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operators

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GREEDY APPROXIMATION OF HIGH-DIMENSIONAL ORNSTEIN–UHLENBECK OPERATORS

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ABSTRACT. We investigate the convergence of a nonlinear approximation method introduced by Ammar et al. (J. Non-Newtonian Fluid Mech. 139:153–176, 2006) for the numerical solution of high-dimensional Fokker–Planck equations featuring in Navier–Stokes–Fokker–Planck systems that arise in kinetic models of dilute polymers. In the case of Poisson’s equation on a rectangular domain in \mathbb{R}^2 , subject to a homogeneous Dirichlet boundary condition, the mathematical analysis of the algorithm was carried out recently by Le Bris, Lelièvre and Maday (Const. Approx. 30:621–651, 2009), by exploiting its connection to greedy algorithms from nonlinear approximation theory, explored, for example, by DeVore and Temlyakov (Adv. Comput. Math. 5:173–187, 1996); hence, the variational version of the algorithm, based on the minimization of a sequence of Dirichlet energies, was shown to converge. Here, we extend the convergence analysis of the pure greedy and orthogonal greedy algorithms considered by Le Bris et al. to a technically more complicated situation, where the Laplace operator is replaced by an Ornstein–Uhlenbeck operator of the kind that appears in Fokker–Planck equations that arise in bead-spring chain type kinetic polymer models with finitely extensible nonlinear elastic potentials, posed on a high-dimensional Cartesian product configuration space $\mathbf{D} = D_1 \times \cdots \times D_N$ contained in \mathbb{R}^{Nd} , where each set D_i , $i = 1, \dots, N$, is a bounded open ball in \mathbb{R}^d , $d = 2, 3$.

1. INTRODUCTION

High-dimensional partial differential equations are ubiquitous in mathematical models in science, engineering and finance. They arise in a number of areas, including, for example, kinetic theory, molecular dynamics, quantum mechanics, and uncertainty quantification based on polynomial chaos expansions, to name only a few.

The purpose of the present paper is to explore the convergence of a numerical algorithm that was recently proposed in the engineering literature in a succession of papers by Ammar, Mokdad, Chinesta, Keunings and collaborators [AMCK06, AMCK07, AND⁺10, GACC10, CALK11], for the numerical solution of high-dimensional Fokker–Planck equations in kinetic models of polymeric fluids under the names *Separated Representation* and *Proper Generalized Decomposition*. A variant with a discretization based on spectral methods instead of the finite element methods preferred by Ammar et al. was presented by Leonenko and Phillips [LP09]. A similar method was considered independently by Nouy [Nou07, Nou08] and Nouy & Le Maître [NLM09] under the name *Power type Generalized Spectral Decomposition*, for the numerical solution of stochastic partial differential equations, although the historical roots of the technique can be traced back to the work of Schmidt [Sch07]. Ammar et al. and Nouy report that the algorithm performs well in numerical experiments and comment that it extends to a large variety of partial differential equations.

In the simplified mathematical setting of Poisson’s equation $-\Delta u = f$ posed on the rectangular domain $\Omega = \Omega_x \times \Omega_y$, where Ω_x and Ω_y are bounded open subintervals of \mathbb{R} , subject to a homogeneous Dirichlet boundary condition on $\partial\Omega$, the convergence of the algorithm was shown in a recent paper by Le Bris, Lelièvre and Maday [LBM09], by drawing on connections with greedy algorithms from nonlinear approximation theory (cf. DeVore and Temlyakov [DT96]). In

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[LBLM09], the solution was represented as a sum

$$u(x, y) = \sum_{n \geq 1} r_n(x) s_n(y) \quad (1.1)$$

by iteratively determining functions $x \in \Omega_x \mapsto r_n(x)$ and $y \in \Omega_y \mapsto s_n(y)$, $n \geq 1$, such that for all n , the product $(x, y) \in \Omega \mapsto r_n(x) s_n(y)$ is the best approximation in the norm of the Sobolev space $H_0^1(\Omega)$ to the solution $(x, y) \in \Omega \mapsto v(x, y)$ of the Poisson equation

$$-\Delta v(x, y) = f(x, y) + \Delta \left(\sum_{k \leq n-1} r_k(x) s_k(y) \right),$$

subject to a homogeneous Dirichlet boundary condition, in terms of a single function of the factorized form $r(x) s(y)$; Le Bris et al. thus show that it is possible to give a sound mathematical basis to the algorithm proposed by Ammar et al., provided that one considers a variational form of the approach that manipulates minimizers of Dirichlet energies instead of stationary points to the associated Euler–Lagrange equations (in the follow-up paper [CEL11] by Cancès, Ehrlicher and Lelièvre it was further shown that one can also work with local—yet still energy-decreasing—minimizers provided that one stays within the two-fold tensor product setting of (1.1)). In order to reformulate the approach in such a variational setting, the arguments in [LBLM09] crucially rely on the fact that the Laplace operator is self-adjoint, and as noted by the authors of [LBLM09], the analysis does not apply exactly to the actual implementation of the method as described in the papers by Ammar et al., where stationary points of the Euler–Lagrange equations associated with the Dirichlet energies are computed instead. Indeed, since minimizers of Dirichlet energies in the approach of Le Bris et al. on the one hand and stationary points of the associated Euler–Lagrange equations in the approach of Ammar et al. on the other are each sought in *nonlinear* manifolds embedded in a Sobolev space, rather than over the entire Sobolev space (which is a normed *linear* space), the two approaches are not equivalent. The authors of [LBLM09] also comment that: “Likewise, it is unclear to us how to provide a mathematical foundation of the approach for nonvariational situations, such as an equation involving a differential operator that is not self-adjoint.” This latter remark is particularly pertinent in the context of Fokker–Planck equations for kinetic bead-spring chain models for dilute polymers, of the kind considered by Ammar et al., where the differential operator in configuration space featuring in the Fokker–Planck equation, a generalized Ornstein–Uhlenbeck operator, is a non-self-adjoint elliptic operator with a drift term that involves an unbounded potential.

It is this last point that the present paper is aimed at addressing: we shall be concerned with the numerical approximation of high-dimensional Fokker–Planck equations that arise in bead-spring chain type kinetic models of dilute polymers on the Cartesian product domain $\Omega \times \mathbf{D}$, where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is the physical (flow) domain, and the *configuration space* \mathbf{D} is the N -fold Cartesian product $\times_{i=1}^N D_i$ of sets $D_i \subset \mathbb{R}^d$, $i = 1, \dots, N$, $N \geq 2$, each of which is a bounded open ball in \mathbb{R}^d . Here, N denotes the number of springs connecting, in a linear fashion, the $N+1$ beads in the bead-spring chain model (cf. Fig. 1.1). Proceeding as in [BS07, BS08, BS09, BS11a, BS11b], we rewrite the Ornstein–Uhlenbeck operator, a non-self-adjoint elliptic operator with respect to the configuration space variable \mathbf{q} featuring in the Fokker–Planck equation whose drift term contains an unbounded potential, as a degenerate, but now self-adjoint, elliptic operator on a Maxwellian-weighted Sobolev space. We then perform a nonlinear approximation of the analytical solution $\psi: (\mathbf{q}_1, \dots, \mathbf{q}_N) \in \mathbf{D} \mapsto \psi(\mathbf{q}_1, \dots, \mathbf{q}_N)$ to this high-dimensional degenerate elliptic boundary-value problem on the appropriate Maxwellian-weighted Sobolev space by separated representations of the form

$$\sum_{k=1}^K \prod_{i=1}^N \psi_k^{(i)}(\mathbf{q}_i),$$

where the factors $\psi_k^{(i)}$, $k = 1, \dots, K$, are defined on the d -dimensional domain D_i , $i = 1, \dots, N$. Instead of being selected from an *a priori* fixed set, the factors $\psi_k^{(i)}$, $i = 1, \dots, N$, are obtained, N at a time, for each $k \in \{1, \dots, K\}$, as the best approximation (in a sense to be made precise in

Section 3) among all possible such factors. The (potentially large) number of terms K is likewise not fixed in advance, but depends on a termination criterion.

