psi_m^E$ and \mathbf{a}^E are all invariant under permutations for these particles. As a consequence, we have

$$\begin{aligned} & B_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) \\ &= \left(\frac{n}{n + |F \cap G|} \right) \tilde{B}_n(\mu_\rho, \mu \llcorner (\square_m)^c, \mu_{F \setminus E}, \mu_{E \setminus G}) \\ &= 0. \end{aligned}$$

We thus established (3.25). Then we put it back to (3.23) and (3.24), which implies that the left-hand side of (3.23) is zero and concludes the proof of (3.21).

We now turn to (3.22). The proof is similar and one can repeat the 4 steps above. The only difference is that we also need to do the expansion according to the number of particles $\mu_\rho(\square_m)$ and we skip the details. \square

Remark 3.4. The proof in fact yields the following stronger result: for all finite sets $E, F \subseteq \mathbb{N}_+$, and $G \subseteq E$, we have that

$$\begin{aligned} \int_{(\square_{m+1})^{E \cup F}} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^{\rho, F} \cdot \mathbf{a}^E \nabla \psi_m^E - \nabla \psi_m^{\rho, F} \cdot q) d(\mu + \mu_G) \right] &= 0, \\ \int_{(\square_{m+1})^{E \cup F}} \mathbb{E} \left[\int_{\square_m} (\nabla \psi_m^F \cdot \mathbf{a}^{\rho, E} \nabla \psi_m^{\rho, E} - \nabla \psi_m^F \cdot q) d(\mu + \mu_G) \right] &= 0. \end{aligned}$$

Remark 3.5. We point out that, choosing $\rho = 0$ in (3.21), we recover the same identity with $\psi_m^{\rho, F}$ replaced by ψ_m^F . From this, we may also change the density of the distribution of μ from ρ_0 to $\rho_0 + \rho$, and obtain the analogue of (3.22) with ψ_m^F replaced by $\psi_m^{\rho, F}$.

Finally, we note that, by linearity, (3.21) and (3.22) are also true if we use test functions of the form $D_F \psi_m^{G \setminus F}$ or $D_F \psi_m^{\rho, G \setminus F}$, $F, G \subseteq \mathbb{N}$ and we replace the outer integrals by $\int_{(\square_{m+1})^{E \cup F \cup G}}$.

4. FIRST-ORDER DIFFERENTIABILITY

In this section we prove Theorem 2.1. We explain at first its main ingredient, and it also gives us the opportunity to exemplify the sort of arguments that will be generalized later to obtain Theorem 2.3.

We recall that we have fixed a vector $q \in \mathbb{R}^d$, and that ψ_m denotes the optimizer in the definition (2.3) of the quantity $\nu_*(\square_m, q, \rho_0)$. We use the notation \lesssim for $\leq C \times$ with the constant C depending only d, Λ and the length of the vector $q \in \mathbb{R}^d$.

The quantity that we will study is the difference between the diffusion coefficients at different densities

$$(4.1) \quad \Delta^\rho(\rho_0) := q \cdot \bar{\mathbf{a}}^{-1}(\rho_0 + \rho)q - q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q,$$

as well as, for each $m \in \mathbb{N}$, its finite-volume analogue

$$(4.2) \quad \Delta_m^\rho(\rho_0) := q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0 + \rho)q - q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0)q.$$

In order to prove Theorem 2.1, we first establish its finite-volume version for $\Delta_m^\rho(\rho_0)$, with estimates that hold uniformly over m , and then pass to the limit. We recall that the notation $\psi_m^{\{1\}}, \mathbf{a}^{\{1\}}$ is defined in (2.9).

Proposition 4.1. *For any $\rho, \rho_0 > 0$ fixed, it holds*

$$(4.3) \quad \Delta^\rho(\rho_0) = \lim_{m \rightarrow \infty} \Delta_m^\rho(\rho_0).$$

Moreover, uniformly over $m \in \mathbb{N}$, we have

$$(4.4) \quad |\Delta_m^\rho(\rho_0) - c_{1,m}(\rho_0)\rho| \lesssim \rho^2,$$

with

$$(4.5) \quad c_{1,m}(\rho_0) := \int_{\mathbb{R}^d} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\{1\}} d\mu \right] dx_1.$$

The proof of Proposition 4.1 relies on two ingredients. The first is the following representation formula for the difference term $\Delta_m^\rho(\rho_0)$.

Lemma 4.2. *For every $m \in \mathbb{N}$ and $\rho > 0$, we have*

$$(4.6) \quad \Delta_m^\rho(\rho_0) = \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho d\mu \right].$$

One may find that (4.6) and (4.5) look quite similar, which explains that $c_{1,m}(\rho_0)$ is indeed its first order approximation. To verify this approximation, we also need some estimate, which is the second ingredient for the proof of Proposition 4.1. The next lemma allows us to compare the behavior of the optimizers ψ_m, ψ_m^ρ when the measures μ or $\mu + \mu_\rho$ are perturbed by one or two additional particles. Given $E \subseteq \mathbb{N}_+$, we recall the definitions (2.10) and (2.11) for the finite difference D_E , and the notation for the integrals \int_{U^E} in (3.19).

Lemma 4.3. *For every $m \in \mathbb{N}$ and $E, F \subseteq \mathbb{N}_+$ with $|E| \leq 2$ and $|F| \leq 1$, we have*

$$(4.7) \quad \int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla D_E \psi_m|^2 d\mu \right] \lesssim 1,$$

$$(4.8) \quad \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^F} \nabla D_F \psi_m \right|^2 d\mu \right] \lesssim 1.$$

Remark 4.4. Applying Lemma 4.3 for an underlying particle density of $\rho_0 + \rho$ instead of ρ , we see that the same estimates as in (4.7) and (4.8) hold if we replace ψ_m by ψ_m^ρ and μ by $\mu + \mu_\rho$.

Proposition 4.1 and Lemma 4.3 will be generalized in Section 5 to prove Theorem 2.3, where a higher-order approximation is needed. Estimate (4.7), indeed, corresponds to Proposition 5.4 with $|F| \leq 2, G = \emptyset$, while (4.8) corresponds to $F = G$ with $|F| = 1$.

We organize the remainder of this section as follows. We finish the introduction with a lemma gathering some basic properties of Poisson point processes. In Subsection 4.1, we prove Lemmas 4.2 and 4.3. Then we devote Subsection 4.2 to the proof of the key result Proposition 4.1. Subsection 4.3 builds upon Proposition 4.1 to conclude for the validity of Theorem 2.1.

Here are some basic estimates for Poisson point processes that we extensively use in the arguments of this section.

Lemma 4.5. *Let $\rho \in (0, +\infty)$. For every measurable $F : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$ such that $\mathbb{E}_\rho[|F|] < +\infty$, $z \in \mathbb{R}^d$, and finite set $E \subseteq \mathbb{N}_+$, we have*

$$(4.9) \quad \begin{aligned} \mathbb{E}_\rho[F(\mu_\rho) \mathbf{1}_{\{\mu_\rho(\square+z)=1\}}] &= \rho \int_{\square+z} \mathbb{E}_\rho[F^{\{1\}}(\mu_\rho) \mathbf{1}_{\{\mu_\rho(\square+z)=0\}}] dx_1, \\ |\mathbb{E}_\rho[F(\mu_\rho) \mathbf{1}_{\{\mu_\rho(\square+z) \geq |E|\}}]| &\leq \rho^{|E|} \int_{(\square+z)^E} \mathbb{E}_\rho[|F^E(\mu_\rho)|]. \end{aligned}$$

For every measurable function $H : \mathcal{M}_\delta(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}$ satisfying the integrability condition $\mathbb{E}_\rho[\int_U |H(\mu_\rho, x)| d\mu_\rho(x)] < +\infty$, we have Mecke's identity (c.f also [15, Chapter 1])

$$(4.10) \quad \mathbb{E}_\rho \left[\frac{1}{\rho |U|} \int_U H(\mu_\rho, x) d\mu_\rho(x) \right] = \int_U \mathbb{E}_\rho[H(\mu_\rho + \delta_x, x)] dx.$$

Proof of Lemma 4.5. Without loss of generality, we may fix $z = 0$ in (4.9). The first identity there follows immediately if we spell out the definition of the expectation \mathbb{E}_ρ and use the independence of increments of the Poisson point process:

$$\begin{aligned} \mathbb{E}_\rho[F(\mu_\rho) \mathbf{1}_{\{\mu_\rho(\square)=1\}}] &= \mathbb{E}_\rho[e^{-\rho} \rho \int_\square F(\delta_{x_1} + \mu_\rho \llcorner (\square)^c) dx_1] \\ &= \rho \int_\square \mathbb{E}_\rho[\mathbf{1}_{\{\mu_\rho(\square)=0\}} F(\delta_{x_1} + \mu_\rho)] dx_1. \end{aligned}$$

For the second estimate in (4.9), we write $n := |E|$ and observe that

$$\mathbb{E}_\rho \left[F(\mu_\rho) \mathbf{1}_{\mu_\rho(\square) \geq |E|} \right] = \mathbb{E}_\rho \left[e^{-\rho} \sum_{k=n}^{\infty} \frac{\rho^k}{k!} \int_{(\square)^k} F\left(\sum_{i=1}^k \delta_{x_i} + \mu_\rho \llcorner (\square)^c\right) dx_1 \cdots dx_k \right].$$

This allows us to bound

$$\begin{aligned} |\mathbb{E}_\rho \left[F(\mu_\rho) \mathbf{1}_{\{\mu_\rho(\square) \geq |E|\}} \right]| &\leq \rho^n \times \\ &\int_{\square^n} \mathbb{E}_\rho \left[\sum_{k=n}^{\infty} e^{-\rho} \frac{\rho^{k-n}}{(k-n)!} \int_{(\square)^{k-n}} |F(\sum_{j=1}^n \delta_{y_j} + \sum_{i=1}^{k-n} \delta_{x_i} + \mu_\rho \llcorner \square^c)| dx_1 \cdots dx_{k-n} \right] dy_1 \cdots dy_n. \end{aligned}$$

which is the second estimate in (4.9). Finally, (4.10) may be obtained from the definition of \mathbb{E}_ρ and the invariance of H under permutations of the atoms in μ . \square

4.1. Representation formula and corrector estimates. In this subsection we prove Lemmas 4.2 and 4.3.

Proof of Lemma 4.2. We use the definition of $\Delta_m^\rho(\rho_0)$ and (3.11) to write

$$\Delta_m^\rho(\rho_0) = \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} q \cdot \nabla \psi_m^\rho d(\mu + \mu_\rho) \right] - \mathbb{E} \left[\frac{1}{\rho_0|\square_m|} \int_{\square_m} q \cdot \nabla \psi_m d\mu \right].$$

Identity (4.10) of Lemma 4.5 applied to $\nabla \psi_m^\rho$, first with density ρ (with respect to μ_ρ) and then ρ_0 (with respect to μ), yields that

$$\mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} q \cdot \nabla \psi_m^\rho d\mu_\rho \right] = \mathbb{E} \left[\frac{\rho}{\rho_0(\rho_0 + \rho)|\square_m|} \int_{\square_m} q \cdot \nabla \psi_m^\rho d\mu \right],$$

and, hence, also

$$(4.11) \quad \Delta_m^\rho(\rho_0) = \mathbb{E} \left[\frac{1}{\rho_0|\square_m|} \int_{\square_m} q \cdot (\nabla \psi_m^\rho - \nabla \psi_m) d\mu \right].$$

To establish representation (4.6) it now only remains to apply (3.22) in Proposition 3.3 and (3.21) with the choice $E = F = \emptyset$. \square

Proof of Lemma 4.3. We start by noting that if $E = F = \emptyset$, then the inequalities of Lemma 4.3 correspond to the basic energy estimate in (3.12). Hence, we only need to focus on the cases $E, F \neq \emptyset$. With no loss of generality, we prove (4.7) with $E = \{1\}$ or $E = \{1, 2\}$ and (4.8) with $F = \{1\}$. We also stress that, since by construction the maximizer ψ_m is $\mathcal{F}_{Q_{3^{m+1}}}$ -measurable, for every non-empty subset $G \subseteq \mathbb{N}$ we have that $D_G \psi_m$ vanishes whenever one of the particles $\{x_j\}_{j \in G}$ does not belong to $Q_{3^{m+1}}$ (c.f. Definitions (2.11) and (2.10)). This implies that in (4.7)-(4.8) we may replace the integrals over \mathbb{R}^d by integrals over any set $U \supseteq Q_{3^{m+1}}$. In line with the notation of Section 3, throughout the proof we fix $U = \square_{m+1}$.

We start with (4.7) when $E = \{1\}$. In view of the previous remarks and spelling out the integrand, this may be rewritten as

$$(4.12) \quad \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0|\square_m|} \int_{\square_m} |\nabla(\psi_m^{\{1\}} - \psi_m)|^2 d\mu \right] dx_1 \lesssim 1,$$

We consider identity (3.21) of Proposition 3.3 with $\rho = 0$, $E = \emptyset$ and $E = \{1\}$ and with test function $D_{\{1\}} \psi_m$ (c.f. Remark 3.5).

$$\begin{aligned} \int_{\square_{m+1}} \mathbb{E} \left[\int_{\square_m} (\nabla D_{\{1\}} \psi_m \cdot \mathbf{a} \nabla \psi_m - \nabla D_{\{1\}} \psi_m \cdot q) d\mu \right] &= 0, \\ \int_{\square_{m+1}} \mathbb{E} \left[\int_{\square_m} (\nabla D_{\{1\}} \psi_m \cdot \mathbf{a}^{\{1\}} \nabla \psi_m^{\{1\}} - \nabla D_{\{1\}} \psi_m \cdot q) d\mu \right] &= 0. \end{aligned}$$

Subtracting the resulting identities yields that

$$(4.13) \quad \begin{aligned} & \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot \mathbf{a}^{\{1\}} \nabla D_{\{1\}} \psi_m \, d\mu \right] dx_1 \\ &= - \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (D_{\{1\}} \mathbf{a}) \nabla \psi_m \, d\mu \right] dx_1. \end{aligned}$$

We now appeal to the uniform ellipticity assumption (2.1) and the Cauchy–Schwarz inequality to infer from (4.13) that

$$\begin{aligned} & \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla D_{\{1\}} \psi_m|^2 \, d\mu \right] dx_1 \\ & \lesssim \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (D_{\{1\}} \mathbf{a})^2 |\nabla \psi_m|^2 \, d\mu \right] dx_1. \end{aligned}$$

We obtain the first inequality in (4.12) after noting that (2.2) and (2.1) for \mathbf{a} imply that also

$$\begin{aligned} & \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (D_{\{1\}} \mathbf{a})^2 |\nabla \psi_m|^2 \, d\mu \right] dx_1 \\ & \lesssim \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square_{+z}} |\nabla \psi_m(\mu, z)|^2 \, dx_1 \, d\mu(z) \right] \stackrel{(3.12)}{\lesssim} 1. \end{aligned}$$

This establishes (4.12).