The paper is structured as follows. After introducing our notational conventions and formulating briefly an alternating direction scheme that separates, by a fractional step method, the full Fokker–Planck equation into a low-dimensional physical space part and a high-dimensional configuration space part, we will concentrate on the latter problem. The central difficulty in the numerical solution of the configuration space problem is the presence of the high-dimensional Ornstein–Uhlenbeck operator, a non-self-adjoint elliptic operator whose drift term contains an unbounded potential. In Section 2 we show that the configuration space problem can be restated, in a Maxwellian-weighted Sobolev space, as the weak formulation of a symmetric degenerate elliptic boundary-value problem on the high-dimensional configuration space \mathcal{D} . Section 3 is devoted to the description of a separated representation strategy for the problem, in the spirit of Le Bris et al. [LBLM09]. Following [LBLM09], we consider a pure greedy algorithm and an orthogonal greedy algorithm. Section 4 concentrates on the convergence of the two algorithms. We shall characterize the convergence rates of the two greedy algorithms by invoking abstract convergence results due to DeVore and Temlyakov [DT96]. In Section 5, we give explicit necessary and sufficient conditions, in terms of Maxwellian-weighted Sobolev spaces, for membership of the space of DeVore and Temlyakov in the case of our degenerate elliptic problem. In Section 6, we provide some conclusions and possible directions for further work.

At an abstract level, our convergence proof follows the arguments in [LBLM09]; however, the verification of certain key properties of the function spaces involved, on the one hand, and the characterization of verifiable sufficient conditions under which the predicted convergence rates of the two greedy algorithms considered are observed, on the other, for the high-dimensional degenerate elliptic problem studied herein are considerably more complicated than in the case of Poisson’s equation studied in [LBLM09]. The former is mostly based on tensorizing the corresponding results for the function spaces associated with the single-spring case (i.e., the *dumbbell*) and the latter relies on shift-theorems for degenerate elliptic operators in Maxwellian-weighted Sobolev spaces and delicate results from the spectral theory of self-adjoint degenerate elliptic operators, which we were unable to find in the literature; these are described in Section 5 and Appendix C, respectively. Appendices A and B collect a number of technical results that are used throughout the paper.

1.1. Notation. We denote by $[k]$ the integer interval $\{i \in \mathbb{N} : 1 \leq i \leq k\}$. We shall denote sequences and arrangements of elements a_i indexed by indices i in an index set \mathcal{I} by $(a_i)_{i \in \mathcal{I}}$.

We shall write $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_N) \in D_1 \times \dots \times D_N = \times_{i \in [N]} D_i =: \mathcal{D}$. Given N real-valued functions f_i , each defined on the corresponding set D_i , we denote by $\bigotimes_{i \in [N]} f_i$ their *tensor product*; i.e., the function

$$\mathbf{q} \in \mathcal{D} \mapsto \prod_{i \in [N]} f_i(\mathbf{q}_i).$$

We extend this notation in three ways. Firstly, as the tensor-product operation is order-dependent, we will use subscripts on the \otimes and the \bigotimes signs to denote where on $\mathbf{q} \in \mathcal{D}$ the function, or functions, following them act; e.g., $\bigotimes_{i \in [N] \setminus \{j\}} f_i \otimes_j f_j$ evaluated on $\mathbf{q} \in \mathcal{D}$ is $f_j(\mathbf{q}_j) \prod_{i \in [N] \setminus \{j\}} f_i(\mathbf{q}_i)$. Secondly, we will use the same notation for the sets resulting from the tensor products of members of function spaces: suppose that F_i is a nonempty set of real-valued functions defined on D_i , $i \in [N]$; we then write $\bigotimes_{i \in [N]} F_i := \{\bigotimes_{i \in [N]} f_i : f_i \in F_i, i \in [N]\}$. Thirdly, if exactly one of the factors is vector-valued, the products involving it at the time of evaluation must be interpreted as scalar-vector products implying that the resulting tensor product will be vector-valued too.

The symbol \Subset will stand for the compact embedding relation. The support of a real-valued function f will be denoted by $\text{supp}(f)$.

Given a measurable and almost everywhere positive real-valued function w defined on an open set $E \subset \mathbb{R}^n$; i.e., a *weight*, we denote by $L_w^2(E)$ the Lebesgue space of square-integrable functions

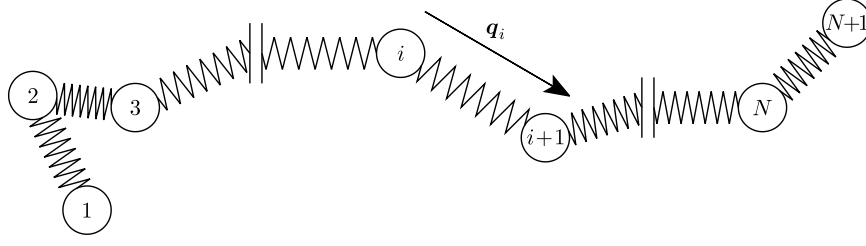


FIGURE 1.1. Bead-spring chain with N springs and $N+1$ beads. Adapted from Figure 11.4-1 of [BCAH87]

with respect to the weight w , equipped with its usual norm,

$$\|\varphi\|_{L_w^2(E)} := \left(\int_E |\varphi|^2 w \right)^{1/2}.$$

We also define the w -weighted Sobolev space $H_w^m(E)$ and its norm $\|\cdot\|_{H_w^m(E)}$ by

$$H_w^m(E) := \{ \varphi \in L_w^2(E) \cap L_{\text{loc}}^1(E) : \partial_\alpha \varphi \in L_w^2(E), |\alpha| \leq m \},$$

$$\|\varphi\|_{H_w^m(E)} := \left(\sum_{|\alpha| \leq m} \|\partial_\alpha \varphi\|_{L_w^2(E)}^2 \right)^{1/2} \quad \forall \varphi \in H_w^m(E).$$

We shall suppose henceforth that Ω is a bounded open set in \mathbb{R}^d with a sufficiently regular (say, Lipschitz continuous) boundary, and denote by \mathbf{n}_x and \mathbf{n}_{q_i} the unit outward normal vector defined (a.e. with respect to the surface measure) on $\partial\Omega$ and ∂D_i , $i \in [N]$, respectively.

1.2. Fokker–Planck equation. The *spring forces* in the model are given by functions $\mathbf{F}_i: D_i \rightarrow \mathbb{R}^d$, which have the form $\mathbf{F}_i(\mathbf{p}) = U_i'(\frac{1}{2}|\mathbf{p}|^2)\mathbf{p}$, $\mathbf{p} \in D_i := B(0, \sqrt{b_i}) \subset \mathbb{R}^d$, $b_i > 0$, $i \in [N]$, and the $U_i: [0, b_i/2) \rightarrow \mathbb{R}$, the *spring potentials*, are such that $U_i(s) \rightarrow +\infty$ as $s \rightarrow b_i/2_-$. It follows that $\mathbf{F}_i(\mathbf{p}) = -\mathbf{F}_i(-\mathbf{p})$ for all $\mathbf{p} \in D_i$. Typical examples include the *FENE (Finitely Extensible Nonlinear Elastic) model* [War72] with

$$U_i(s) = -\frac{b_i}{2} \ln \left(1 - \frac{2s}{b_i} \right) \quad \text{and} \quad \mathbf{F}_i(\mathbf{q}_i) = \frac{1}{1 - |\mathbf{q}_i|^2/b_i} \mathbf{q}_i, \quad (1.2)$$

where $b_i > 0$ is a parameter, and *Cohen's Padé approximant to the Inverse Langevin (CPAIL) model* [Coh91] with

$$U_i(s) = \frac{s}{3} - \frac{b_i}{3} \ln \left(1 - \frac{2s}{b_i} \right) \quad \text{and} \quad \mathbf{F}_i(\mathbf{q}_i) = \frac{1 - |\mathbf{q}_i|^2/(3b_i)}{1 - |\mathbf{q}_i|^2/b_i} \mathbf{q}_i, \quad (1.3)$$

where $b_i > 0$ is again a parameter. We note in passing that both of these force laws are approximations to the *Inverse Langevin force law* [KG42]

$$\mathbf{F}_i(\mathbf{q}_i) = \frac{\sqrt{b_i}}{3} L^{-1} \left(\frac{|\mathbf{q}_i|}{\sqrt{b_i}} \right) \frac{\mathbf{q}_i}{|\mathbf{q}_i|},$$

where the *Langevin function* L is defined by $L(t) := \coth(t) - 1/t$ on $[0, \infty)$. As L is strictly monotonic increasing on $[0, \infty)$ and tends to 1 as its argument tends to ∞ , it follows that the function $|\mathbf{q}_i| \in [0, \sqrt{b_i}) \mapsto L^{-1}(|\mathbf{q}_i|/\sqrt{b_i}) \in [0, \infty)$ is strictly monotonic increasing, with a vertical asymptote at $|\mathbf{q}_i| = \sqrt{b_i}$.

Remark 1. An important spring force model, which is excluded from our considerations, is the simple *Hookean model* described by

$$D_i = \mathbb{R}^d, \quad U_i(s) = s \quad \text{and} \quad \mathbf{F}_i(\mathbf{q}_i) = \mathbf{q}_i.$$

However, in many practically relevant flow regimes the physically unrealistic allowance of the Hookean model for indefinitely extended springs outweighs its mathematical convenience.

The Fokker-Planck equation under consideration for the probability density function ψ has the following form (cf. [BS07, BS08, BS09, BS11b, BS11a]):

$$\begin{aligned} \frac{\partial \psi}{\partial t} + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\psi) + \sum_{i=1}^N \operatorname{div}_{\mathbf{q}_i} \left[(\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}_i \psi - \frac{1}{4\operatorname{Wi}} \sum_{j=1}^N A_{ij} (\mathbf{F}_j(\mathbf{q}_j) \psi + \nabla_{\mathbf{q}_j} \psi) \right] \\ = \frac{(l_0/L_0)^2}{4\operatorname{Wi}(N+1)} \Delta_{\mathbf{x}} \psi, \quad (\mathbf{x}, \mathbf{q}, t) \in \Omega \times \mathbf{D} \times (0, T], \end{aligned} \quad (1.4a)$$

with initial and no-flux boundary conditions

$$\psi(\cdot, \cdot, 0) = \psi_0, \quad (\mathbf{x}, \mathbf{q}) \in \Omega \times \mathbf{D}, \quad (1.4b)$$

$$\frac{(l_0/L_0)^2}{4\operatorname{Wi}(N+1)} \nabla_{\mathbf{x}} \psi \cdot \mathbf{n}_{\mathbf{x}} = 0, \quad (\mathbf{x}, \mathbf{q}, t) \in \partial\Omega \times \mathbf{D} \times (0, T], \quad (1.4c)$$

and

$$\left[(\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}_i \psi - \frac{1}{4\operatorname{Wi}} \sum_{j=1}^N A_{ij} (\mathbf{F}_j(\mathbf{q}_j) \psi + \nabla_{\mathbf{q}_j} \psi) \right] \cdot \mathbf{n}_{\mathbf{q}_i} = 0, \quad i \in [N], \quad (\mathbf{x}, \mathbf{q}, t) \in \Omega \times \partial\mathbf{D} \times (0, T]. \quad (1.4d)$$

Here, $\mathbf{u}: \bar{\Omega} \times [0, T] \rightarrow \mathbb{R}^d$ is the flow velocity, $\operatorname{Wi} := \lambda U_0 / L_0$ is the (nondimensional) Weissenberg number, l_0 is the characteristic length-scale of a spring, λ is the characteristic relaxation time of a spring and L_0 and U_0 are the characteristic macroscopic length and velocity, respectively (thus, Wi is the ratio of the microscopic to macroscopic time scales). The matrix $A = (A_{ij})_{i,j \in [N]}$ is symmetric and positive definite; we denote the smallest eigenvalue of A by λ_{\min} .

We remark that the boundary condition (1.4d) is an ensemble of N boundary conditions, which collectively account for the full $(Nd - 1)$ -dimensional measure of $\partial\mathbf{D}$.

We define the partial Maxwellians M_i and the (full) Maxwellian \mathbf{M} by

$$M_i(\mathbf{p}) := Z_i^{-1} \exp\left(-U_i\left(\frac{1}{2}|\mathbf{p}|^2\right)\right), \quad \mathbf{p} \in D_i, \quad i \in [N]; \quad (1.5)$$

$$\mathbf{M}(\mathbf{q}) := \prod_{i=1}^N M_i(\mathbf{q}_i), \quad \mathbf{q} \in \mathbf{D}; \quad (1.6)$$

that is, $\mathbf{M} = \bigotimes_{i \in [N]} M_i$. Here, each Z_i is a positive constant chosen so that $\int_{D_i} M_i = 1$ (we can do so because of Hypothesis A, below). Thereby, $\int_{\mathbf{D}} \mathbf{M} = 1$. We note that since U_i is assumed to tend to $+\infty$ as \mathbf{q}_i approaches ∂D_i , the corresponding partial Maxwellian M_i tends to 0 as \mathbf{q}_i approaches ∂D_i , $i \in [N]$; consequently, \mathbf{M} tends to 0 as \mathbf{q} approaches $\partial\mathbf{D}$. The fact that the Maxwellian factorizes—which comes from the fact that the energy stored in the chain is the sum of the potential energies stored in each spring—will be crucial throughout the rest of this paper. For a start, this fact allows us to write

$$\mathbf{F}_j(\mathbf{q}_j) \psi + \nabla_{\mathbf{q}_j} \psi = \psi \nabla_{\mathbf{q}_j} U_j\left(\frac{1}{2}|\mathbf{q}_j|^2\right) + \nabla_{\mathbf{q}_j} \psi = \mathbf{M} \nabla_{\mathbf{q}_j} \left(\frac{\psi}{\mathbf{M}}\right). \quad (1.7)$$

Multiplying (1.4a) by φ/\mathbf{M} , using (1.7) and (formally) integrating by parts, the corresponding weak form of (1.4) is: Find $\psi = \psi(\mathbf{x}, \mathbf{q}, t)$ such that

$$\begin{aligned} \int_{\Omega \times \mathbf{D}} \left\{ \frac{\partial \psi}{\partial t} \frac{\varphi}{\mathbf{M}} + \operatorname{div}_{\mathbf{x}}(\mathbf{u}\psi) \frac{\varphi}{\mathbf{M}} - \sum_{i=1}^N \left[(\nabla_{\mathbf{x}} \mathbf{u}) \mathbf{q}_i \psi - \sum_{j=1}^N \frac{A_{ij}}{4\operatorname{Wi}} \mathbf{M} \nabla_{\mathbf{q}_j} \left(\frac{\psi}{\mathbf{M}}\right) \right] \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{\mathbf{M}}\right) \right. \\ \left. + \frac{(l_0/L_0)^2}{4\operatorname{Wi}(N+1)} \nabla_{\mathbf{x}} \psi \cdot \nabla_{\mathbf{x}} \varphi \frac{1}{\mathbf{M}} \right\} = 0 \end{aligned} \quad (1.8)$$

for all $\varphi = \varphi(\mathbf{x}, \mathbf{q})$ in a suitable function space.

For the sake of convenience we define the following bilinear forms:

$$\tilde{\mathcal{T}}(\mathbf{u}; \sigma, \tau) := \int_{\Omega \times \mathbf{D}} \operatorname{div}_{\mathbf{x}}(\mathbf{u}\sigma) \frac{\tau}{\mathbf{M}}, \quad \tilde{\mathcal{K}}(\sigma, \tau) := \frac{(l_0/L_0)^2}{4W\mathbf{i}(N+1)} \int_{\Omega \times \mathbf{D}} \nabla_{\mathbf{x}}\sigma \cdot \nabla_{\mathbf{x}}\tau \frac{1}{\mathbf{M}}, \quad (1.9)$$

$$\mathcal{T}(\mathbf{u}; \sigma, \tau) := - \int_{\Omega \times \mathbf{D}} \sum_{i=1}^N (\nabla_{\mathbf{x}}\mathbf{u})_{\mathbf{q}_i} \sigma \cdot \nabla_{\mathbf{q}_i} \left(\frac{\tau}{\mathbf{M}} \right), \quad (1.10)$$

$$\mathcal{K}(\sigma, \tau) := \int_{\Omega \times \mathbf{D}} \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4W\mathbf{i}} \mathbf{M} \nabla_{\mathbf{q}_j} \left(\frac{\sigma}{\mathbf{M}} \right) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\tau}{\mathbf{M}} \right). \quad (1.11)$$

Then, (1.8) can be written concisely as

$$\left\langle \frac{\partial \psi}{\partial t}, \varphi / \mathbf{M} \right\rangle + \tilde{\mathcal{T}}(\mathbf{u}; \psi, \varphi) + \tilde{\mathcal{K}}(\psi, \varphi) + \mathcal{T}(\mathbf{u}; \psi, \varphi) + \mathcal{K}(\psi, \varphi) = 0 \quad (1.12)$$

for all $\varphi = \varphi(\mathbf{x}, \mathbf{q})$ in a suitable function space. We note that $\tilde{\mathcal{T}}$ and $\tilde{\mathcal{K}}$ involve partial derivatives of their arguments with respect to the *spatial* variable \mathbf{x} only. Analogously, \mathcal{T} and \mathcal{K} involve partial derivatives of their arguments with respect to the *configuration* space variable \mathbf{q} only. This motivates the use of the alternating direction scheme based on operator splitting whose informal description is given in the next subsection.