The proof of (4.7) when $E = \{1, 2\}$ follows a similar argument. Observe that

$$D_{\{1,2\}} \psi_m = \psi_m^{\{1,2\}} - \psi_m^{\{1\}} - \psi_m^{\{2\}} + \psi_m,$$

we may add and subtract suitable combinations of identity (3.21) in Proposition 3.3 with $E \in \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}$ and test function $\nabla D_{\{1,2\}} \psi_m$ (c.f. Remark 3.5) to infer that

$$(4.14) \quad \begin{aligned} & \int_{(\square_{m+1})^2} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1,2\}} \psi_m \cdot \mathbf{a}^{\{1,2\}} \nabla D_{\{1,2\}} \psi_m \, d\mu \right] dx_1 \, dx_2 \\ &= \sum_{i=1}^2 \int_{(\square_{m+1})^2} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1,2\}} \psi_m \cdot (\mathbf{a}^{\{i\}} - \mathbf{a}^{\{1,2\}}) \nabla D_{\{i\}} \psi_m \, d\mu \right] dx_1 \, dx_2 \\ & \quad - \int_{(\square_{m+1})^2} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1,2\}} \psi_m \cdot (D_{\{1,2\}} \mathbf{a}) \nabla \psi_m \, d\mu \right] dx_1 \, dx_2. \end{aligned}$$

From this, we obtain (4.7) when $E = \{1, 2\}$ as was done in the case $E = \{1\}$. This time, besides the Cauchy–Schwarz inequality and (2.1)–(2.2), we also rely on inequality (4.12) for $|E| = 1$ that was proved above.

To conclude the proof of this lemma, it remains to establish inequality (4.8). As argued at the beginning of the proof of this lemma, this can be reduced to

$$(4.15) \quad \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\int_{(\square_{m+1})^{\{1\}}} \nabla D_{\{1\}} \psi_m|^2 \, d\mu \right] \lesssim 1.$$

We appeal again to Proposition 3.3: we subtract (3.21) with $E = \emptyset$ and test function $D_{\{2\}} \psi_m$ (c.f. Remark 3.5) from the same identity with $E = \{1\}$ and test function $D_{\{2\}} \psi_m$. This yields

$$\begin{aligned} & \int_{(\square_{m+1})^{\{1,2\}}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{2\}} \psi_m \cdot \mathbf{a} \nabla D_{\{1\}} \psi_m \, d\mu \right] \\ &= - \int_{(\square_{m+1})^{\{1,2\}}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{2\}} \psi_m \cdot (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\{1\}} \, d\mu \right]. \end{aligned}$$

Appealing to Fubini's theorem and observing that, by a simple relabelling of the integration variable, it holds that $\int_{(\square_{m+1})^{\{1\}}} D_{\{1\}} \psi_m = \int_{(\square_{m+1})^{\{2\}}} D_{\{2\}} \psi_m$, we infer that

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \left(\int_{(\square_{m+1})^{\{1\}}} D_{\{1\}} \psi_m \right) \cdot \mathbf{a} \nabla \left(\int_{(\square_{m+1})^{\{1\}}} D_{\{1\}} \psi_m \right) d\mu \right] \\ &= -\mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \left(\int_{(\square_{m+1})^{\{1\}}} D_{\{1\}} \psi_m \right) \cdot \left(\int_{(\square_{m+1})^{\{1\}}} (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\{1\}} \right) d\mu \right]. \end{aligned}$$

By (2.1) and the Cauchy–Schwarz inequality, this also implies that

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_{m+1})^{\{1\}}} \nabla D_{\{1\}} \psi_m \right|^2 d\mu \right] \\ & \leq \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_{m+1})^{\{1\}}} (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\{1\}} \right|^2 d\mu \right]. \end{aligned}$$

We thus conclude the proof of (4.15) provided that the term on the right-hand side above is $\lesssim 1$: by the triangle inequality we have that

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_{m+1})^{\{1\}}} (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\{1\}} \right|^2 d\mu \right] \\ & \leq \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_{m+1})^{\{1\}}} (D_{\{1\}} \mathbf{a}) \nabla D_{\{1\}} \psi_m \right|^2 d\mu \right] \\ & \quad + \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_{m+1})^{\{1\}}} (\mathbf{a} - \mathbf{a}^{\{1\}}) \right|^2 |\nabla \psi_m|^2 d\mu \right]. \end{aligned}$$

The second term on the right-hand side is immediately bounded by $\lesssim 1$ due to assumptions (2.1)–(2.2) on \mathbf{a} and (3.12). The first term admits the same upper bound thanks to the Cauchy–Schwarz inequality, (2.1)–(2.2), and (4.12). The proof of Lemma 4.3 is complete. \square

4.2. Proof of Proposition 4.1. In this section we use Lemmas 4.2 and 4.3 to show Proposition 4.1.

Proof of Proposition 4.1. Limit (4.3) follows immediately from definitions (4.1), (4.2) and (2.5). We thus turn to (4.4) and prove this inequality in three different steps.

Step 1. We claim that

$$\begin{aligned} & \left| \Delta_m^\rho(\rho_0) - \rho c_{1,m}(\rho_0) \right| \lesssim \rho^2 \\ (4.16) \quad & + \rho \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (D_{\{1\}} \mathbf{a}) (\nabla \psi_m^{\rho, \{1\}} - \nabla \psi_m^{\{1\}}) d\mu \right] dx_1 \right|. \end{aligned}$$

We begin by using the representation formula for $\Delta_m^\rho(\rho_0)$ of Lemma 4.2, the definition of the expectation \mathbb{E} and assumption (2.2) for \mathbf{a} to rewrite

$$\begin{aligned} (4.17) \quad \Delta_m^\rho(\rho_0) &= \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho \left[\mathbf{1}_{\mu_\rho(\square+z) \geq 1} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho \right] d\mu(z) \right] \\ &= \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho \left[\mathbf{1}_{\mu_\rho(\square+z) = 1} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho \right] d\mu(z) \right] \\ & \quad + \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho \left[\mathbf{1}_{\mu_\rho(\square+z) \geq 2} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho \right] d\mu(z) \right]. \end{aligned}$$

We claim that the second term on the right-hand side above is bounded by a constant multiple of ρ^2 : using the Cauchy–Schwarz inequality, the bound (3.12), and the

second inequality in (4.9) of Lemma 4.5 with $E = \{1, 2\}$, we infer that

$$(4.18) \quad \left| \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho [\mathbf{1}_{\mu_\rho(\square+z) \geq 2} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho] d\mu \right] \right| \\ \lesssim \rho^2 \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\square+z)^2} |\nabla \psi_m^{\rho, \{1,2\}}|^2 dx_1 dx_2 \right) d\mu(z) \right],$$

and the right-hand side is $\lesssim \rho^2$, as one can see by writing

$$\psi_m^{\rho, \{1,2\}} = D_{\{1,2\}} \psi_m^\rho - D_{\{1\}} \psi_m^\rho - D_{\{2\}} \psi_m^\rho + \psi_m^\rho,$$

and then applying the triangle inequality and Lemma 4.3. Inserting this into (4.17), we have that

$$(4.19) \quad \left| \Delta_m^\rho(\rho_0) - \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho [\mathbf{1}_{\mu_\rho(\square+z)=1} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho] d\mu(z) \right] \right| \lesssim \rho^2.$$

We now apply the first inequality of (4.9) to the inner expectation in the term on the left-hand side above. This, together with the locality (2.2) of \mathbf{a} , yields that

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \mathbb{E}_\rho [\mathbf{1}_{\mu_\rho(\square+z)=1} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho] d\mu(z) \right] \\ &= \rho \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \left(\int_{\square+z} \mathbb{E}_\rho [\mathbf{1}_{\mu_\rho(\square+z)=0} (\mathbf{a} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\rho, \{1\}}] dx_1 \right) d\mu(z) \right] \\ &\stackrel{(4.5)}{=} \rho c_{m,1} - \rho \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \left(\int_{\square+z} (D_{\{1\}} \mathbf{a}) (\nabla \psi_m^{\rho, \{1\}} - \nabla \psi_m^{\{1\}}) dx_1 \right) d\mu(z) \right] \\ &+ \rho \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \left(\int_{\square+z} \mathbb{E}_\rho [\mathbf{1}_{\mu_\rho(\square+z) \geq 1} (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\rho, \{1\}}] dx_1 \right) d\mu(z) \right]. \end{aligned}$$

To conclude from this and (4.19) that inequality (4.16) holds, it remains to prove that the last term above is $\lesssim \rho^2$. This may be done using again the second inequality in (4.9) and Lemma 4.3, as done for the term in (4.18).

Step 2. We now argue that the term appearing on the right-hand side of (4.16) may be rewritten as follows:

$$(4.20) \quad \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \nabla \psi_m \cdot (D_{\{1\}} \mathbf{a}) (\nabla \psi_m^{\rho, \{1\}} - \nabla \psi_m^{\{1\}}) d\mu \right] dx_1 \\ = \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\rho, \{1\}} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\rho, \{1\}} d\mu \right] dx_1.$$

We appeal to Proposition 3.3: we subtract (3.21) with $E = F = \{1\}$ from (3.21) with $E = \emptyset$ and $F = \{1\}$. This, together with the symmetry of \mathbf{a} , yields that

$$\begin{aligned} & - \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (D_{\{1\}} \mathbf{a}) \nabla \psi_m^{\rho, \{1\}} d\mu \right] dx_1 \\ &= \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{\rho, \{1\}} \cdot \mathbf{a}^{\{1\}} \nabla D_{\{1\}} \psi_m d\mu \right] dx_1. \end{aligned}$$

We now subtract this inequality from the same one with $\rho = 0$ (see also the discussion in Remark 3.5) and conclude that

$$(4.21) \quad \begin{aligned} & \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (D_{\{1\}} \mathbf{a}) (\nabla \psi_m^{\rho, \{1\}} - \nabla \psi_m^{\{1\}}) d\mu \right] dx_1 \\ &= \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (\nabla \psi_m^{\{1\}} - \nabla \psi_m^{\rho, \{1\}}) \cdot \mathbf{a}^{\{1\}} \nabla D_{\{1\}} \psi_m d\mu \right] dx_1. \end{aligned}$$

We now treat the term on the right-hand side above in an analogous way. We consider (3.21) and (3.22) in Proposition 3.3 with $E = \{1\}$ and test function $D_{\{1\}} \psi_m$ (this is possible by Remark 3.5). This yields

$$(4.22) \quad \begin{aligned} & \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot \mathbf{a}^{\{1\}} (\nabla \psi_m^{\{1\}} - \nabla \psi_m^{\rho, \{1\}}) d\mu \right] dx_1 \\ &= \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\rho, \{1\}} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\rho, \{1\}} d\mu \right] dx_1. \end{aligned}$$

We compare the two displays (4.21) and (4.22), which give (4.20) and thus conclude the proof of Step 2.

Step 3. In this step, we give an estimate that

$$(4.23) \quad \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_{m+z}} \nabla \psi_m \cdot (D_{\{1\}} \mathbf{a}) (\nabla \psi_m^{\rho, \{1\}} - \nabla \psi_m^{\{1\}}) d\mu \right] dx_1 \right| \lesssim \rho.$$

This, together with the result (4.16) of Step 1, will establish Proposition 4.1.

Appealing to Step 2, the proof of this step can be reduced to establishing that

$$(4.24) \quad \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\rho, \{1\}} - \mathbf{a}^{\{1\}}) \nabla \psi_m^{\rho, \{1\}} d\mu \right] dx_1 \right| \lesssim \rho.$$

We use the triangle inequality to split

$$(4.25) \quad \begin{aligned} & \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho, \{1\}}) \nabla \psi_m^{\rho, \{1\}} d\mu \right] dx_1 \right| \\ & \leq \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho, \{1\}}) \nabla D_{\{1\}} \psi_m^{\rho} d\mu \right] dx_1 \right| \\ & \quad + \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho, \{1\}}) \nabla \psi_m^{\rho} d\mu \right] dx_1 \right|, \end{aligned}$$

and treat separately the two integrals above.