1.3. Alternating direction scheme. Let Δt be such that $M := T/\Delta t \in \mathbb{N}$ and define $t^n := n\Delta t$ for $n \in \{0, \dots, M\}$. We will consider the following *alternating-direction* semidiscretization of (1.8): We initialize the scheme by defining $\psi^0 := \psi_0$; for $n \in \{0, \dots, M-1\}$ and then define the ‘intermediate’ function $\psi^{n+1/2}$ and the approximation ψ^{n+1} to $\psi(t^{n+1}, \cdot, \cdot)$, respectively, by

$$\begin{aligned} \left\langle \frac{\psi^{n+1/2} - \psi^n}{\Delta t/2}, \frac{\varphi}{\mathbf{M}} \right\rangle + \tilde{\mathcal{T}}(\mathbf{u}(\cdot, t^{n+1}); \psi^{n+1/2}, \varphi) + \tilde{\mathcal{K}}(\psi^{n+1/2}, \varphi) \\ = -\mathcal{T}(\mathbf{u}(\cdot, t^n); \psi^n, \varphi) - \mathcal{K}(\psi^n, \varphi) \end{aligned} \quad (1.13a)$$

and

$$\begin{aligned} \left\langle \frac{\psi^{n+1} - \psi^{n+1/2}}{\Delta t/2}, \frac{\varphi}{\mathbf{M}} \right\rangle + \mathcal{K}(\psi^{n+1}, \varphi) = -\mathcal{T}(\mathbf{u}(\cdot, t^n); \psi^n, \varphi) \\ - \tilde{\mathcal{T}}(\mathbf{u}(\cdot, t^{n+1}); \psi^{n+1/2}, \varphi) - \tilde{\mathcal{K}}(\psi^{n+1/2}, \varphi), \end{aligned} \quad (1.13b)$$

for all $\varphi = \varphi(\mathbf{x}, \mathbf{q})$ in a suitable function space. In (1.13a) the spatial bilinear forms $\tilde{\mathcal{T}}$ and $\tilde{\mathcal{K}}$ are treated implicitly while the configuration space bilinear forms \mathcal{T} and \mathcal{K} are treated explicitly. In (1.13b) the spatial bilinear forms $\tilde{\mathcal{T}}$ and $\tilde{\mathcal{K}}$ and the configuration space bilinear form \mathcal{T} associated with the drag term are treated explicitly, while the bilinear form \mathcal{K} is treated implicitly.

Let $\left((\mathbf{q}^{(k)}, w_{\mathbf{D}}^{(k)}) \right)_{k \in [Q_{\mathbf{D}}]}$ and $\left((\mathbf{x}^{(k)}, w_{\Omega}^{(k)}) \right)_{k \in [Q_{\Omega}]}$ be $\frac{1}{\mathbf{M}}$ - and 1-weighted quadrature rules on \mathbf{D} and Ω , respectively. We then approximate (1.13a) by performing numerical integration over the configuration space, which results in

$$\begin{aligned} \sum_{k=1}^{Q_{\mathbf{D}}} w_{\mathbf{D}}^{(k)} \int_{\Omega} \frac{\psi^{n+1/2}(\cdot, \mathbf{q}^{(k)}) - \psi^n(\cdot, \mathbf{q}^{(k)})}{\Delta t/2} \varphi(\cdot, \mathbf{q}^{(k)}) \\ + \sum_{k=1}^{Q_{\mathbf{D}}} w_{\mathbf{D}}^{(k)} \int_{\Omega} \operatorname{div}_{\mathbf{x}} \left(\mathbf{u}(\cdot, t^{n+1}) \psi^{n+1/2}(\cdot, \mathbf{q}^{(k)}) \right) \varphi(\cdot, \mathbf{q}^{(k)}) \\ + \sum_{k=1}^{Q_{\mathbf{D}}} w_{\mathbf{D}}^{(k)} \frac{(l_0/L_0)^2}{4W\mathbf{i}(N+1)} \int_{\Omega} \nabla_{\mathbf{x}} \psi^{n+1/2}(\cdot, \mathbf{q}^{(k)}) \cdot \nabla_{\mathbf{x}} \varphi(\cdot, \mathbf{q}^{(k)}) \\ \approx \sum_{k=1}^{Q_{\mathbf{D}}} w_{\mathbf{D}}^{(k)} \int_{\Omega} \sum_{i=1}^N \mathbf{M}(\mathbf{q}^{(k)}) (\nabla_{\mathbf{x}} \mathbf{u}(\cdot, t^n))_{\mathbf{q}_i}^{(k)} \psi^n(\cdot, \mathbf{q}^{(k)}) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{\mathbf{M}} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})} \end{aligned}$$

$$- \sum_{k=1}^{Q_D} w_D^{(k)} \int_{\Omega} \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4Wi} M(\mathbf{q}^{(k)}) \nabla_{\mathbf{q}_j} \left(\frac{\psi^n}{M} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})} \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{M} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})},$$

for all $\varphi = \varphi(\mathbf{x}, \mathbf{q})$ in a suitable function space. Here, the symbol \approx denotes equality, up to quadrature errors. By selecting Q_D linearly independent functions $\zeta_{(m)}$, $m \in [Q_D]$, of $\mathbf{q} \in D$ such that $\zeta_{(m)}(\mathbf{q}^{(k)}) = \delta_{km}$, $k, m \in [Q_D]$, and taking successively $\varphi = \varphi_{(m)}$, where $\varphi_{(m)}(\mathbf{x}, \mathbf{q}) := \chi(\mathbf{x})\zeta_{(m)}(\mathbf{q})$, in the equality above, we obtain a total of Q_D independent variational problems, each posed over the d -dimensional domain Ω , of the form:

$$\begin{aligned} & \frac{1}{\Delta t/2} \int_{\Omega} \psi^{n+1/2}(\cdot, \mathbf{q}^{(m)}) \chi + \int_{\Omega} \operatorname{div}_{\mathbf{x}} \left(\mathbf{u}(\cdot, t^{n+1}) \psi^{n+1/2}(\cdot, \mathbf{q}^{(m)}) \right) \chi \\ & + \frac{(l_0/L_0)^2}{4Wi(N+1)} \int_{\Omega} \nabla_{\mathbf{x}} \psi^{n+1/2}(\cdot, \mathbf{q}^{(m)}) \cdot \nabla_{\mathbf{x}} \chi \approx \frac{1}{\Delta t/2} \int_{\Omega} \psi^n(\cdot, \mathbf{q}^{(m)}) \chi \\ & + \frac{1}{w_D^{(m)}} \sum_{k=1}^{Q_D} w_D^{(k)} \left[\int_{\Omega} \sum_{i=1}^N M(\mathbf{q}^{(k)}) (\nabla_{\mathbf{x}} \mathbf{u}(\cdot, t^n)) \mathbf{q}_i^{(k)} \psi^n(\cdot, \mathbf{q}^{(k)}) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\zeta_{(m)}}{M} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})} \chi \right. \\ & \left. - \int_{\Omega} \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4Wi} M(\mathbf{q}^{(k)}) \nabla_{\mathbf{q}_j} \left(\frac{\psi^n}{M} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})} \cdot \nabla_{\mathbf{q}_i} \left(\frac{\zeta_{(m)}}{M} \right) \Big|_{(\cdot, \mathbf{q}^{(k)})} \chi \right] \\ & =: \mathfrak{M}_{(m)}(\psi^n; \chi) \quad \forall m \in [Q_D], \quad (1.14) \end{aligned}$$

for all $\chi = \chi(\mathbf{x})$ in a suitable function space, where each $\mathfrak{M}_{(m)}(\psi^n; \cdot)$, $m \in [Q_D]$, is a linear functional. Thus, (1.14) amounts to solving Q_D mutually independent linear convection-diffusion problems over Ω .

In turn, we can approximate (1.13b) by performing numerical quadrature over Ω , resulting in

$$\begin{aligned} & \sum_{k=1}^{Q_{\Omega}} w_{\Omega}^{(k)} \int_D \frac{\psi^{n+1}(\mathbf{x}^{(k)}, \cdot) - \psi^{n+1/2}(\mathbf{x}^{(k)}, \cdot)}{\Delta t/2} \frac{\varphi(\mathbf{x}^{(k)}, \cdot)}{M} \\ & - \sum_{k=1}^{Q_{\Omega}} w_{\Omega}^{(k)} \int_D \sum_{i=1}^N (\nabla_{\mathbf{x}} \mathbf{u}(\mathbf{x}^{(k)}, t^n)) \mathbf{q}_i \psi^n(\mathbf{x}^{(k)}, \cdot) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi(\mathbf{x}^{(k)}, \cdot)}{M} \right) \\ & + \sum_{k=1}^{Q_{\Omega}} w_{\Omega}^{(k)} \int_D \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4Wi} M \nabla_{\mathbf{q}_j} \left(\frac{\psi^{n+1}(\mathbf{x}^{(k)}, \cdot)}{M} \right) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi(\mathbf{x}^{(k)}, \cdot)}{M} \right) \\ & \approx - \sum_{k=1}^{Q_{\Omega}} w_{\Omega}^{(k)} \int_D \operatorname{div}_{\mathbf{x}} \left(\mathbf{u}(\cdot, t^{n+1}) \psi^{n+1/2} \right) \Big|_{(\mathbf{x}^{(k)}, \cdot)} \frac{\varphi(\mathbf{x}^{(k)}, \cdot)}{M} \\ & - \sum_{k=1}^{Q_{\Omega}} w_{\Omega}^{(k)} \frac{(l_0/L_0)^2}{4Wi(N+1)} \int_D \nabla_{\mathbf{x}} \psi^{n+1/2} \Big|_{(\mathbf{x}^{(k)}, \cdot)} \cdot \nabla_{\mathbf{x}} \varphi \Big|_{(\mathbf{x}^{(k)}, \cdot)} \frac{1}{M}, \end{aligned}$$

for all $\varphi = \varphi(\mathbf{x}, \mathbf{q})$ in a suitable function space. By selecting Q_{Ω} linearly independent functions $\chi_{(m)}$, $m \in [Q_{\Omega}]$, of $\mathbf{x} \in \Omega$ such that $\chi_{(m)}(\mathbf{x}^{(k)}) = \delta_{km}$, $k, m \in [Q_{\Omega}]$, and taking successively $\varphi = \varphi_{(m)}$, where $\varphi_{(m)}(\mathbf{x}, \mathbf{q}) := \chi_{(m)}\zeta(\mathbf{q})$, in the equality above, we obtain a total of Q_{Ω} independent variational problems over the Nd -dimensional domain D of the form:

$$\begin{aligned} & \frac{1}{\Delta t/2} \int_D \psi^{n+1}(\mathbf{x}^{(m)}, \cdot) \frac{\zeta}{M} + \int_D \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4Wi} M \nabla_{\mathbf{q}_j} \left(\frac{\psi^{n+1}(\mathbf{x}^{(m)}, \cdot)}{M} \right) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\zeta}{M} \right) \\ & \approx \left[\frac{1}{\Delta t/2} \int_D \psi^{n+1/2}(\mathbf{x}^{(m)}, \cdot) \frac{\zeta}{M} + \int_D \sum_{i=1}^N (\nabla_{\mathbf{x}} \mathbf{u}(\mathbf{x}^{(m)}, t^n)) \mathbf{q}_i \psi^n(\mathbf{x}^{(m)}, \cdot) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\zeta}{M} \right) \right. \\ & \left. - \int_D \operatorname{div}_{\mathbf{x}} \left(\mathbf{u}(\cdot, t^{n+1}) \psi^{n+1/2} \right) \Big|_{(\mathbf{x}^{(m)}, \cdot)} \frac{\zeta}{M} \right] \end{aligned}$$

$$-\frac{1}{w_\Omega^{(m)}} \sum_{k=1}^{Q_\Omega} w_\Omega^{(k)} \frac{(l_0/L_0)^2}{4W_i(N+1)} \int_D \nabla_{\mathbf{x}} \psi^{n+1/2} \Big|_{(\mathbf{x}^{(k)}, \cdot)} \cdot \nabla_{\mathbf{x}} \chi(m) \Big|_{(\mathbf{x}^{(k)}, \cdot)} \frac{\zeta}{\mathbf{M}} \Big] \\ =: \mathfrak{N}_{(m)}(\psi^{n+1/2}; \zeta) \quad \forall m \in [Q_\Omega], \quad (1.15)$$

for all $\zeta = \zeta(\mathbf{q})$ in a suitable function space, where each $\mathfrak{N}_{(m)}(\psi^{n+1/2}; \cdot)$, $m \in [Q_\Omega]$, is a linear functional. Thus, (1.15) amounts to solving $[Q_\Omega]$ mutually independent linear elliptic variational problems, each posed on the high-dimensional configurational domain $D = D_1 \times \cdots \times D_N \subset \mathbb{R}^{Nd}$. It is the approximate solution of (1.15) by greedy algorithms that this paper is concerned with.

2. THE CONFIGURATION SPACE OPERATOR

2.1. Variational formulation and function spaces. The form of the problem (1.15) motivates us to consider the linear elliptic variational problem

$$a(\psi, \varphi) = f(\varphi), \quad (2.1)$$

posed on the high-dimensional configurational domain $D = D_1 \times \cdots \times D_N \subset \mathbb{R}^{Nd}$, where

$$a(\psi, \varphi) := \int_D \sum_{i=1}^N \sum_{j=1}^N \frac{A_{ij}}{4W_i} \mathbf{M} \nabla_{\mathbf{q}_j} \left(\frac{\psi}{\mathbf{M}} \right) \cdot \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{\mathbf{M}} \right) + c \int_D \frac{\psi \varphi}{\mathbf{M}}, \quad (2.2)$$

the parameter c is positive and f is a linear functional. The natural function space associated with problem (2.1) is

$$H(D; \mathbf{M}) := \left\{ \varphi \in L_{1/\mathbf{M}}^2(D) \cap \mathbf{M} L_{\text{loc}}^1(D) : \nabla_{\mathbf{q}_i}(\varphi/\mathbf{M}) \in [L_{\mathbf{M}}^2(D)]^d \quad \forall i \in [N] \right\},$$

equipped with the norm

$$\|\varphi\|_{H(D; \mathbf{M})} := \left(\|\varphi\|_{L_{1/\mathbf{M}}^2(D)}^2 + \sum_{i=1}^N \|\nabla_{\mathbf{q}_i}(\varphi/\mathbf{M})\|_{[L_{\mathbf{M}}^2(D)]^d}^2 \right)^{1/2}.$$

The spaces $L_{1/\mathbf{M}}^2(D)$ and $H(D; \mathbf{M})$ are isometrically isomorphic to, respectively, $L_{\mathbf{M}}^2(D)$ and $H_{\mathbf{M}}^1(D)$ via the relations

$$L_{1/\mathbf{M}}^2(D) = \mathbf{M} L_{\mathbf{M}}^2(D), \quad \|\cdot\|_{L_{1/\mathbf{M}}^2(D)} = \|\mathbf{M}^{-1} \cdot\|_{L_{\mathbf{M}}^2(D)}, \quad (2.3a)$$

$$H(D; \mathbf{M}) = \mathbf{M} H_{\mathbf{M}}^1(D), \quad \|\cdot\|_{H(D; \mathbf{M})} = \|\mathbf{M}^{-1} \cdot\|_{H_{\mathbf{M}}^1(D)}. \quad (2.3b)$$

Later, we will make use of the spaces $H(D_i; M_i)$, $i \in [N]$, each of which is the i -th partial Maxwellian analogue of $H(D; \mathbf{M})$. That is,

$$H(D_i; M_i) := \left\{ \varphi \in L_{1/M_i}^2(D_i) \cap M_i L_{\text{loc}}^1(D_i) : \nabla(\varphi/M_i) \in [L_{M_i}^2(D_i)]^d \right\},$$

equipped with the norm $\|\varphi\|_{H(D_i; M_i)} := \left(\|\varphi\|_{L_{1/M_i}^2(D_i)}^2 + \|\nabla(\varphi/M_i)\|_{[L_{M_i}^2(D_i)]^d}^2 \right)^{1/2}$.

Remark 2.