We begin with the first one and argue similarly to (4.17) of Step 1: we use (2.2), Lemma 4.9 and the Cauchy–Schwarz inequality to control

$$\begin{aligned} & \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho, \{1\}}) \nabla D_{\{1\}} \psi_m^{\rho} d\mu \right] dx_1 \right| \\ & \leq \rho \left(\int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla D_{\{1\}} \psi_m|^2 d\mu \right] dx_1 \right)^{\frac{1}{2}} \\ & \quad \times \left(\int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square_{m+z}} |\nabla D_{\{1\}} \psi_m^{\rho, 2}|^2 dx_2 d\mu(z) \right] dx_1 \right)^{\frac{1}{2}} \\ & \stackrel{\text{Lemma 4.3}}{\lesssim} \rho \left(\int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square_{m+z}} |\nabla D_{\{1\}} \psi_m^{\rho, 2}|^2 dx_2 d\mu(z) \right] dx_1 \right)^{\frac{1}{2}}. \end{aligned}$$

Writing

$$D_{\{1\}}\psi_m^{\rho,2} = \psi_m^{\rho,\{1,2\}} - \psi_m^{\rho,\{2\}} = D_{\{1,2\}}\psi_m^\rho - D_{\{1\}}\psi_m^\rho,$$

and appealing again to the triangle inequality and to the estimates of Lemma 4.3, we infer that

$$(4.26) \quad \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho,\{1\}}) \nabla D_{\{1\}} \psi_m^\rho d\mu \right] dx_1 \right| \lesssim \rho.$$

The second integral in (4.25) may be treated in a similar way, if we split

$$\begin{aligned} & \left| \int_{\square_{m+1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla D_{\{1\}} \psi_m \cdot (\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho,\{1\}}) \nabla \psi_m^\rho d\mu \right] dx_1 \right| \\ & \leq \left| \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square_{m+1} \setminus (\square+z)} \nabla D_{\{1\}} \psi_m \cdot \mathbb{E}_\rho[(\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho,\{1\}}) \nabla \psi_m^\rho] dx_1 d\mu \right] \right| \\ & \quad + \left| \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square+z} \nabla D_{\{1\}} \psi_m \cdot \mathbb{E}_\rho[(\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho,\{1\}}) \nabla \psi_m^\rho] dx_1 d\mu \right] \right|. \end{aligned}$$

The second term may be bounded by $\lesssim \rho$ using again (2.2) and an argument analogous to the one used for (4.26). On the other hand, since by (2.2), for every $z \in \square_m$ and $x \in \square_m \setminus (\square+z)$ we have that

$$\mathbf{a}^{\{1\}}(\mu, z) - \mathbf{a}^{\rho,\{1\}}(\mu, z) = \mathbf{1}_{\{\mu_\rho(\square+z) \geq 1\}} (\mathbf{a}(\mu, z) - \mathbf{a}^\rho(\mu, z)),$$

the first term on the right-hand side above may be rewritten as

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square_{m+1} \setminus (\square+z)} \nabla D_{\{1\}} \psi_m \cdot \mathbb{E}_\rho[(\mathbf{a}^{\{1\}} - \mathbf{a}^{\rho,\{1\}}) \nabla \psi_m^\rho] dx_1 d\mu \right] \\ & = \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{\square_{m+1} \setminus (\square+z)} \nabla D_{\{1\}} \psi_m dx_1 \right) \cdot \mathbb{E}_\rho[\mathbf{1}_{\{\mu_\rho(\square+z) \geq 1\}} (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho] d\mu \right]. \end{aligned}$$

We may bound this term by $\lesssim \rho$ by appealing once again to the Cauchy–Schwarz inequality and Lemmas 4.3 and 4.9. This yields that also the second integral in (4.25) is bounded by $\lesssim \rho$. This establishes (4.24) and concludes the proof of Step 3. Proposition 4.1 is therefore proved. \square

4.3. Proof of Theorem 2.1. Equipped with Proposition 4.1, we are now ready to prove the main result of this section.

Proof of Theorem 2.1. A first consequence of Proposition 4.1 is that $\{c_{1,m}(\rho_0)\}_{m \in \mathbb{N}}$ in (4.5) is uniformly bounded over $m \in \mathbb{N}$. Indeed, by definition (4.5), assumptions (2.1)–(2.2) on \mathbf{a} and the Cauchy–Schwarz inequality, we have that

$$\begin{aligned} |c_{1,m}(\rho_0)| &= \left| \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot \int_{(\square+z)} (\mathbf{a}^{\{1\}} - \mathbf{a}) \nabla \psi_m^{\{1\}} dx_1 d\mu(z) \right] \right| \\ &\leq \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla \psi_m|^2 d\mu \right]^{\frac{1}{2}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{\square+z} |\nabla \psi_m^{\{1\}}|^2 d\mu \right]^{\frac{1}{2}}. \end{aligned}$$

The first factor on the right-hand side above is bounded thanks to (3.12). The second one can be controlled by the triangle inequality, Lemma 4.3 and again (3.12).

Let $\rho_0 > 0$ be fixed. The uniform bound for $\{c_{1,m}(\rho_0)\}_{m \in \mathbb{N}}$ implies that we may find a subsequence (possibly depending on ρ_0) and a number $c_1^*(\rho_0)$ such that

$$\lim_{j \rightarrow +\infty} c_{1,m_j}(\rho_0) := c_1^*(\rho_0).$$

Passing to the limit along this subsequence in the inequality (4.4) of Proposition 4.1 and using (4.3), we infer that for every $\rho > 0$

$$(4.27) \quad |\Delta^\rho(\rho_0) - c_1^*(\rho_0)\rho| \lesssim \rho^2.$$

On the one hand, the arbitrariness of $\rho > 0$ in this inequality implies that the value $c_1^*(\rho_0)$ is the limit for the full sequence $\{c_{m,1}(\rho_0)\}_{m \in \mathbb{N}}$, which we denote by $c_1(\rho_0)$. On the other hand, definition (4.1) allows to immediately infer that for every $\rho_0 > 0$ fixed and $\rho \geq 0$ tending to zero, we have

$$(4.28) \quad q \cdot \bar{\mathbf{a}}^{-1}(\rho_0 + \rho)q = q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q + c_1(\rho_0)\rho + O(\rho^2).$$

To conclude the proof of Theorem 2.1, it thus remains to extend (4.28) to negative values of ρ that tend to zero. We do this by applying (4.28) with the pair $(\rho_0, \rho_0 + \rho)$ substituted with $(\rho_0 - \rho, \rho_0)$ to get that, as $\rho \geq 0$ tends to zero,

$$(4.29) \quad q \cdot \bar{\mathbf{a}}^{-1}(\rho_0 - \rho)q = q \cdot \bar{\mathbf{a}}^{-1}(\rho_0)q - c_1(\rho_0 - \rho)\rho + O(\rho^2).$$

To conclude the desired expansion, it remains to show that we may replace $c_1(\rho_0 - \rho)$ by $c_1(\rho_0)$ in this display. Defining $f(\cdot) := q \cdot \bar{\mathbf{a}}^{-1}(\cdot)q$ and appealing to identity (4.28), we write

$$\begin{aligned} c_1(\rho_0 - \rho) &= \frac{f(\rho_0) - f(\rho_0 - \rho)}{\rho} + O(\rho) \\ &= \frac{f(\rho_0) - f(\rho_0 + \rho)}{\rho} + \frac{f(\rho_0 + \rho) - f(\rho_0 - \rho)}{\rho} + O(\rho) \\ &= -c_1(\rho_0) + 2c_1(\rho_0 - \rho) + O(\rho). \end{aligned}$$

In the last line, we apply (4.28) at ρ_0 for the first term, and (4.28) at $(\rho_0 - \rho)$ for the second term with step size 2ρ . The notation $O(\rho)$ is valid as the hidden constant is independent from the density. The equation above gives us

$$c_1(\rho_0 - \rho) = c_1(\rho_0) + O(\rho).$$

Inserting this into (4.29) yields that (4.28) holds also for negative perturbations ρ . This completes the proof of Theorem 2.1. \square

5. HIGHER-ORDER DIFFERENTIABILITY

The goal of this section is to generalize the results of the previous section, and ultimately prove Theorem 2.3 stating that the mapping $\rho_0 \mapsto \bar{\mathbf{a}}(\rho_0)$ is infinitely differentiable.

As a preparation, we recall that the notation f^E and D_E is introduced in (2.9), (2.11) and state basic algebraic properties of these operators.

Proposition 5.1 (Algebraic properties). *For every $f, g : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$ and every finite set $E \subseteq \mathbb{N}_+$, the following identities hold.*

- *Inclusion-exclusion formula*

$$(5.1) \quad D_E f = \sum_{F \subseteq E} (-1)^{|E \setminus F|} f^F.$$

- *Telescoping formula*

$$(5.2) \quad f^E = \sum_{F \subseteq E} D_F f.$$

- *Leibniz formulas*

$$(5.3) \quad D_E(fg) = \sum_{F \subseteq E} (D_F f)(D_{E \setminus F} g^F),$$

and

$$(5.4) \quad D_E(fg) = \sum_{F, G \subseteq E, F \cup G = E} (D_F f)(D_G g).$$

Proof. These elementary identities can be proved by induction. We show (5.3) for illustration. Without loss of generality, we can assume that $E = \llbracket 1, n \rrbracket$ for some integer $n \in \mathbb{N}_+$. The case $n = 1$ is clear:

$$(5.5) \quad D_1(fg) = f^{\{1\}} g^{\{1\}} - fg = (D_1 f) g^{\{1\}} + f(D_1 g).$$

Assuming that the formula is valid for $E = \llbracket 1, n \rrbracket$, we can then write

$$\begin{aligned} D_{\llbracket 1, n+1 \rrbracket}(fg) &= D_{n+1}(D_{\llbracket 1, n \rrbracket}(fg)) \\ &= D_{n+1} \left(\sum_{F \subseteq \llbracket 1, n \rrbracket} (D_F f)(D_{\llbracket 1, n \rrbracket \setminus F} g^F) \right) \\ &= \sum_{F \subseteq \llbracket 1, n \rrbracket} D_{n+1} \left((D_F f)(D_{\llbracket 1, n \rrbracket \setminus F} g^F) \right). \end{aligned}$$

We then use (5.5) to assert that

$$\begin{aligned} &D_{n+1} \left((D_F f)(D_{\llbracket 1, n \rrbracket \setminus F} g^F) \right) \\ &= (D_{F \cup \{n+1\}} f)(D_{\llbracket 1, n \rrbracket \setminus F} g^{F \cup \{n+1\}}) + (D_F f)(D_{\llbracket 1, n+1 \rrbracket \setminus F} g^F) \\ &= (D_{F \cup \{n+1\}} f)(D_{\llbracket 1, n+1 \rrbracket \setminus (F \cup \{n+1\})} g^{F \cup \{n+1\}}) + (D_F f)(D_{\llbracket 1, n+1 \rrbracket \setminus F} g^F). \end{aligned}$$

Combining the two previous displays yields the claim. \square

5.1. Main strategy. In this section, we present the structure of the proof of Theorem 2.3. We will in fact mostly focus on the following finite-volume version of this statement. Recall the definitions of Δ^ρ and Δ_m^ρ in (4.1) and (4.2), and we know from (4.1) that $\Delta^\rho = \lim_{m \rightarrow \infty} \Delta_m^\rho$. In order to lighten the expressions appearing below, we use the notation in (3.19) to simplify the integration with respect to several particles.

Proposition 5.2 (Smoothness in finite volume). *For every $\rho_0 > 0$ and $k, m \in \mathbb{N}_+$, we define*

$$(5.6) \quad c_{k,m}(\rho_0) := \int_{(\mathbb{R}^d)^{\llbracket 1, k \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_{\llbracket 1, k \rrbracket} ((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) d\mu \right].$$

There exists a positive constant $C_k(d, \Lambda) < \infty$ such that for every $m \in \mathbb{N}_+$ and $\rho_0 > 0$,

$$(5.7) \quad |c_{k,m}(\rho_0)| \leq C_k.$$

Moreover, the quantity $\Delta_m^\rho(\rho_0)$ defined in (4.2) satisfies that, for every $k \in \mathbb{N}_+$,

$$(5.8) \quad \Delta_m^\rho(\rho_0) = \sum_{j=1}^k c_{j,m}(\rho_0) \frac{\rho^j}{j!} + R_k(m, \rho_0, \rho),$$

where $R_k(m, \rho_0, \rho)$ is such that, as $\rho > 0$ tends to zero and uniformly over m and ρ_0 ,

$$R_k(m, \rho_0, \rho) = O(\rho^{k+1}).$$

In Subsection 5.6, we will obtain our main result Theorem 2.3 as a corollary of Proposition 5.2. For now, we present the structure of the proof of this proposition.

The first step of the proof of Proposition 5.2 consists in identifying a convenient expansion for Δ_m^ρ . As a starting point, one can check that if a function $f : \mathcal{M}_\delta(\mathbb{R}^d) \rightarrow \mathbb{R}$ is bounded and local, then we have

$$\mathbb{E}[f(\mu + \mu_\rho)] = \sum_{k=0}^{\infty} \frac{\rho^k}{k!} \left(\int_{(\mathbb{R}^d)^{[1,k]}} \mathbb{E}[D_{[1,k]} f] \right).$$

(See for instance [16, Theorem 19.2]; a self-contained argument is given below.) Generalizing this observation, it is natural to expect that Δ_m^ρ can be rewritten from (4.6) as

$$\sum_{k=1}^{\infty} \frac{\rho^k}{k!} \left(\int_{(\mathbb{R}^d)^{[1,k]}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_{[1,k]} ((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) d\mu \right] \right),$$

where we dropped the summand indexed by $k = 0$, which vanishes. Notice that in the formula above, we could replace $\int_{(\mathbb{R}^d)^{[1,k]}}$ with $\int_{(\square_{m+1})^{[1,k]}}$, because ψ_m is $\mathcal{F}_{Q_{3m+1}}$ -measurable, \mathbf{a} is also local and the perturbation by adding particles outside \square_{m+1} will not contribute; this observation will be applied several times in the sequel. The following lemma states that the expansion formula is indeed valid for Δ_m^ρ ; its proof is provided in Subsection 5.2.

Lemma 5.3 (Expansion of Δ_m^ρ). *For each $m \in \mathbb{N}$, the quantity Δ_m^ρ is an analytic function of ρ and satisfies*

$$(5.9) \quad \Delta_m^\rho = \sum_{k=1}^{\infty} \frac{\rho^k}{k!} \left(\int_{(\mathbb{R}^d)^{[1,k]}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_{[1,k]} ((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) d\mu \right] \right).$$

The remainder of the proof of Proposition 5.2 consists in the analysis of the summands in the expansion provided Lemma 5.3. Applying the Leibniz formula (5.9) to these summands:

$$(5.10) \quad D_{[1,k]} ((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) = \sum_{E \cup F = [1,k]} D_E (\mathbf{a} - \mathbf{a}^\#) (D_F \nabla \psi_m),$$

we are led to the expansion

$$(5.11) \quad \Delta_m^\rho = \sum_{k=1}^{\infty} \frac{\rho^k}{k!} \sum_{E \cup F = [1,k]} I(m, \rho_0, E, F),$$

where the quantity $I(m, \rho_0, E, F)$ is defined for E, F finite subsets of \mathbb{N}_+ ,

$$(5.12) \quad I(m, \rho_0, E, F) := \int_{(\mathbb{R}^d)^{[1,k]}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_E (\mathbf{a} - \mathbf{a}^\#) D_F (\nabla \psi_m) d\mu \right].$$

It suffices to give a uniform estimate for the quantity $I(m, \rho_0, E, F)$ with respect to m and ρ_0 . Heuristically, the k derivatives act either on the conductance or on the corrector, and they compensate with the integration $\int_{(\mathbb{R}^d)^{[1,k]}}$. With some more reduction, the estimation of these terms will be based on the following key result.

Proposition 5.4 (Key estimate). *There exists a family of constants $\{C(i, j)\}_{i \geq j \geq 0}$ such that for every finite sets $G \subseteq F \subseteq \mathbb{N}_+$, $m \in \mathbb{N}_+$ and $\rho_0 > 0$, we have*

$$(5.13) \quad \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right|^2 d\mu \right] \leq C(|F|, |G|).$$

The proof of this proposition is based on an induction argument. The base case, for $F = G = \emptyset$, is the standard Dirichlet energy estimate (3.12) for ψ_m . Although this is not necessary, for greater clarity we first present the easier proof of the special case with $G = \emptyset$ and arbitrary F in Subsection 5.3. We then give a proof for the general case in Subsection 5.4. This requires a more careful use of Fubini's lemma and some inclusion-exclusion argument. The proof of Proposition 5.2 is then carried out in Subsection 5.5, by combining the results above according to the outline just discussed.

5.2. Expansion in finite volume. We prove Lemma 5.3 in this part.

Proof of Lemma 5.3. We start by decomposing the expression for Δ_m^ρ with respect to $\mu_\rho \llcorner \square_{m+1}$, as the particles outside \square_{m+1} will not contribute to the perturbation

$$\begin{aligned} \Delta_m^\rho &\stackrel{(4.6)}{=} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^\rho) \nabla \psi_m^\rho d\mu \right] \\ &= e^{-\rho |\square_{m+1}|} \sum_{j=0}^{\infty} \frac{(\rho |\square_{m+1}|)^j}{j!} \left(\int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket} d\mu \right] \right). \end{aligned}$$

We establish first that the series in the above expression converges absolutely. Indeed, using the Cauchy–Schwarz inequality and applying the bound (3.12) on the Dirichlet energy, we can write

$$\begin{aligned} &\left| \int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket} d\mu \right] \right| \\ &\leq \left(\int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |(\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket}|^2 d\mu \right] \right)^{\frac{1}{2}} \\ (5.14) \quad &\times \left(\int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla \psi_m|^2 d\mu \right] \right)^{\frac{1}{2}} \\ &\leq \left(\int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |(\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket}|^2 d\mu \right] \right)^{\frac{1}{2}}. \end{aligned}$$

We introduce the notation

$$A_j := \int_{(\square_{m+1})^{\llbracket 1, j \rrbracket}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |(\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket}|^2 d\mu \right].$$

We can further split the integrals contributing to A_j according to the subset $E \subseteq \llbracket 1, j \rrbracket$ of particles outside of \square_m , leading to

$$\begin{aligned} (5.15) \quad A_j &= \sum_{E \subseteq \llbracket 1, j \rrbracket} \left(\frac{|\square_{m+1} \setminus \square_m|}{|\square_{m+1}|} \right)^{|E|} \left(\frac{|\square_m|}{|\square_{m+1}|} \right)^{j-|E|} B_{j,E}, \\ B_{j,E} &:= \int_{(\square_{m+1} \setminus \square_m)^E} \int_{(\square_m)^{\llbracket 1, j \rrbracket \setminus E}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |(\mathbf{a} - \mathbf{a}^{\llbracket 1, j \rrbracket}) \nabla \psi_m^{\llbracket 1, j \rrbracket}|^2 d\mu \right]. \end{aligned}$$

Now for (Lebesgue) almost every $(x_i)_{i \in E} \in (\square_{m+1} \setminus \square_m)^E$ fixed, they can be treated together with $\mu \llcorner (\square_m)^c$ as the “outer environment”, and we apply the improved energy inequality (3.18) for $(\mu(\square_m) + j - |E|)$ particles to obtain that

$$\int_{(\square_m)^{\llbracket 1, j \rrbracket \setminus E}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |\nabla \psi_m^{\llbracket 1, j \rrbracket}|^2 d\mu \right] \mu(\square_m), \mu \llcorner (\square_m)^c \leq \frac{(\mu(\square_m) + j - |E|)}{\rho_0 |\square_m|}.$$

From this expression and the uniform ellipticity assumption (2.1), one obtains that

$$B_{j,E} \leq C \frac{\rho_0 |\square_m| + j - |E|}{\rho_0 |\square_m|},$$

and thus

$$A_j \leq C \sum_{\ell=0}^j \binom{j}{\ell} 3^{-d(j-\ell)} (1-3^{-d})^\ell \left(1 + \frac{j-\ell}{\rho_0 |\square_m|}\right) \leq C \left(1 + \frac{j}{\rho_0 |\square_m|}\right).$$

We use this estimate with (5.14) to get that

$$\begin{aligned} \sum_{j=0}^{\infty} \frac{(\rho |\square_{m+1}|)^j}{j!} \left| \mathcal{f}_{(\square_{m+1})[[1,j]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{[[1,j]]}) \nabla \psi_m^{[[1,j]]} d\mu \right] \right| \\ \leq C \sum_{j=0}^{\infty} \frac{(\rho |\square_{m+1}|)^j}{j!} \left(1 + \frac{j}{\rho_0 |\square_m|}\right)^{\frac{1}{2}} < \infty, \end{aligned}$$

which implies that the series is absolutely convergent. Since $e^{-\rho |\square_{m+1}|}$ is analytic with respect to ρ , their product Δ_m^ρ is also an analytic function of ρ . Then we expand $e^{-\rho |\square_{m+1}|}$ into its Talyor series

$$\begin{aligned} \Delta_m^\rho = \sum_{l=0}^{\infty} \frac{(-\rho |\square_{m+1}|)^l}{l!} \sum_{j=0}^{\infty} \frac{(\rho |\square_{m+1}|)^j}{j!} \\ \times \left(\mathcal{f}_{(\square_{m+1})[[1,j]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{[[1,j]]}) \nabla \psi_m^{[[1,j]]} d\mu \right] \right), \end{aligned}$$

and the absolute convergence allows us to reorganize the summations according to

$$\begin{aligned} \Delta_m^\rho = \sum_{k=0}^{\infty} \sum_{\substack{l,j \in \mathbb{N}, \\ l+j=k}} \frac{(-1)^l (\rho |\square_{m+1}|)^k}{l! j!} \\ \times \left(\mathcal{f}_{(\square_{m+1})[[1,j]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{[[1,j]]}) \nabla \psi_m^{[[1,j]]} d\mu \right] \right). \end{aligned}$$

We also observe that the part $\mathcal{f}_{(\square_{m+1})[[1,j]]}(\dots)$ means the adding of j particles in \square_{m+1} , but the indices do not play a specific role. Thus we have

$$\begin{aligned} \mathcal{f}_{(\square_{m+1})[[1,j]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^{[[1,j]]}) \nabla \psi_m^{[[1,j]]} d\mu \right] \\ = \binom{k}{j}^{-1} \sum_{E \subseteq [[1,k]], |E|=j} \mathcal{f}_{(\square_{m+1})[[1,k]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^E) \nabla \psi_m^E d\mu \right]. \end{aligned}$$

This leads to

$$\begin{aligned} \Delta_m^\rho &= \sum_{k=0}^{\infty} \sum_{\substack{l,j \in \mathbb{N}, \\ l+j=k}} \frac{(-1)^l \rho^k}{k!} \sum_{E \subseteq [[1,k]], |E|=j} \left(\mathcal{f}_{(\square_{m+1})[[1,k]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^E) \nabla \psi_m^E d\mu \right] \right) \\ &= \sum_{k=0}^{\infty} \sum_{E \subseteq [[1,k]]} \frac{(-1)^{k-|E|} \rho^k}{k!} \left(\mathcal{f}_{(\square_{m+1})[[1,k]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot (\mathbf{a} - \mathbf{a}^E) \nabla \psi_m^E d\mu \right] \right) \\ &= \sum_{k=1}^{\infty} \frac{\rho^k}{k!} \left(\mathcal{f}_{(\square_{m+1})[[1,k]]} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_{[[1,k]]}((\mathbf{a} - \mathbf{a}^\#) \nabla \psi_m^\#) d\mu \right] \right). \end{aligned}$$

From the second to the third line, we use the inclusion-exclusion formula (5.1). The term $k = 0$ can be dropped since it vanishes. Finally, we can extend $\int_{(\square_{m+1})^{[1,k]}}$ to $\int_{(\mathbb{R}^d)^{[1,k]}}$ and this is the desired result (5.9). \square

5.3. Key estimate for base case. In this part, for clarity of exposition, we prove (5.13) in the simpler case $G = \emptyset$. That is, we show that for every finite $F \subseteq \mathbb{N}_+$,

$$(5.16) \quad \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_F \nabla \psi_m|^2 d\mu \right] \leq C(|F|, 0).$$

We start by introducing some notation (that will mostly be useful in the more general case treated in the next subsection). For $x, z \in \mathbb{R}^d$, we write $\Upsilon(E, z)$ to denote the indicator function

$$(5.17) \quad \Upsilon(E, z)(x) := \prod_{i \in E} \mathbf{1}_{\{x_i \in z + \square\}}.$$

We record a handful of elementary observations concerning Υ : for every finite sets $E, F \subseteq \mathbb{N}_+$ and $z \in \mathbb{R}^d$, we have

$$(5.18) \quad \Upsilon(E, z) \Upsilon(F, z) = \Upsilon(E \cup F, z),$$

$$(5.19) \quad \int_{(\mathbb{R}^d)^F} \Upsilon(E, z) \leq \int_{(\mathbb{R}^d)^{F \setminus E}} \Upsilon(E \setminus F, z),$$

and

$$(5.20) \quad |D_E \mathbf{a}(\mu, z)| \leq 2^{|E|} \Lambda \Upsilon(E, z).$$

Proof of (5.16). The case $F = \emptyset$ is basic energy estimate in (3.12), so we now assume that $F \neq \emptyset$. By Proposition 3.3 for $\rho = 0$, we have for any finite $E_1, E_2 \subseteq \mathbb{N}_+$ that

$$(5.21) \quad \begin{aligned} \int_{(\square_{m+1})^{E_1 \cup E_2}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E_2} \cdot \mathbf{a}^{E_1} \nabla \psi_m^{E_1} d\mu \right] \\ = \int_{(\square_{m+1})^{E_1 \cup E_2}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E_2} \cdot q d\mu \right]. \end{aligned}$$

We apply this with $E_1, E_2 \subseteq F$, thus we can extend as an average over particles in F that

$$(5.22) \quad \begin{aligned} \int_{(\square_{m+1})^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E_2} \cdot \mathbf{a}^{E_1} \nabla \psi_m^{E_1} d\mu \right] \\ = \int_{(\square_{m+1})^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E_2} \cdot q d\mu \right]. \end{aligned}$$

We do the linear combination of (5.22) over all the $E_1 \subseteq F$ and apply the inclusion-exclusion formula (5.1) to obtain

$$(5.23) \quad \int_{(\square_{m+1})^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E_2} \cdot D_F (\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

Here the sum on the right-hand side is zero thanks to the inclusion-exclusion formula and $F \neq \emptyset$. We extend the integration $\int_{(\square_{m+1})^F}$ to $\int_{(\mathbb{R}^d)^F}$ and then apply the linear combination of (5.23) over all the $E_2 \subseteq F$ to obtain

$$(5.24) \quad \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} D_F (\nabla \psi_m) \cdot D_F (\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

Now we use the Leibniz's formula in (5.3) and obtain that

$$D_F(\mathbf{a}^\# \nabla \psi_m^\#) = \sum_{G \subseteq F} D_{F \setminus G}(\mathbf{a}^G)(D_G \nabla \psi_m).$$

We put this back to (5.24), and keep the term $(D_F \nabla \psi_m) \cdot \mathbf{a}^F(D_F \nabla \psi_m)$ on the left-hand side, while moving the other terms to the right-hand side

$$\begin{aligned} & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (D_F \nabla \psi_m) \cdot \mathbf{a}^F(D_F \nabla \psi_m) d\mu \right] \\ &= - \sum_{G \not\subseteq F} \left(\int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (D_F \nabla \psi_m) \cdot D_{F \setminus G}(\mathbf{a}^G)(D_G \nabla \psi_m) d\mu \right] \right). \end{aligned}$$

Using Young's inequality, we obtain that

$$\begin{aligned} & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_F \nabla \psi_m|^2 d\mu \right] \\ & \leq \sum_{G \not\subseteq F} \left(\int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_{F \setminus G}(\mathbf{a}^G)| |D_G \nabla \psi_m|^2 d\mu \right] \right). \end{aligned}$$

Then we use Fubini's lemma to pass $\int_{(\mathbb{R}^d)^{F \setminus G}}$

$$\begin{aligned} & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_{F \setminus G}(\mathbf{a}^G)| |D_G \nabla \psi_m|^2 d\mu \right] \\ &= \int_{(\mathbb{R}^d)^G} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^{F \setminus G}} |D_{F \setminus G}(\mathbf{a}^G)| \right) |D_G \nabla \psi_m|^2 d\mu \right]. \end{aligned}$$

The last line uses the fact that $D_G \nabla \psi_m$ does not involve the particle in $F \setminus G$. A varied version of (5.20) and (5.19) gives us that

$$\int_{(\mathbb{R}^d)^{F \setminus G}} |D_{F \setminus G}(\mathbf{a}^G)| \leq 2^{|F \setminus G|} \Lambda \int_{(\mathbb{R}^d)^{F \setminus G}} \Upsilon(F \setminus G, \cdot) \leq 2^{|F \setminus G|} \Lambda.$$

Therefore, we obtain an estimate that

$$\begin{aligned} (5.25) \quad & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_F \nabla \psi_m|^2 d\mu \right] \\ & \leq \sum_{G \not\subseteq F} \left(2^{|F \setminus G|} \Lambda \int_{(\mathbb{R}^d)^G} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_G \nabla \psi_m|^2 d\mu \right] \right). \end{aligned}$$

This estimate allows us to justify the induction argument. Indeed, the case $|F| = 0$ is the Dirichlet energy estimate. Suppose (5.16) is valid for $|F| = n$, then for $|F| = n + 1$, we apply (5.25). As the quantity on the right-hand side only relies on $G \not\subseteq F$, which implies $|G| \leq n$, we can invoke (5.16) for lower order. This completes the proof of (5.16). \square

5.4. Key estimate for the general case. In this part, we now treat the general case of (5.13).

Proof of Proposition 5.4. We decompose the proof into three steps and we suppose $F \neq \emptyset$.