- (1) For $i \in [N]$, $H(D_i; M_i)$ is exactly $H(D; \mathbf{M})$ if $N = 1$ and $\mathbf{M} = M_i$. None of the results involving $H(D; \mathbf{M})$ appearing below depend on restrictions on N and thereby remain valid for $H(D_i; M_i)$. Just like (2.3), $\varphi \mapsto M_i \varphi$ is an isometric isomorphism between $L_{M_i}^2(D_i)$ and $L_{1/M_i}^2(D_i)$ and between $H_{M_i}^1(D_i)$ and $H(D_i; M_i)$.
- (2) The definitions above can be extended to open subsets of D and of the D_i , $i \in [N]$, in the usual way.

Before listing our structural hypotheses and proving the properties we need of $H(D; \mathbf{M})$ we fully state the weak formulation of our model problem:

Given $f \in H(D; \mathbf{M})'$, find $\psi \in H(D; \mathbf{M})$ such that

$$a(\psi, \varphi) = f(\varphi) \quad \forall \varphi \in H(D; \mathbf{M}). \quad (2.4)$$

We adopt the following structural hypotheses.

Hypothesis A. For each $i \in [N]$, the spring potential U_i belongs to $C^1([0, \frac{b_i}{2}))$, where $b_i > 0$, and satisfies $\lim_{s \rightarrow b_i/2-} U(s) = +\infty$.

Immediate consequences of Hypothesis A are that $M \in C(\overline{D}) \cap C^1(D)$ and that, for any $K \Subset D$, there exist positive constants c_K and C_K such that $c_K \leq M(\mathbf{q}) \leq C_K$, for all $\mathbf{q} \in K$.

Hypothesis B. For each $i \in [N]$, $H_{M_i}^1(D_i)$ is compactly embedded in $L_{M_i}^2(D_i)$.

Remark 3. It is easy to check that springs obeying any of the example force models (1.2) and (1.3) comply with Hypothesis A.

In Step 1 of section A.1 of [BS08] it is proved that springs obeying the FENE model (1.2) satisfy Hypothesis B, under the condition $b_i \geq 2$. The compliance with Hypothesis B of springs obeying the CPAIL model (1.3) is shown in Lemma A.1 in Appendix A under the condition $b_i \geq 3$.

Lemma 2.1. $L_M^2(D)$, $H_M^m(D)$ for $m \in \mathbb{N}$, $L_{1/M}^2(D)$ and $H(D; M)$ are separable Hilbert spaces.

Proof. The operation $\varphi \in L_M^2(D) \mapsto \varphi/\sqrt{M}$ defines an isometric isomorphism between $L_M^2(D)$ and $L^2(D)$. Therefore the first space inherits its separability from the latter. On noting that $M^{-1} \in L_{\text{loc}}^1(D)$, Theorem 1.11 of [KO84] guarantees the completeness of $H_M^m(D)$ (this source actually states the result for the case $m = 1$ only; however, the proof carries over to higher m in this single-weight case) and thus, $H_M^m(D)$ is separable by an argument along the lines of [AF03, ¶3.5]. The spaces $L_{1/M}^2(D)$ and $H(D; M)$ inherit these properties via the isometric isomorphism (2.3). Finally, as their respective norms obey the parallelogram law, these spaces are Hilbert spaces. \square

Lemma 2.2. $H_M^1(D)$ is compactly embedded in $L_M^2(D)$, and $H(D; M)$ is compactly embedded in $L_{1/M}^2(D)$.

Proof. Throughout this proof we will assume, for ease of exposition, that $N = 2$; the argument carries over to higher N without difficulties. Let $u \in H_M^1(D)$. As, by (1.6), $M = M_1 \otimes M_2$, it follows from Fubini's theorem that, for almost all $\mathbf{q}_1 \in D_1$,

$$u(\mathbf{q}_1, \cdot) \in L_{M_2}^2(D_2) \cap L_{\text{loc}}^1(D_2) \quad \text{and} \quad \partial_\alpha u(\mathbf{q}_1, \cdot) \in L_{M_2}^2(D_2),$$

where α is any multi-index in $[\mathbb{N}_0]^d$ with $0 \leq |\alpha| \leq 1$. Fubini's theorem, again, ensures that, given $\varphi_2 \in C_0^\infty(D_2)$ and $\alpha_2 \in [\mathbb{N}_0]^d$, $0 \leq \alpha_2 \leq 1$,

$$\int_{D_1} \left[(-1) \int_{D_2} u(\mathbf{q}_1, \cdot) \partial_{\alpha_2} \varphi_2 \right] \varphi_1 d\mathbf{q}_1 = \int_{D_1} \left[\int_{D_2} \partial_{(0, \alpha_2)} u(\mathbf{q}_1, \cdot) \varphi_2 \right] \varphi_1 d\mathbf{q}_1,$$

for all $\varphi_1 \in C_0^\infty(D_1)$. Therefore, $\partial_{\alpha_2}[u(\mathbf{q}_1, \cdot)] = \partial_{(0, \alpha_2)} u(\mathbf{q}_1, \cdot)$ in the weak sense on D_2 for almost all $\mathbf{q}_1 \in D_1$. As $\partial_{(0, \alpha_2)} u(\mathbf{q}_1, \cdot)$ lies in $L_{M_2}^2(D_2)$ for almost all $\mathbf{q}_1 \in D_1$, we have that

$$u(\mathbf{q}_1, \cdot) \in H_{M_2}^1(D_2) \quad \text{for almost all } \mathbf{q}_1 \in D_1. \quad (2.5)$$

In the same way it can be proved that $u(\cdot, \mathbf{q}_2) \in H_{M_1}^1(D_1)$ for almost all $\mathbf{q}_2 \in D_2$.

Let us define, for $i \in \{1, 2\}$, the sequence $(D_{i,(n)})_{n \geq 1}$ of bounded and proper subsets of D_i by $D_{i,(n)} := B(0, \frac{\sqrt{b_i n}}{n+1})$. Then,

$$D_{i,(n)} \subset D_{i,(n+1)}, \quad n \in \mathbb{N}, \quad \bigcup_{n=1}^{\infty} D_{i,(n)} = D_i \quad \text{and} \quad H_{M_i}^1(D_{i,(n)}) \Subset L_{M_i}^2(D_{i,(n)}).$$

This last relation is a consequence of the corresponding relation for the unweighted case, $H^1(D_{i,(n)}) \Subset L^2(D_{i,(n)})$ —in turn a consequence of the boundedness and Lipschitz continuity of $D_{i,(n)}$ —on account of the existence of positive lower and upper bounds for M_i on $D_{i,(n)}$, whereupon there is algebraic and topological equivalence between $H_{M_i}^1(D_{i,(n)})$ and $H^1(D_{i,(n)})$ and between $L_{M_i}^2(D_{i,(n)})$ and $L^2(D_{i,(n)})$.

Letting, for $n \in \mathbb{N}$, $D_{(n)} := \times_{i=1}^2 D_{i,(n)} \subsetneq D$, the above properties get inherited:

$$D_{(n)} \subset D_{(n+1)}, \quad n \in \mathbb{N}, \quad \bigcup_{n=1}^{\infty} D_{(n)} = D \quad \text{and} \quad H_M^1(D_{(n)}) \Subset L_M^2(D_{(n)}).$$

The third statement follows from the fact that the $D_{(n)}$, being Cartesian products of bounded Lipschitz domains, are also bounded Lipschitz domains¹. Let us define $D_i^{(n)} := D_i \setminus D_{i,(n)}$ and $D^{(n)} := D \setminus D_{(n)}$. Thanks to [OK90, Theorem 17.6], the above compact embeddings on members of a nested covering imply the following characterizations (the first, for $i \in \{1, 2\}$):

$$H_{M_i}^1(D_i) \subseteq L_{M_i}^2(D_i) \iff \lim_{n \rightarrow \infty} \sup_{u \in H_{M_i}^1(D_i) \setminus \{0\}} \int_{D_i^{(n)}} u^2 M_i / \|u\|_{H_{M_i}^1(D_i)}^2 = 0, \quad (2.6)$$

$$H_M^1(D) \subseteq L_M^2(D) \iff \lim_{n \rightarrow \infty} \sup_{u \in H_M^1(D) \setminus \{0\}} \int_{D^{(n)}} u^2 M / \|u\|_{H_M^1(D)}^2 = 0. \quad (2.7)$$

From Hypothesis B, the left-hand side of (2.6) holds; hence, its right-hand side also holds. Using (2.5) and (2.6) with $i = 2$, we deduce that for each $\varepsilon > 0$ there exists some $\tilde{n} = \tilde{n}(\varepsilon) \in \mathbb{N}$ such that $n \geq \tilde{n}$ implies

$$\begin{aligned} \int_{D_1 \times D_2^{(n)}} u^2 M &= \int_{D_1} \left[\int_{D_2^{(n)}} u^2(\mathbf{q}_1, \cdot) M_2 \right] M_1(\mathbf{q}_1) d\mathbf{q}_1 \\ &\leq \varepsilon \int_{D_1} \|u(\mathbf{q}_1, \cdot)\|_{H_{M_2}^1(D_2)}^2 M_1(\mathbf{q}_1) d\mathbf{q}_1 \\ &= \varepsilon \int_{D_1} \left[\int_{D_2} \left(u^2(\mathbf{q}_1, \cdot) + |\nabla_{\mathbf{q}_2} u(\mathbf{q}_1, \cdot)|^2 \right) M_2 \right] M_1(\mathbf{q}_1) d\mathbf{q}_1 \leq \varepsilon \|u\|_{H_M^1(D)}^2. \end{aligned}$$

An analogous result can be proved for the M -weighted integral of u^2 on $D_1^{(n)} \times D_2$. Then, since $D^{(n)} = (D_1 \times D_2^{(n)}) \cup (D_1^{(n)} \times D_2)$, the right-hand side of (2.7) holds; hence, so does its left-hand side.

Finally, the embedding $H(D; M) \subseteq L_{1/M}^2(D)$ follows directly from the embedding $H_M^1(D) \subseteq L_M^2(D)$ on account of the isometric isomorphism (2.3). \square

Lemma 2.3. *The following inclusion holds: $C_0^1(D) \subset H(D; M)$.*

Proof. Let $\varphi \in C_0^1(D)$ and $K := \text{supp}(\varphi) \Subset D$. Then, trivially, $\varphi \in L_{1/M}^2(D)$, since

$$\int_D \varphi^2 \frac{1}{M} = \int_K \varphi^2 \frac{1}{M} \leq |K| \sup_{\mathbf{q} \in K} \frac{\varphi(\mathbf{q})^2}{M(\mathbf{q})} < \infty,$$

which, in turn, stems from the fact that M is positively bounded from below on each compact subset of D . Similarly, for all $K' \Subset D$,

$$\int_{K'} \left| \frac{\varphi}{M} \right| \leq |K' \cap K| \sup_{\mathbf{q} \in K' \cap K} \frac{|\varphi(\mathbf{q})|}{M(\mathbf{q})} < \infty$$

on account of which $\varphi \in M L_{\text{loc}}^1(D)$. The latter implies that φ/M defines a regular distribution in the usual way. Then, for each $i \in [N]$, $\nabla_{\mathbf{q}_i}(\varphi/M)$ exists as a distribution and coincides with the classical i -th component gradient of φ/M , which belongs to $[C(D)]^d$ because of Hypothesis A. Then,

$$\int_D \left| \nabla_{\mathbf{q}_i} \left(\frac{\varphi}{M} \right) \right|^2 M \leq |K| \sup_{\mathbf{q} \in K} \left| \nabla_{\mathbf{q}_i} \left(\frac{\varphi(\mathbf{q})}{M(\mathbf{q})} \right) \right|^2 M(\mathbf{q}) < \infty$$

and that proves the lemma. \square

¹This follows by combining Theorem 3.1 in the Ph.D. Thesis of Reinhard Hochmuth: *Randwertproblem einer nicht hypoelliptischen linearen partiellen Differentialgleichung. Dissertation, Freie Universität Berlin, 1989*, which implies that the Cartesian product of a finite number of bounded domains, each satisfying the uniform cone property, is a bounded domain satisfying the uniform cone property, and Theorem 1.2.2.2 in the book of Grisvard [Gri85], which states that a bounded open set in \mathbb{R}^n has the uniform cone property if, and only if, its boundary is Lipschitz. In the special case of the domain $D_{(n)}$ an alternative proof is to note that, as a Cartesian product of bounded open convex sets, $D_{(n)}$ is a bounded open convex set in \mathbb{R}^n (cf. [HUL01], p. 23), and then apply Corollary 1.2.2.3 in Grisvard [Gri85], which states that a bounded open convex set in \mathbb{R}^n has Lipschitz boundary.

2.2. Properties of tensor products.

Lemma 2.4. *Suppose that $T \in \mathcal{D}'(\mathbf{D})$ is a distribution such that*

$$T\left(\bigotimes_{i=1}^N \varphi^{(i)}\right) = 0 \quad \forall (\varphi^{(1)}, \dots, \varphi^{(N)}) \in \prod_{i \in [N]} C_0^\infty(D_i).$$

Then, $T = 0$ in $\mathcal{D}'(\mathbf{D})$.

Further, for any ensemble of sequences of distributions $(R_n^{(i)})_{n \geq 1}$, $i \in [N]$, with $R_n^{(i)} \in \mathcal{D}'(D_i)$ and such that $\lim_{n \rightarrow \infty} R_n^{(i)} = R^{(i)}$ in $\mathcal{D}'(D_i)$ for $i \in [N]$, we have that

$$\lim_{n \rightarrow \infty} \bigotimes_{i \in [N]} R_n^{(i)} = \bigotimes_{i \in [N]} R^{(i)} \quad \text{in } \mathcal{D}'(\mathbf{D}).$$

Proof. These are standard results from the theory of distributions, so we omit the proofs and refer the reader to Section 1.3.2 of the book of Vladimirov [Vla02], for example. \square

Lemma 2.5. *The following statements hold:*

- (1) *For any ensemble $r^{(i)} \in H(D_i; M_i)$, $i \in [N]$, $\bigotimes_{i \in [N]} r^{(i)} \in H(\mathbf{D}; \mathbf{M})$.*
- (2) *Suppose that $r^{(i)}: D_i \rightarrow \mathbb{R}$, $i \in [N]$, are measurable functions. Then, the next two statements are equivalent:*
 - (a) *$r^{(i)} \in H(D_i; M_i) \setminus \{0\}$ for all $i \in [N]$;*
 - (b) *$\bigotimes_{i \in [N]} r^{(i)} \in H(\mathbf{D}; \mathbf{M}) \setminus \{0\}$.*

Proof. (1) It is immediate from the factorization of \mathbf{M} that $\bigotimes_{i \in [N]} r^{(i)}$ belongs to $L_{1/\mathbf{M}}^2(\mathbf{D})$. Thanks to Lemma 2.4, the identity

$$\nabla_{q_j} \left(\frac{\bigotimes_{i=1}^N r^{(i)}}{\mathbf{M}} \right) = \bigotimes_{\substack{i=1 \\ i \neq j}}^N \left(\frac{r^{(i)}}{M_i} \right) \otimes_j \nabla \left(\frac{r^{(j)}}{M_j} \right) \quad (2.8)$$

holds in the distributional sense. Then, as $r^{(i)}/M_i \in L_{M_i}^2(D_i)$ for $i \in [N] \setminus \{j\}$, and $\nabla(r^{(j)}/M_j) \in [L_{M_j}^2(D_j)]^d$, the factorization of the Maxwellian \mathbf{M} implies that, for $j \in [N]$, $\nabla_{q_j}(\bigotimes_{i=1}^N r^{(i)}/\mathbf{M}) \in [L_{\mathbf{M}}^2(\mathbf{D})]^d$. That completes the proof of Part (1).

(2) We shall prove the second part by showing that (b) is both necessary and sufficient for (a).

(a) \implies (b): This is immediate from the first part and the fact that the tensor product of the $r^{(i)}$, $i \in [N]$, cannot be null if none of its factors is.