Step 1: Expansion. We start once again from (5.22), and apply a “doubling variables trick”. For $G \subseteq F \subseteq \mathbb{N}_+$, we add another set $G' \subseteq \mathbb{N}_+ \setminus F$ such that $|G'| = |G|$,

and consider (5.22) for some $E_1 \subseteq F$ and $E'_2 \subseteq (F \setminus G) \sqcup G'$. Then $(E_1 \cup E'_2) \subseteq (F \sqcup G')$ and (5.22) becomes

$$\begin{aligned} \int_{(\square_{m+1})^{F \sqcup G'}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E'_2} \cdot \mathbf{a}^{E_1} \nabla \psi_m^{E_1} d\mu \right] \\ = \int_{(\square_{m+1})^{F \sqcup G'}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E'_2} \cdot q d\mu \right]. \end{aligned}$$

Then we apply the inclusion-exclusion formula (5.1) over all $E_1 \subseteq F$ and obtain that

$$\int_{(\square_{m+1})^{F \sqcup G'}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m^{E'_2} \cdot D_F(\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

From this line, we can extend $\int_{(\square_{m+1})^{F \sqcup G'}}$ to $\int_{(\mathbb{R}^d)^{F \sqcup G'}}$. We then apply the inclusion-exclusion formula (5.1) over all $E'_2 \subseteq (F \setminus G) \sqcup G'$ and obtain

$$\int_{(\mathbb{R}^d)^{F \sqcup G'}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} (D_{(F \setminus G) \sqcup G'} \nabla \psi_m) \cdot D_F(\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

Notice that the particles in G' only act on the term $(D_{(F \setminus G) \sqcup G'} \nabla \psi_m)$, we can pass $\int_{(\mathbb{R}^d)^{G'}}$ to the interior and this equation becomes

$$\int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^{G'}} D_{(F \setminus G) \sqcup G'} \nabla \psi_m \right) \cdot D_F(\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

Up to a relabelling of the particles, we can write

$$\int_{(\mathbb{R}^d)^{G'}} D_{(F \setminus G) \sqcup G'} \nabla \psi_m = \int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m,$$

and obtain a counter-part of (5.24) that

$$\int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) \cdot D_F(\mathbf{a}^\# \nabla \psi_m^\#) d\mu \right] = 0.$$

Like (5.24), we do an expansion for this identity for the term $D_F(\mathbf{a}^\# \nabla \psi_m^\#)$, but we need to treat it more carefully. We apply (5.4) on $D_F(\mathbf{a}^\# \nabla \psi_m^\#)$ and obtain that

$$D_F(\mathbf{a}^\# \nabla \psi_m^\#) = \sum_{F_1 \cup F_2 = F} D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m).$$

We keep the term

$$\{F_1 \cup F_2 = F\} \cap \{F_2 \subseteq (F \setminus G)\} \cap \{F_1 = F\},$$

on the left-hand side, while putting the other terms

$$\{F_1 \cup F_2 = F\} \cap (\{F_2 \cap G \neq \emptyset\} \cup \{F_1 \not\subseteq F\}),$$

on the right-hand side. We also notice (5.2) that

$$\sum_{F_2 \subseteq (F \setminus G)} D_{F_2}(\mathbf{a}) = \mathbf{a}^{F \setminus G},$$

so we obtain that

$$\begin{aligned} (5.26) \quad & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) \cdot \mathbf{a}^{F \setminus G} (D_F \nabla \psi_m) d\mu \right] \\ & = \sum_{\substack{F_1 \cup F_2 = F \\ F_2 \cap G \neq \emptyset, \text{ or } F_1 \not\subseteq F}} - \left(\int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) \cdot D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m) d\mu \right] \right). \end{aligned}$$

Because $\mathbf{a}^{F \setminus G}$, $\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m$ and $d\mu$ do not depend on the particles indexed by G , we can apply Fubini's lemma to pass $\int_{(\mathbb{R}^d)^G}$ to interior, thus the left-hand side of (5.26) becomes

$$\begin{aligned} & \int_{(\mathbb{R}^d)^F} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) \cdot \mathbf{a}^{F \setminus G} (D_F \nabla \psi_m) d\mu \right] \\ &= \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) \cdot \mathbf{a}^{F \setminus G} \left(\int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right) d\mu \right] \\ &\geq \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right|^2 d\mu \right]. \end{aligned}$$

For the right-hand side, we argue similarly and use Young's inequality to obtain that

$$\begin{aligned} (5.27) \quad & \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_F \nabla \psi_m \right|^2 d\mu \right] \\ &\leq C \sum_{\substack{F_1 \cup F_2 = F \\ F_2 \cap G \neq \emptyset, \text{ or } F_1 \not\subseteq F}} \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m) \right|^2 d\mu \right]. \end{aligned}$$

Step 2: Simplification and recurrence inequality. The final goal is to get a recurrence like (5.25), but (5.27) still needs some further simplification. We focus on the term

$$\int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m).$$

Since $F_1 \cup F_2 = F$, we use the disjoint decomposition that

$$F = (F_2 \setminus F_1) \sqcup (F_1 \setminus F_2) \sqcup (F_2 \cap F_1),$$

which also induces the decomposition of G

$$G = ((G \cap F_2) \setminus F_1) \sqcup ((G \cap F_1) \setminus F_2) \sqcup (G \cap F_2 \cap F_1).$$

Thus, we can decompose

$$\int_{(\mathbb{R}^d)^G} = \int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}},$$

and pass them respectively to the proper term

$$\begin{aligned} & \int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m) \\ &= \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} D_{F_2}(\mathbf{a}) \right) \left(\int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right) \right). \end{aligned}$$

Let $z \in \text{supp}(\mu)$ be the particle at which the gradient is computed, then we use the notation (5.17) and the estimate (5.20) to give its bound

$$\begin{aligned} & \left| \int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a}) D_{F_1} \nabla \psi_m \right|^2(z) \\ &\leq \left| \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} |D_{F_2}(\mathbf{a})| \right) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right| \right) \right|^2(z) \\ &\leq 4^{|F_2|} \Lambda^2 \left| \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, z) \right) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right| \right) \right|^2(z). \end{aligned}$$

Next, we use the property that $\Upsilon(F_2, z)$ requires all the particles in F_2 to live in $z + \square$

$$\begin{aligned}
& \left| \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, z) \right) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right| \right) \right|^2 (z) \\
&= \left| \int_{(z + \square)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, \cdot) \right) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right| \right) \right|^2 (z) \\
&\leq \int_{(z + \square)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, \cdot) \right)^2 \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) (z) \\
&= \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\left(\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, \cdot) \right)^2 \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) (z).
\end{aligned}$$

From the second line to the third line, we use the Cauchy–Schwarz inequality, and from the third line to the fourth line, we reapply the property of $\Upsilon(F_2, z)$. So in this step we gain a small factor for Cauchy–Schwarz inequality. Now, we use the property (5.19)

$$\int_{(\mathbb{R}^d)^{(G \cap F_2) \setminus F_1}} \Upsilon(F_2, z) \leq \Upsilon(F_2 \setminus ((G \cap F_2) \setminus F_1), z).$$

We put all these estimates back to the right-hand side of (5.27) to obtain that

$$\begin{aligned}
(5.28) \quad & \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a}) (D_{F_1} \nabla \psi_m) \right|^2 d\mu \right] \\
& \leq 4^{|F_2|} \Lambda^2 \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \right. \\
& \quad \left. \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\Upsilon(F_2 \setminus ((G \cap F_2) \setminus F_1), \cdot) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right].
\end{aligned}$$

In this integral, we can continue some simplification with $\Upsilon(F_2 \setminus ((G \cap F_2) \setminus F_1), \cdot)$. We have the following disjoint union

$$F \setminus G = ((F_2 \cap F_1) \setminus G) \sqcup ((F_2 \setminus F_1) \setminus G) \sqcup ((F_1 \setminus F_2) \setminus G),$$

which implies that

$$(5.29) \quad \int_{(\mathbb{R}^d)^{F \setminus G}} = \int_{(\mathbb{R}^d)^{(F_2 \cap F_1) \setminus G}} + \int_{(\mathbb{R}^d)^{(F_2 \setminus F_1) \setminus G}} + \int_{(\mathbb{R}^d)^{(F_1 \setminus F_2) \setminus G}}.$$

Because $\int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m$ only involves a subset of particles in F_1 , which is disjoint from $(F_2 \setminus F_1) \setminus G$, we use Fubini's lemma to pass the integration of $\int_{(\mathbb{R}^d)^{(F_2 \setminus F_1) \setminus G}}$

to the inside

$$\begin{aligned}
& \int_{(\mathbb{R}^d)^{(F_2 \setminus F_1) \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \right. \\
& \quad \left. \left(\Upsilon(F_2 \setminus ((G \cap F_2) \setminus F_1), \cdot) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right] \\
&= \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \right. \\
& \quad \left. \left(\left(\int_{(\mathbb{R}^d)^{(F_2 \setminus F_1) \setminus G}} \Upsilon(F_2 \setminus ((G \cap F_2) \setminus F_1), \cdot) \right) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right] \\
&= \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \left(\Upsilon(F_2 \cap F_1, \cdot) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right] \\
&= \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\Upsilon(F_2 \cap F_1, \cdot) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right].
\end{aligned}$$

From the second line to the third line, we used (5.19) and the decomposition

$$F_2 \setminus ((G \cap F_2) \setminus F_1) = (F_2 \cap F_1) \sqcup ((F_2 \setminus F_1) \setminus G).$$

See the Venn diagram in Figure 1 to help check this equation. From the third line to the fourth line, we put the integral $\int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}}$ outside the expectation using Fubini's lemma. We combine this integral together with the rest of integrals in (5.29) and we observe that

$$(5.30) \quad \int_{(\mathbb{R}^d)^{(F_2 \cap F_1) \setminus G}} \int_{(\mathbb{R}^d)^{(F_1 \setminus F_2) \setminus G}} \int_{(\mathbb{R}^d)^{G \cap F_2 \cap F_1}} = \int_{(\mathbb{R}^d)^{F_1 \setminus ((G \cap F_1) \setminus F_2)}}.$$

because of the identity (see Figure 1 to help check this equation)

$$((F_2 \cap F_1) \setminus G) \sqcup ((F_1 \setminus F_2) \setminus G) \sqcup (G \cap F_2 \cap F_1) = F_1 \setminus ((G \cap F_1) \setminus F_2).$$

Therefore, one term in the right-hand side of (5.27) can be bounded

$$\begin{aligned}
& \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^G} D_{F_2}(\mathbf{a})(D_{F_1} \nabla \psi_m) \right|^2 d\mu \right] \\
& \leq \int_{(\mathbb{R}^d)^{F_1 \setminus ((G \cap F_1) \setminus F_2)}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\Upsilon(F_2 \cap F_1, \cdot) \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 \right) d\mu \right].
\end{aligned}$$

We can further drop out the indicator $\Upsilon(F_2 \cap F_1, \cdot)$, and put it back to (5.27) to obtain that

$$\begin{aligned}
(5.31) \quad & \int_{(\mathbb{R}^d)^{F \setminus G}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\square_m)^G} (D_F \nabla \psi_m) \right|^2 d\mu \right] \\
& \leq \sum_{\substack{F_1 \cup F_2 = F \\ F_2 \cap G \neq \emptyset, \text{ or } F_1 \not\subseteq F}} 4^{|F_2|} \Lambda^2 \int_{(\mathbb{R}^d)^{F_1 \setminus ((G \cap F_1) \setminus F_2)}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^{(G \cap F_1) \setminus F_2}} D_{F_1} \nabla \psi_m \right|^2 d\mu \right].
\end{aligned}$$

Step 3: Induction argument. Equation (5.31) is the analogue of (5.25) for the general case. In this step, we describe the induction argument, which consists in obtaining a bound for the constant $C(i, j)$ in (5.13) in terms of a linear combination of the $C(i', j')$ with $i' \leq i$, $j' \leq j$, and $i' + j' < i + j$. An illustration is in Figure 2.

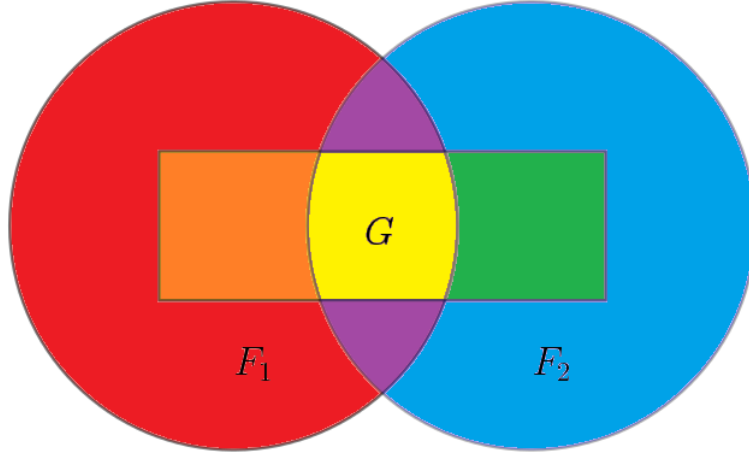


FIGURE 1. A Venn diagram for illustration. The disk on the left represents F_1 and the disk on the right represents F_2 . The rectangle is G . We use different colors for the partition of $F = F_1 \cup F_2$, and it has the following bijections.

$$\begin{aligned}
 F_1 \cap F_2 &= \{\text{yellow, purple}\}, \\
 G \cap F_1 \cap F_2 &= \{\text{yellow}\}, \\
 (F_1 \cap F_2) \setminus G &= \{\text{purple}\}, \\
 (F_1 \setminus F_2) \setminus G &= \{\text{red}\}, \\
 (F_2 \setminus F_1) \setminus G &= \{\text{blue}\}, \\
 F_1 \setminus ((G \cap F_1) \setminus F_2) &= \{\text{red, yellow, purple}\}, \\
 F_2 \setminus ((G \cap F_2) \setminus F_1) &= \{\text{blue, yellow, purple}\}.
 \end{aligned}$$

We denote by $\tilde{I}(m, \rho_0, F, G)$ the left-hand side of (5.31). This equation can be rewritten as

$$(5.32) \quad \tilde{I}(m, \rho_0, F, G) \leq 4^{|F_2|} \Lambda^2 \sum_{\substack{F_1 \cup F_2 = F \\ F_2 \cap G \neq \emptyset, \text{ or } F_1 \not\subseteq F}} \tilde{I}(m, \rho_0, F_1, (G \cap F_1) \setminus F_2).$$

For sets F_1, F_2 as in the summands above, we clearly have

$$|F_1| + |(G \cap F_1) \setminus F_2| \leq |F| + |G|.$$

In fact, the inequality is always strict. Indeed, a possible case of equality would require that $F_1 = F$, since $F_1 \subseteq F$ and $(G \cap F_1) \setminus F_2 \subseteq G$. But if $F_1 = F$, then we must have $F_2 \cap G \neq \emptyset$, and thus

$$|(G \cap F_1) \setminus F_2| = |G \setminus F_2| \leq |G| - 1.$$

So all the summands on the right side of (5.32) are such that

$$|F_1| + |(G \cap F_1) \setminus F_2| < |F| + |G|.$$

The induction argument is then clear: the case when $F = G = \emptyset$ is the basic Dirichlet energy estimate. Next, assuming the boundedness of $\tilde{I}(m, \rho_0, F, G)$ for $|F| + |G| \leq k$, we can obtain the result for $|F| + |G| = k + 1$ by an application of (5.32). This completes the proof of Proposition 5.4. \square

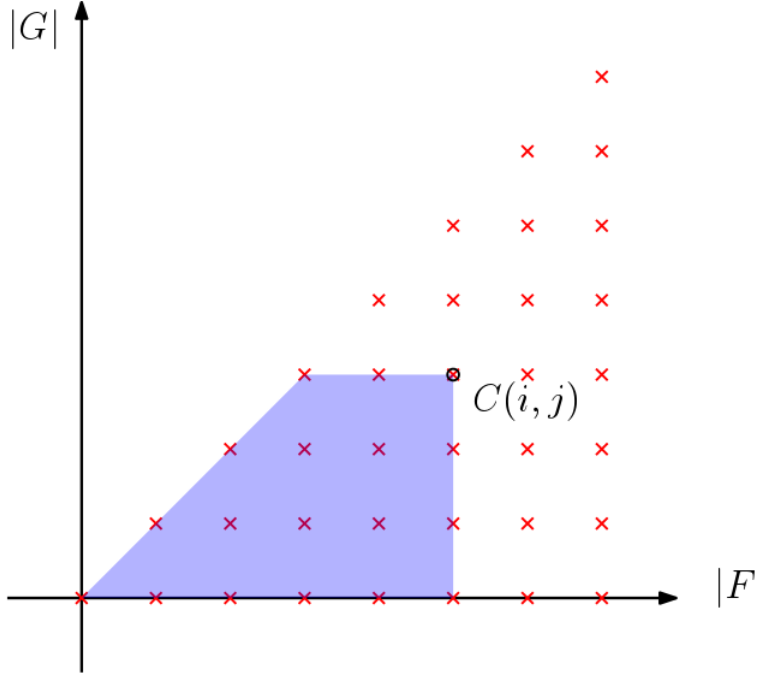


FIGURE 2. An illustration of the recurrence argument. The constant $C(i, j)$ can be bounded by a linear combination of the $C(i', j')$ with $j' \leq j$, $i' \leq i$, and $i' + j' < i + j$.

5.5. Smoothness in finite volume. We can now combine Lemma 5.3 and Proposition 5.4 to complete the proof of Proposition 5.2.

Proof of Proposition 5.2. We decompose the proof into three steps.

Step 1: Decomposition and expansion. As stated in Subsection 5.1, we first expand Δ_m^ρ with respect to ρ as in (5.9) and use the Leibniz formula (5.4) to get that

$$(5.33) \quad \Delta_m^\rho(\rho_0) = \sum_{k=1}^{\infty} \frac{\rho^k}{k!} c_{k,m}(\rho_0) = \sum_{k=1}^{\infty} \frac{\rho^k}{k!} \sum_{E \cup F = \llbracket 1, k \rrbracket} I(m, \rho_0, E, F),$$

with $c_{k,m}$ defined in (5.6) and $I(m, \rho_0, E, F)$ defined in (5.12). Lemma 5.3 ensures that this series converges, and that $\rho \mapsto \Delta_m^\rho$ is analytic. In the next step, we aim to give a bound to $I(m, \rho_0, E, F)$ which is uniform with respect to m and ρ_0 .

Step 2: Reduction of $I(m, \rho_0, E, F)$. Recall the expression of $I(m, \rho_0, E, F)$ in (5.12), we use Fubini's lemma and pass the integration $\llbracket 1, k \rrbracket \setminus E$ inside. Notice that we have $\llbracket 1, k \rrbracket \setminus E = F \setminus E$ thanks to $E \cup F = \llbracket 1, k \rrbracket$. Since the particles in the set $F \setminus E$ do not appear in $D_E(\mathbf{a} - \mathbf{a}^\#)$, we have

$$I(m, \rho_0, E, F) = \int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \nabla \psi_m \cdot D_E(\mathbf{a} - \mathbf{a}^\#) \left(\int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \, d\mu \right) \right].$$

We apply the Cauchy–Schwarz inequality and obtain that

$$\begin{aligned} |I(m, \rho_0, E, F)| &\leq \left(\int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_E(\mathbf{a} - \mathbf{a}^\#)| |\nabla \psi_m|^2 \, d\mu \right] \right)^{\frac{1}{2}} \\ &\quad \times \left(\int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_E(\mathbf{a} - \mathbf{a}^\#)| \left| \int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \, d\mu \right|^2 \, d\mu \right] \right)^{\frac{1}{2}}. \end{aligned}$$

The first term is easy to treat since we can use Fubini's lemma that

$$\begin{aligned} & \int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_E(\mathbf{a} - \mathbf{a}^\#)| |\nabla \psi_m|^2 d\mu \right] \\ &= \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^E} |D_E(\mathbf{a} - \mathbf{a}^\#)| \right) |\nabla \psi_m|^2 d\mu \right] \\ &\leq 2^{|E|} \Lambda. \end{aligned}$$

In the last step, we apply (5.20) and (5.19) that

$$\int_{(\mathbb{R}^d)^E} |D_E(\mathbf{a} - \mathbf{a}^\#)| \leq 2^{|E|} \Lambda \int_{(\mathbb{R}^d)^E} \Upsilon(E, \cdot) \leq 2^{|E|} \Lambda.$$

For the second term, we use the decomposition

$$D_E = D_{E \setminus F} \circ D_{E \cap F}, \quad \int_{(\mathbb{R}^d)^E} = \int_{(\mathbb{R}^d)^{E \setminus F}} \int_{(\mathbb{R}^d)^{E \cap F}},$$

and pass the integration $\int_{(\mathbb{R}^d)^{E \setminus F}}$ inside

$$\begin{aligned} & \int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_E(\mathbf{a} - \mathbf{a}^\#)| \left| \int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \right|^2 d\mu \right] \\ &= \int_{(\mathbb{R}^d)^{E \cap F}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left(\int_{(\mathbb{R}^d)^{E \setminus F}} |D_E(\mathbf{a} - \mathbf{a}^\#)| \right) \left| \int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \right|^2 d\mu \right]. \end{aligned}$$

We apply once again the estimate (5.19) and (5.20) that

$$\int_{(\mathbb{R}^d)^{E \setminus F}} |D_E(\mathbf{a} - \mathbf{a}^\#)| \leq 2^{|E|} \int_{(\mathbb{R}^d)^{E \setminus F}} \Upsilon(E, \cdot) \leq 2^{|E|} \Lambda \Upsilon(E \cap F, \cdot) \leq 2^{|E|} \Lambda.$$

Therefore, we bound the second term by

$$\begin{aligned} & \int_{(\mathbb{R}^d)^E} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} |D_E(\mathbf{a} - \mathbf{a}^\#)| \left| \int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \right|^2 d\mu \right] \\ &\leq 2^{|E|} \Lambda \int_{(\mathbb{R}^d)^{E \cap F}} \mathbb{E} \left[\frac{1}{\rho_0 |\square_m|} \int_{\square_m} \left| \int_{(\mathbb{R}^d)^{F \setminus E}} D_F \nabla \psi_m \right|^2 d\mu \right]. \end{aligned}$$

Here we apply the key estimate Proposition 5.4 to conclude the proof a the uniform bound of $I(m, \rho_0, E, F)$ with respect to m and ρ_0 . This also implies the uniform bound (5.7) for $c_{k,m}(\rho_0)$.

Step 3: Control of the tail R_k . In this step, we need to control the tail in the expansion of $\Delta_m^\rho(\rho_0)$. In fact, the estimate in Step 2 allows us to obtain the uniform bound of $|c_{k,m}(\rho_0)| \leq C_k$ defined in Proposition 5.2, but the best available bound in k is that $C_k \sim (k!)^2$ if one checks the proof of Proposition 5.4 carefully. Thus, when we put this bound into (5.9), the series $\sum_{j>k} \frac{C_j}{j!} \rho^j$ will not be summable. On the other hand, we know the function $\rho \mapsto \Delta_m^\rho(\rho_0)$ is indeed analytic for any fixed $\rho_0 \in \mathbb{R}_+$ (using a naive bound of $c_{k,m}$ depending on m , see Lemma 5.3 and its proof in Subsection 5.2), so for $c_{j,m}$ defined in Proposition 5.2 and $\rho_0 > 0$, we have

$$c_{j,m}(\rho_0) = \left(\frac{d}{d\rho} \right)_{\rho=0}^j \Delta_m^\rho(\rho_0).$$

We also write $\partial^j \Delta_m^\rho$ as a shorthand notation for the j -th derivative at ρ ,

$$\partial^j \Delta_m^\rho(\rho_0) := \left(\frac{d}{d\rho} \right)^j \Delta_m^\rho(\rho_0).$$

Then we apply Taylor's expansion for the function $\rho \mapsto \Delta_m^\rho(\rho_0)$ until order k

$$(5.34) \quad \Delta_m^\rho(\rho_0) = \sum_{j=0}^k \frac{\partial^j \Delta_m^0(\rho_0)}{j!} \rho^j + \int_0^\rho \frac{\partial^{k+1} \Delta_m^s(\rho_0)}{k!} s^k ds.$$

Recalling the definition of Δ_m^ρ in (4.2), we have

$$\begin{aligned} \partial^{k+1} \Delta_m^s(\rho_0) &= \left(\frac{d}{d\rho} \right)_{|\rho=s}^j (q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0 + \rho) q - q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0) q) \\ &= \left(\frac{d}{d\rho} \right)_{|\rho=0}^j (q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0 + s + \rho) q - q \cdot \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0 + s) q) \\ &= \partial^{k+1} \Delta_m^0(\rho_0 + s). \end{aligned}$$

Since $\partial^{k+1} \Delta_m^0(\rho_0 + s) = c_{k+1,m}(\rho_0 + s)$, upon inserting this back into (5.34), it follows that

$$(5.35) \quad \Delta_m^\rho(\rho_0) = \sum_{j=0}^k \frac{c_{j,m}(\rho_0)}{j!} \rho^j + \int_0^\rho \frac{c_{k+1,m}(\rho_0 + s)}{k!} s^k ds.$$

This gives us an expression for the remainder of order k in (5.8), which is

$$(5.36) \quad R_k(m, \rho_0, \rho) := \int_0^\rho \frac{c_{k+1,m}(\rho_0 + s)}{k!} s^k ds.$$

Using the uniform estimate (5.7) of $c_{k+1,m}(\rho_0 + s)$ with respect to $\rho_0 + s$ and m , the remainder is of order $O(\rho^{k+1})$ independent of ρ_0 and m . This finishes our proof of Proposition 5.2. \square

5.6. Proof of the main theorem. In this final subsection, we conclude the proof of the main Theorem 2.3, using Proposition 5.2.

Proof of Theorem 2.3. As a first step, we show the existence of the limit in (2.12). Let $k \geq 2$ and assume by induction that the existence of $c_j(\rho_0)$ is established for $1 \leq j \leq k-1$ and $\rho_0 > 0$ (recall that the existence of $c_1(\rho_0)$ follows from Theorem 2.1). For $\rho_0 > 0$, the sequence $\{c_{k,m}(\rho_0)\}_{m \in \mathbb{N}}$ defined in (5.6) is bounded by some positive constant $C_k(d, \Lambda)$ using Proposition 5.2. Thus, there exists a subsequence $\{c_{k,m_\ell}(\rho_0)\}_{\ell \in \mathbb{N}}$ (possibly depending on ρ_0) such that

$$c_k^*(\rho_0) := \lim_{\ell \rightarrow +\infty} c_{k,m_\ell}(\rho_0)$$

exists. By (5.8), one has for $\rho > 0$

$$\left| \Delta_{m_\ell}^\rho(\rho_0) - \sum_{j=1}^{k-1} \frac{c_{j,m_\ell}(\rho_0) \rho^j}{j!} - \frac{c_{k,m_\ell}(\rho_0)}{k!} \rho^k \right| \leq |R_k(m_\ell, \rho_0, \rho)|,$$

and passing to the limit $\ell \rightarrow \infty$ yields (upon using Proposition 5.2, the induction hypothesis and (4.3))

$$(5.37) \quad \sup_{\rho_0 \in (0, \infty)} \left| \Delta^\rho(\rho_0) - \sum_{j=1}^{k-1} \frac{c_j(\rho_0) \rho^j}{j!} - \frac{c_k^*(\rho_0)}{k!} \rho^k \right| \leq O(\rho^{k+1}), \quad \text{for } \rho > 0.$$

In particular, (5.37) implies that $c_k^*(\rho_0)$ is the unique limit of the full sequence $\{c_{k,m}(\rho_0)\}_{m \in \mathbb{N}}$, and we denote it by $c_k(\rho_0)$. This proves (2.12). We note in passing that

$$(5.38) \quad c_1, \dots, c_k : (0, \infty) \rightarrow \mathbb{R} \text{ are bounded functions,}$$

which follows by (2.12) and $|c_{k,m}| \leq C_k(d, \Lambda)$, see Proposition 5.2. Thus, we can write

$$(5.39) \quad \Delta^\rho(\rho_0) = \sum_{j=1}^k \frac{c_j(\rho_0)}{j!} \rho^j + O(\rho^{k+1}), \quad \text{for } \rho > 0,$$

with the error term independent of ρ_0 . We now turn to the proof of the expansion (2.13), which extends the previous display to $\rho \in (-\rho_0, 0)$. To simplify notation, we again set $f(\cdot) := q \cdot \bar{\mathbf{a}}^{-1}(\cdot)q$. We claim that the expansion (5.39) implies that

$$(5.40) \quad c_1, \dots, c_k : (0, \infty) \rightarrow \mathbb{R} \text{ are Lipschitz-continuous,}$$

and moreover

$$(5.41) \quad f \text{ has } k \text{ derivatives, and } f^{(j)}(\rho_0) = c_j(\rho_0), \quad 1 \leq j \leq k, \quad \rho_0 > 0.$$

We first define the forward difference of order ℓ of f at $\rho_0 > 0$, $\ell \in \mathbb{N}_+$, with step size $\rho \geq 0$ as

$$(5.42) \quad \Delta^{\ell, \rho}[f](\rho_0) = \Delta^{\ell, \rho}(\rho_0) := \sum_{i=0}^{\ell} \binom{\ell}{i} (-1)^{\ell-i} f(\rho_0 + i\rho),$$

(note that with our fixed choice of f , $\Delta^{1, \rho}(\rho_0) = \Delta^\rho(\rho_0)$). We claim that these quantities fulfill for $1 \leq \ell \leq k$, $\rho_0 > 0$ and $\rho \geq 0$,

$$(5.43) \quad \Delta^{\ell, \rho}(\rho_0) = c_\ell(\rho_0) \rho^\ell + O(\rho^{\ell+1}),$$

with the error term independent of ρ_0 , and for $1 \leq \ell < k$, $\rho_0 > 0$ and $\rho \geq 0$,

$$(5.44) \quad \Delta^{\ell, \rho}(\rho_0 + \rho) - \Delta^{\ell, \rho}(\rho_0) = \Delta^{\ell+1, \rho}(\rho_0).$$

We prove (5.43). To this end, we infer from (5.39) that

$$(5.45) \quad f(\rho_0 + i\rho) = \sum_{j=0}^k \frac{c_j(\rho_0)}{j!} (i\rho)^j + O(\rho^{k+1}), \quad \text{for } \rho > 0, 1 \leq i \leq k,$$

where we defined for convenience $c_0(\rho_0) := f(\rho_0)$. Equation (5.45) is now inserted into (5.42), which yields for $\rho_0 > 0$, $\rho \geq 0$ and $1 \leq \ell \leq k$ that

$$\begin{aligned} \Delta^{\ell, \rho}(\rho_0) &= \sum_{i=0}^{\ell} \binom{\ell}{i} (-1)^{\ell-i} \left\{ \sum_{j=0}^{\ell} \frac{c_j(\rho_0)}{j!} (i\rho)^j + \sum_{j=\ell+1}^k \frac{c_j(\rho_0)}{j!} (i\rho)^j + O(\rho^{k+1}) \right\} \\ &= \sum_{j=0}^{\ell} \frac{c_j(\rho_0)}{j!} \rho^j \left(\sum_{i=0}^{\ell} \binom{\ell}{i} (-1)^{\ell-i} i^j \right) + O(\rho^{\ell+1}) \\ &= c_\ell(\rho_0) \rho^\ell + O(\rho^{\ell+1}). \end{aligned}$$

Here, we combined the terms involving ρ^j with $j \in \{\ell+1, \dots, k\}$ and $O(\rho^{k+1})$ into a contribution $O(\rho^{\ell+1})$ and using (5.38) in going from the first to the second line. From the second to the third line, we use the fact that for any polynomial P with real coefficients A_0, \dots, A_k , i.e., $P(X) = A_\ell X^\ell + \dots + A_0$ of degree smaller or equal to ℓ , one has $\sum_{i=0}^{\ell} \binom{\ell}{i} (-1)^{\ell-i} P(i) = \ell! A_\ell$. Equation (5.44) also follows directly from elementary

properties of binomial coefficients. Indeed:

$$\begin{aligned}
\Delta^{\ell,\rho}(\rho_0 + \rho) - \Delta^{\ell,\rho}(\rho_0) &= \sum_{i=0}^{\ell} (-1)^{\ell-i} \binom{\ell}{i} f(\rho_0 + (i+1)\rho) - \sum_{i=0}^{\ell} (-1)^{\ell-i} \binom{\ell}{i} f(\rho_0 + i\rho) \\
&= \sum_{i=1}^{\ell+1} (-1)^{\ell-i+1} \binom{\ell}{i-1} f(\rho_0 + i\rho) + \sum_{i=0}^{\ell} (-1)^{\ell-i+1} \binom{\ell}{i} f(\rho_0 + i\rho) \\
&= \sum_{i=0}^{\ell+1} (-1)^{\ell+1-i} \left\{ \binom{\ell}{i-1} + \binom{\ell}{i} \right\} f(\rho_0 + i\rho) \\
&= \sum_{i=0}^{\ell+1} (-1)^{\ell+1-i} \binom{\ell+1}{i} f(\rho_0 + i\rho) = \Delta^{\ell+1,\rho}(\rho_0).
\end{aligned}$$

Identity (5.43) is now used at $\rho_0 + \rho$ and ρ_0 on the left-hand side of (5.44), and at ρ_0 on the right-hand side of the same equation (recall that the $O(\rho^\ell)$ resp. $O(\rho^{\ell+1})$ terms do not depend on ρ_0):

$$\begin{aligned}
(5.46) \quad & \frac{1}{\rho^\ell} (\Delta^{\ell,\rho}(\rho_0 + \rho) - \Delta^{\ell,\rho}(\rho_0)) = \frac{1}{\rho^\ell} \Delta^{\ell+1,\rho}(\rho_0) \\
\Rightarrow & c_\ell(\rho_0 + \rho) - c_\ell(\rho_0) = c_{\ell+1}(\rho_0)\rho + O(\rho), \quad \text{for } \rho > 0.
\end{aligned}$$

By the boundedness of $c_{\ell+1}$ (5.38), this establishes the Lipschitz-continuity (5.40) of c_ℓ .

Now we prove the differentiability (5.41): By induction, suppose that we already established that $f^{(\ell-1)}(\rho_0) = c_{\ell-1}(\rho_0)$ for all $\rho_0 \in (0, \infty)$, and $1 \leq \ell < k$. Now, for $\rho > 0$, one has

$$\begin{aligned}
(5.47) \quad \Delta^{\ell-1,\rho}(\rho_0) &= \sum_{i=0}^{\ell-1} \binom{\ell-1}{i} (-1)^{\ell-1-i} \left\{ \sum_{j=0}^{\ell-1} \frac{c_j(\rho_0)}{j!} (i\rho)^j + \frac{c_\ell(\rho_0)}{\ell!} (i\rho)^\ell \right\} + O(\rho^{\ell+1}) \\
&= c_{\ell-1}(\rho_0)\rho^{\ell-1} + \underbrace{\sum_{i=0}^{\ell-1} \binom{\ell-1}{i} (-1)^{\ell-1-i} \frac{i^\ell}{\ell!} c_\ell(\rho_0)}_{=: C(\ell)} \rho^\ell + O(\rho^{\ell+1}),
\end{aligned}$$

having used the same arguments as in the proof of (5.43), with $C(\ell) \in \mathbb{R}$ some numerical constant. The latter gives us that for $\rho > 0$,

$$\begin{aligned}
(5.48) \quad & \frac{1}{\rho^\ell} \Delta^{\ell,\rho}(\rho_0) \stackrel{(5.44)}{=} \frac{1}{\rho} \left\{ \frac{1}{\rho^{\ell-1}} \Delta^{\ell-1}(\rho_0 + \rho) - \frac{1}{\rho^{\ell-1}} \Delta^{\ell-1}(\rho_0) \right\} \\
&= \frac{1}{\rho} (c_{\ell-1}(\rho_0 + \rho) - c_{\ell-1}(\rho_0)) + C(\ell)(c_\ell(\rho_0 + \rho) - c_\ell(\rho_0)) + O(\rho). \\
&\quad \underbrace{\hspace{10em}}_{= \frac{1}{\rho} (f^{(\ell-1)}(\rho_0 + \rho) - f^{(\ell-1)}(\rho_0))}
\end{aligned}$$

On the other hand, the left-hand side of the equation above is also equal to $c_\ell(\rho_0) + O(\rho)$. Letting $\rho \downarrow 0$ then shows that the right-derivative of $f^{(\ell-1)}$ at ρ_0 exists and equals $c_\ell(\rho_0)$, upon using (5.40) for c_ℓ . Replacing ρ_0 by $\rho_0 - \rho$ in (5.48) then gives

$$(5.49) \quad \frac{1}{\rho} (f^{(\ell-1)}(\rho_0) - f^{(\ell-1)}(\rho_0 - \rho)) = c_\ell(\rho_0 - \rho) + O(\rho),$$

from which one can then infer the left-derivative of $f^{(\ell-1)}$ as well (using once more (5.40)). This finishes the proof of (5.41). Since $k \in \mathbb{N}_+$ was arbitrary, f is smooth, and therefore the expansion (2.13) holds by Taylor expansion (see also Step 4 of the proof of Proposition 5.2). \square

6. LOCAL UNIFORM CONVERGENCE

The aim of this section is to strengthen the pointwise convergence of the sequences $(\bar{\mathbf{a}}(\square_m, \rho_0))_{m \geq 1}$ and $(\bar{\mathbf{a}}_*(\square_m, \rho_0))_{m \geq 1}$ towards $\bar{\mathbf{a}}(\rho_0)$ for each fixed $\rho_0 > 0$ (see (2.5) and below) to a locally uniform convergence, that is to show the following statement.

Proposition 6.1. *The mappings $\bar{\mathbf{a}}(\square_m, \cdot)$ and $\bar{\mathbf{a}}_*(\square_m, \cdot)$ both converge to $\bar{\mathbf{a}}(\cdot)$ locally uniformly over $[0, \infty)$ as m tends to infinity. Moreover, for every $k \in \mathbb{N}_+$, the sequence of approximate derivatives $c_{k,m}$ converges locally uniformly to c_k , as m tends to infinity (recall (5.6) and (2.12) for the respective definitions).*

The local uniform convergence of $\bar{\mathbf{a}}(\square_m, \cdot)$ and $\bar{\mathbf{a}}_*(\square_m, \cdot)$ could in fact be obtained as a consequence of the quantitative estimate (2.6) and the observation that the exponent $\alpha > 0$ and the constant $C < \infty$ appearing there can be chosen locally uniformly over $\rho_0 > 0$. However, we think it useful to point out that Proposition 6.1 is actually a rather straightforward consequence of the qualitative statement that, for each fixed $\rho_0 > 0$,

$$(6.1) \quad \bar{\mathbf{a}}(\rho_0) = \lim_{m \rightarrow \infty} \bar{\mathbf{a}}(\square_m, \rho_0) = \lim_{m \rightarrow \infty} \bar{\mathbf{a}}_*(\square_m, \rho_0).$$

As will be seen, once (6.1) is granted, the fact that these sequences converge locally uniformly as ρ_0 varies is an application of Dini's theorem.

Since we will need to show the continuity of $\bar{\mathbf{a}}(\square_m, \cdot)$, we first need to develop some version of Lemma 3.1 geared towards $\nu(U, p, \rho_0)$ instead of $\nu_*(U, q, \rho_0)$. To state it, we define for a bounded open $U \subseteq \mathbb{R}^d$ the function space $\mathcal{D}(U)$ to consist of sequences of functions $f = (f_n)_{n \geq 0}$, where $f_n : U^n \rightarrow \mathbb{R}$ satisfy

- (1) f_0 is a constant and for every $n \in \mathbb{N}_+$, $f_n \in C^\infty(U^n)$;
- (2) There exists a compact set $K \subseteq U$ such that for any $x_i \notin K$

$$f_n(x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_n) = f_{n-1}(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n).$$

The canonical projection in (3.2) is an injection from $\mathcal{C}_c^\infty(U)$ to $\mathcal{D}(U)$; in other words, we can think of $\mathcal{C}_c^\infty(U)$ as a subset of $\mathcal{D}(U)$.

We then define a version of the minimization problem in the first line of (2.3) with $\mathcal{D}(U)$ replacing $\mathcal{H}_0^1(U)$. Define for $f \in \mathcal{D}(U)$ the quantity

$$(6.2) \quad \mathcal{K}(f, U, p, \rho_0) := \frac{e^{-\rho_0|U|}}{2\rho_0|U|} \sum_{n=0}^{\infty} \frac{(\rho_0|U|)^n}{n!} \left(\int_{U^n} \sum_{i=1}^n (p + \nabla_{x_i} f_n) \cdot \mathbf{a} \left(\sum_{k=1}^n \delta_{x_k}, x_i \right) (p + \nabla_{x_i} f_n) dx_1 \cdots dx_n \right).$$

With this definition, one has the following result.

Lemma 6.2. *For every bounded open set U , $\nu(U, p, \rho_0) = \inf_{f \in \mathcal{D}(U)} \mathcal{K}(f, U, p, \rho_0)$.*

Proof. For every $f = (f_n)_{n \geq 0} \in \mathcal{D}(U)$, we consider the symmetrization $\tilde{f} = (\tilde{f}_n)_{n \geq 0}$ by defining $\tilde{f}_n = \frac{1}{n!} \sum_{\sigma \in S_n} f(x_{\sigma(1)}, \dots, x_{\sigma(n)})$. This function fulfills $\tilde{f} \in \mathcal{D}(U)$: Indeed $\tilde{f}_n \in C^\infty(U^n)$ follows directly from the definition, and letting $K \subseteq U$ be the compact set associated with f , one has e.g. for the case $x_1 \notin K$

$$\begin{aligned} \tilde{f}_n(x_1, x_2, \dots, x_n) &= \frac{1}{n!} \sum_{\sigma \in S_n} f_n(x_{\sigma(1)}, x_{\sigma(2)}, \dots, x_{\sigma(n)}) \\ &= \frac{1}{(n-1)!} \sum_{\sigma \in S_{n-1}(\{2, \dots, n\})} f_{n-1}(x_{\sigma(2)}, x_{\sigma(3)}, \dots, x_{\sigma(n)}) \\ &= \tilde{f}_{n-1}(x_2, \dots, x_n). \end{aligned}$$

Here, from the first line to the second line, we can remove x_1 in the function, and make use of the natural n -to-1 bijection from the group of permutations S_n to the group of permutations $S_{n-1}(\{2, \dots, n\})$. This establishes the second condition for functions in $\mathcal{D}(U)$, so $\tilde{f} \in \mathcal{D}(U)$.

By an application of Jensen's inequality, it follows that

$$\begin{aligned} \mathcal{K}(\tilde{f}, U, p, \rho_0) &\leq \frac{e^{-\rho_0|U|}}{2\rho_0|U|} \sum_{n=0}^{\infty} \frac{(\rho_0|U|)^n}{n!} \frac{1}{n!} \sum_{\sigma \in S_n} \left(\int_{U^n} \sum_{i=1}^n ((p + \nabla_{x_i} f_n(x_{\sigma(1)}, \dots, x_{\sigma(n)})) \right. \\ &\quad \cdot \mathbf{a} \left(\sum_{k=1}^n \delta_{x_k}, x_i \right) (p + \nabla_{x_i} f_n(x_{\sigma(1)}, \dots, x_{\sigma(n)})) \Big) dx_1 \cdots dx_n \Big), \end{aligned}$$

which implies that $\mathcal{K}(\tilde{f}, U, p, \rho_0) \leq \mathcal{K}(f, U, p, \rho_0)$. This establishes that the value $\inf_{f \in \mathcal{D}(U)} \mathcal{K}(f, U, p, \rho_0)$ can be attained on the subspace with invariance by permutation, which can be identified as $\mathcal{C}_c^\infty(U)$. \square

Proof of Proposition 6.1. We need to verify that

$$(6.3) \quad \text{For fixed } m \in \mathbb{N}, \bar{\mathbf{a}}(\square_m, \cdot) \text{ and } \bar{\mathbf{a}}_*(\square_m, \cdot) \text{ are continuous.}$$

Once (6.3) is established, the uniform convergence follows from Dini's theorem, which states that if a decreasing or increasing sequence of continuous functions $(f_n)_{n \geq 1}$ converges pointwisely to a continuous function f , then the convergence is a locally uniform. Recall that $(\bar{\mathbf{a}}(\square_m, \cdot))_{m \geq 1}$ is decreasing and $(\bar{\mathbf{a}}_*(\square_m, \cdot))_{m \geq 1}$ is increasing and the common limit (6.1) is ensured by [11, Theorem 1.1]. Moreover, note that $\bar{\mathbf{a}}(\cdot)$ is continuous by Theorem 2.3 (in fact, to establish the continuity of $\bar{\mathbf{a}}(\cdot)$ it suffices to establish its upper and lower semicontinuity, which follows from the monotone convergence of $\bar{\mathbf{a}}(\square_m, \cdot)$ and $\bar{\mathbf{a}}_*(\square_m, \cdot)$, respectively). Therefore, it suffices to justify the continuity condition (6.3).

Step 1: Continuity of $\bar{\mathbf{a}}_(\square_m, \cdot)$.* The continuity of $\bar{\mathbf{a}}_*^{-1}(\square_m, \cdot)$ follows immediately from (4.4), and this implies the continuity of $\bar{\mathbf{a}}_*(\square_m, \cdot)$.

Step 2: Continuity of $\bar{\mathbf{a}}(\square_m, \cdot)$. We use the exact expression of the subadditive quantity

$$\begin{aligned} \nu(\square_m, p, \rho_0 + \rho) &= p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho) p \\ &= \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} (p + \nabla \phi_m^\rho) \cdot \mathbf{a}^\rho(p + \nabla \phi_m^\rho) d(\mu + \mu_\rho) \right], \end{aligned}$$

for $m \in \mathbb{N}$, $p \in \mathbb{R}^d$ and ϕ_m^ρ denotes the minimizer in the definition of $\nu(\square_m, p, \rho_0 + \rho)$. We now derive an upper bound on the above expression. Using Lemma 6.2, we know that $\phi_m(\mu)$ is a sub-minimizer for the problem $\nu(\square_m, p, \rho_0 + \rho)$ with density $\rho + \rho_0$. Also with the help of Mecke's identity (4.10), we obtain that

$$\begin{aligned} &p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho) p \\ &\leq \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} (p + \nabla \phi_m(\mu, \cdot)) \cdot \mathbf{a}(\mu + \mu_\rho, \cdot) (p + \nabla \phi_m(\mu, \cdot)) d(\mu + \mu_\rho) \right] \\ &\leq \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} (p + \nabla \phi_m(\mu, \cdot)) \cdot \mathbf{a}(\mu + \mu_\rho, \cdot) (p + \nabla \phi_m(\mu, \cdot)) d\mu \right] + \frac{\rho \Lambda |p|^2}{\rho_0 + \rho} \\ &= \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} (p + \nabla \phi_{m,\xi}(\mu, \cdot)) \cdot (\mathbf{a}(\mu + \mu_\rho, \cdot) - \mathbf{a}(\mu, \cdot)) (p + \nabla \phi_m(\mu, \cdot)) d\mu \right] \\ &\quad + \left(\frac{\rho_0}{\rho_0 + \rho} \right) p \cdot \bar{\mathbf{a}}(\square_m, \rho_0) p + \left(\frac{\rho}{\rho_0 + \rho} \right) \Lambda |p|^2. \end{aligned}$$

For the first term, we perform an expansion with respect to μ_ρ , and note that $\mathbf{a}(\mu + \mu_\rho, \cdot) - \mathbf{a}(\mu) = 0$ on the event $\{\mu_\rho = 0\}$. Therefore,

$$\begin{aligned} & \mathbb{E} \left[\frac{1}{(\rho_0 + \rho)|\square_m|} \int_{\square_m} (p + \nabla \phi_m(\mu, \cdot)) \cdot (\mathbf{a}(\mu + \mu_\rho, \cdot) - \mathbf{a}(\mu, \cdot)) (p + \nabla \phi_m(\mu, \cdot)) d\mu \right] \\ &= e^{-\rho|\square_m|} \sum_{k=1}^{\infty} \left(\frac{(\rho|\square_m|)^k}{k!} \frac{1}{(\rho_0 + \rho)|\square_m|} \right. \\ & \quad \times \int_{(\square_m)^k} \mathbb{E}_{\rho_0} \left[\int_{\square_m} (p + \nabla \phi_m(\mu, \cdot)) \cdot \left(\mathbf{a}(\mu + \sum_{i=1}^k \delta_{x_i}, \cdot) - \mathbf{a}(\mu, \cdot) \right) (p + \nabla \phi_m(\mu, \cdot)) d\mu \right] dx_1 \cdots dx_k \Big) \\ &\leq \rho|\square_m| \left(e^{-\rho|\square_m|} \sum_{k=1}^{\infty} \frac{(\rho|\square_m|)^{(k-1)}}{(k-1)!} \Lambda^2 |p|^2 \right) \\ &= \rho|\square_m| \Lambda^2 |p|^2. \end{aligned}$$

This gives us

$$\begin{aligned} (6.4) \quad & p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho)p - p \cdot \bar{\mathbf{a}}(\square_m, \rho_0)p \\ & \leq \rho|\square_m| \Lambda^2 |p|^2 + \left(\frac{\rho}{\rho_0 + \rho} \right) \Lambda |p|^2 - \left(\frac{\rho}{\rho_0 + \rho} \right) p \cdot \bar{\mathbf{a}}(\square_m, \rho_0)p. \end{aligned}$$

Taking $\rho \searrow 0$ we obtain that

$$(6.5) \quad \lim_{\rho \searrow 0} \bar{\mathbf{a}}(\square_m, \rho_0 + \rho) \leq \bar{\mathbf{a}}(\square_m, \rho_0).$$

We now establish that $\lim_{\rho \searrow 0} \bar{\mathbf{a}}(\square_m, \rho_0 + \rho) = \bar{\mathbf{a}}(\square_m, \rho_0)$. To this end, we drop out the part of integration against μ_ρ and obtain

$$\begin{aligned} (6.6) \quad & p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho)p \\ & \geq \frac{\rho_0}{\rho_0 + \rho} \mathbb{E} \left[\frac{1}{\rho_0|\square_m|} \int_{\square_m} (p + \nabla \phi_m^\rho) \cdot \mathbf{a}(\mu + \mu_\rho, \cdot) (p + \nabla \phi_m^\rho) d\mu \right]. \end{aligned}$$

We compare this with the following minimization problem, in which we fix $\mathcal{M}_\delta(\mathbb{R}^d)$, $p \in \mathbb{R}^d$ and $U \subseteq \mathbb{R}^d$ a bounded domain,

$$(6.7) \quad \nu(U, p; \mu_\rho) := \inf_{v \in \mathcal{H}_0^1(U)} \int \left(\frac{1}{\rho|U|} \int_U \frac{1}{2} (p + \nabla v) \cdot \mathbf{a}(\mu + \mu_\rho, \cdot) (p + \nabla v) d\mu \right) d\mathbb{P}_{\rho_0}(\mu).$$

This can always be seen as the problem like (2.3), but with a perturbation with a fixed point process μ_ρ . We denote by $\mu \mapsto \phi_m(\mu; \mu_\rho) \in \mathcal{H}_0^1(U)$ its minimizer, and for every fixed $\mu_\rho \in \mathcal{M}_\delta(\mathbb{R}^d)$, $\phi_m^\rho(\cdot + \mu_\rho)$ is a sub-minimizer for (6.7). Therefore, (6.6) gives that

$$\begin{aligned} & p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho)p \\ & \geq \frac{\rho_0}{\rho_0 + \rho} \mathbb{E}_{\rho_0} \left[\frac{1}{\rho_0|\square_m|} \int_{\square_m} (p + \nabla \phi_m(\mu; \mu_\rho)) \cdot \mathbf{a}(\mu + \mu_\rho, \cdot) (p + \nabla \phi_m(\mu; \mu_\rho)) d\mu \right]. \end{aligned}$$

We perform an expansion with respect to μ_ρ and notice that, when $\mu_\rho = 0$ the problem (6.7) is exactly the same as (2.3) and $\phi_m(\mu; 0) = \phi_m(\mu)$, so we obtain that

$$(6.8) \quad p \cdot \bar{\mathbf{a}}(\square_m, \rho_0 + \rho)p \geq \left(\frac{\rho_0 e^{-\rho|\square_m|}}{\rho_0 + \rho} \right) p \cdot \bar{\mathbf{a}}(\square_m, \rho_0)p.$$

This also concludes that

$$(6.9) \quad \lim_{\rho \searrow 0} \bar{\mathbf{a}}(\square_m, \rho_0 + \rho) \geq \bar{\mathbf{a}}(\square_m, \rho_0).$$

Combining (6.9) and (6.5) yields the right continuity of $\bar{\mathbf{a}}(\square_m, \cdot)$.

We also need to verify the left continuity. We define $\rho_1 := \rho_0 + \rho$ which is fixed, then (6.4) becomes

$$p \cdot \bar{\mathbf{a}}(\square_m, \rho_1)p - p \cdot \bar{\mathbf{a}}(\square_m, \rho_0)p \leq \rho |\square_m| \Lambda^2 |p|^2 + \left(\frac{\rho}{\rho_1}\right) \Lambda |p|^2 - \left(\frac{\rho}{\rho_1}\right) |p|^2.$$

We let $\rho_1 \nearrow \rho_0$ and obtain that

$$\bar{\mathbf{a}}(\square_m, \rho_1) \leq \lim_{\rho_0 \nearrow \rho_1} \bar{\mathbf{a}}(\square_m, \rho_0).$$

Similarly, we put fixed $\rho_1 = \rho_0 + \rho$ into (6.8) and get

$$p \cdot \bar{\mathbf{a}}(\square_m, \rho_1)p - p \cdot \bar{\mathbf{a}}(\square_m, \rho_0)p \geq \left(\frac{\rho_0 e^{-\rho |\square_m|}}{\rho_1} - 1\right) \Lambda |p|^2,$$

which means that

$$\bar{\mathbf{a}}(\square_m, \rho_1) \geq \lim_{\rho_0 \nearrow \rho_1} \bar{\mathbf{a}}(\square_m, \rho_0).$$

These prove the left continuity of $\bar{\mathbf{a}}(\square_m, \cdot)$, establishing that $\bar{\mathbf{a}}(\square_m, \cdot)$ is continuous.

Step 3: Locally uniform convergence of $c_{k,m}$. We now turn to the proof of the locally uniform convergence of $\{c_{k,m}\}_{m \in \mathbb{N}}$. Let $K > 0$ and $\rho > 0$. For the case $k = 1$, by (5.8) and (5.39), we find that

$$\begin{aligned} \sup_{\rho_0 \in [0, K]} |c_{1,m}(\rho_0) - c_1(\rho_0)| &\leq \frac{1}{\rho} \sup_{\rho_0 \in [0, K]} |R_1(m, \rho_0, \rho)| + O(\rho) \\ &\quad + \frac{1}{\rho} \sup_{\rho_0 \in [0, K]} |q \cdot (\bar{\mathbf{a}}^{-1}(\rho_0 + \rho) - \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0 + \rho))q| \\ &\quad + \frac{1}{\rho} \sup_{\rho_0 \in [0, K]} |q \cdot (\bar{\mathbf{a}}^{-1}(\rho_0) - \bar{\mathbf{a}}_*^{-1}(\square_m, \rho_0))q|. \end{aligned}$$

Using the statement of Proposition 5.2, the first line on the right-hand side of the previous display is uniformly bounded by a constant $O(\rho)$ independent of m and ρ_0 , and the locally uniform convergence of $(\bar{\mathbf{a}}_*(\square_m, \cdot))_{m \geq 1}$ towards $\bar{\mathbf{a}}$ makes the second line and third line vanish when m tends to infinity. Thus, we obtain

$$\limsup_{m \rightarrow \infty} \sup_{\rho_0 \in [0, K]} |c_{1,m}(\rho_0) - c_1(\rho_0)| \leq O(\rho).$$

Since the left hand side of the display above does not depend on ρ , we can let ρ be arbitrarily small, which proves the locally uniform convergence of $\{c_{1,m}\}_{m \in \mathbb{N}}$. For the case $k \geq 2$, the claim about $\{c_{k,m}\}_{m \in \mathbb{N}}$ follows in the same manner by induction. \square

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