(b) \implies (a): Suppose that $\bigotimes_{i=1}^N r^{(i)} \in H(\mathbf{D}; \mathbf{M}) \setminus \{0\}$; then, because of the tensor-product structure of \mathbf{M} , the positivity of M_i on compact subsets of D_i for $i \in [N]$ and Fubini's theorem, $r^{(i)} \in M_i L_{\text{loc}}^1(D_i) \cap L_{1/M_i}^2(D_i)$, $i \in [N]$. Hence, each $r^{(i)}/M_i$ defines a regular distribution in $\mathcal{D}'(D_i)$. Again, Lemma 2.4 makes (2.8) valid and thus,

$$\left\| \bigotimes_{i=1}^N r^{(i)} \right\|_{H(\mathbf{D}; \mathbf{M})}^2 = \prod_{i=1}^N \left\| r^{(i)} \right\|_{L_{1/M_i}^2(D_i)}^2 + \sum_{j=1}^N \left[\prod_{\substack{i=1 \\ i \neq j}}^N \left\| r^{(i)} \right\|_{L_{1/M_i}^2(D_i)}^2 \right] \left\| \nabla \left(\frac{r^{(j)}}{M_j} \right) \right\|_{[L_{M_j}^2(D_j)]^d}^2. \quad (2.9)$$

Now, none of the $r^{(i)}$ can be null (otherwise their tensor product would be null). On combining this with their $1/M_i$ -weighted square integrability, the identity (2.9) yields $\|\nabla(r^{(i)}/M_i)\|_{[L_{M_i}^2(D_i)]^d} < \infty$ for all $i \in [N]$. Hence $r^{(i)} \in H(D_i; M_i) \setminus \{0\}$ for $i \in [N]$. \square

3. SEPARATED REPRESENTATION

3.1. Two algorithms. The existence of a unique weak solution to (2.1) is an immediate consequence of the Lax–Milgram theorem via the facts that $H(\mathbf{D}; \mathbf{M})$ is a Hilbert space (cf. Lemma 2.1) and a is a bounded and coercive bilinear form on $H(\mathbf{D}; \mathbf{M})$. By virtue of the Riesz representation theorem, there exists a bounded linear operator $\mathcal{A}: H(\mathbf{D}; \mathbf{M}) \rightarrow H(\mathbf{D}; \mathbf{M})'$, defined by

$(\mathcal{A}\psi)(\varphi) = a(\psi, \varphi)$ for all $\varphi \in H(D; M)$. Thanks to the symmetry of a , the weak formulation (2.1) can be restated as the following, equivalent, energy minimization problem:

$$\psi := \arg \min_{\varphi \in H(D; M)} J_f(\varphi) \quad \text{where} \quad J_f(\varphi) := \frac{1}{2} a(\varphi, \varphi) - f(\varphi). \quad (3.1)$$

We observe that, with $\psi \in H(D; M)$ as in (3.1),

$$J_f(\varphi) = \frac{1}{2} a(\varphi - \psi, \varphi - \psi) - \frac{1}{2} a(\psi, \psi) \quad \forall \varphi \in H(D; M). \quad (3.2)$$

Following the work of Le Bris, Lelièvre and Maday [LBLM09] concerning the numerical solution of high-dimensional Poisson equations, we consider two numerical methods.

Algorithm 1. (Pure Greedy Algorithm)

0. Define: $f_0 := f \in H(D; M)'$.
1. For $n \geq 1$ do:
 - 1.1 Find $r_n^{(i)} \in H(D_i; M_i)$, $i \in [N]$, such that

$$(r_n^{(1)}, \dots, r_n^{(N)}) \in \arg \min_{(s^{(1)}, \dots, s^{(N)}) \in \times_{i=1}^N H(D_i; M_i)} J_{f_{n-1}} \left(\bigotimes_{i=1}^N s^{(i)} \right). \quad (3.3)$$

- 1.2 Define: $f_n := f_{n-1} - \mathcal{A} \left(\bigotimes_{i=1}^N r_n^{(i)} \right) \in H(D; M)'$.
- 1.3 If $\|f_n\|_{H(D; M)'} \geq \text{TOL}$, then proceed to iteration $n + 1$; else, stop.

Algorithm 2. (Orthogonal Greedy Algorithm)

0. Define: $f_0 := f \in H(D; M)'$.
1. For $n \geq 1$ do:
 - 1.1 Find $r_n^{(i)} \in H(D_i; M_i)$, $i \in [N]$, such that

$$(r_n^{(1)}, \dots, r_n^{(N)}) \in \arg \min_{(s^{(1)}, \dots, s^{(N)}) \in \times_{i=1}^N H(D_i; M_i)} J_{f_{n-1}} \left(\bigotimes_{i=1}^N r^{(i)} \right). \quad (3.4)$$

- 1.2 Minimize J_f on the span of $\left(\bigotimes_{i=1}^N r_k^{(i)} \right)_{k \in [n]}$; i.e., find $\alpha^{(n)} \in \mathbb{R}^n$ such that

$$\alpha^{(n)} = \arg \min_{\beta \in \mathbb{R}^n} J_f \left(\sum_{k=1}^n \beta_k \bigotimes_{i=1}^N r_k^{(i)} \right). \quad (3.5)$$

- 1.3 Define: $f_n := f - \mathcal{A} \left(\sum_{k=1}^n \alpha_k^{(n)} \bigotimes_{i=1}^N r_k^{(i)} \right) \in H(D; M)'$.
- 1.4 If $\|f_n\|_{H(D; M)'} \geq \text{TOL}$, then proceed to iteration $n + 1$; else, stop.

For future reference, we define $\psi_n \in H(D; M)$ as the unique solution of the problem

$$a(\psi_n, \varphi) = f_n(\varphi) \quad \forall \varphi \in H(D; M).$$

Clearly, for all n up to the (existing or not) termination of the corresponding algorithm,

$$\psi_n = \begin{cases} \psi_{n-1} - \bigotimes_{i=1}^N r_n^{(i)} & \text{for the Pure Greedy Algorithm,} \\ \psi - \sum_{k=1}^n \alpha_k^{(n)} \bigotimes_{i=1}^N r_k^{(i)} & \text{for the Orthogonal Greedy Algorithm,} \end{cases} \quad (3.6)$$

where $\psi = \psi_0$ is the unique solution of (3.1). Proving the convergence of the algorithms amounts to showing that the sequences $(\psi_n)_{n \geq 0}$ defined by (3.6) converge to 0 in $H(D; M)$.

3.2. Correctness of the algorithms. The proof of the correctness of Algorithm 1 (respectively Algorithm 2) amounts to showing that, given $f_{n-1} \in H(D; M)'$ (respectively $(f_{n-1}, \alpha^{(n-1)}) \in H(D; M)' \times \mathbb{R}^{n-1}$), the loop 1 returns a well-defined member of $H(D; M)'$ (resp. $H(D; M)' \times \mathbb{R}^n$).

We start by observing that, thanks to the first part of Lemma 2.5, the set of N -way tensor products of ensembles of functions $H(D_i; M_i)$, $i \in [N]$, is a subset of $H(D; M)$, thereby rendering the minimization problems (3.3) and (3.4) sound. However, the existence of solutions $(r_n^{(1)}, \dots, r_n^{(N)})$ to these problems is quite another matter: it will be proved using Lemma 3.1 and Theorem 3.2 below.

Lemma 3.1. *Suppose that $f \in H(D; M)' \setminus \{0\}$ and consider the functional J_f , as in (3.1). Then, there exists $(r^{(1)}, \dots, r^{(N)})$ in $\times_{i=1}^N H(D_i; M_i)$ such that*

$$J_f \left(\bigotimes_{i=1}^N r^{(i)} \right) < 0.$$

Proof. Consider any functional $f \in H(D; M)' \setminus \{0\}$ and assume that the thesis is false; i.e., $J_f \left(\bigotimes_{i=1}^N r^{(i)} \right) \geq 0$ for all ensembles $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N H(D_i; M_i)$; then,

$$\frac{1}{2} a \left(\bigotimes_{i=1}^N r^{(i)}, \bigotimes_{i=1}^N r^{(i)} \right) \geq f \left(\bigotimes_{i=1}^N r^{(i)} \right) \quad \forall (r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N H(D_i; M_i).$$

Given a particular ensemble $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N H(D_i; M_i)$, we can replace $r^{(1)}$ with $\varepsilon r^{(1)}$ and, by virtue of the bilinearity of a and the linearity of f , we obtain

$$\frac{1}{2} \varepsilon^2 a \left(\bigotimes_{i=1}^N r^{(i)}, \bigotimes_{i=1}^N r^{(i)} \right) \geq \varepsilon f \left(\bigotimes_{i=1}^N r^{(i)} \right). \quad (3.7)$$

By combining the inequalities resulting from dividing both sides of (3.7) by positive ε and taking the one-sided limit $\varepsilon \rightarrow 0_+$ and from dividing (3.7) by a negative ε and taking the one-sided limit $\varepsilon \rightarrow 0_-$ we get that

$$f \left(\bigotimes_{i=1}^N r^{(i)} \right) = 0.$$

As this is valid for any ensemble $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N H(D_i; M_i)$, Lemma 2.3 implies that it is valid, in particular, for any ensemble $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N C_0^\infty(D_i)$, whence Lemma 2.4 implies that $f = 0$. As this contradicts the hypotheses of the lemma, its thesis holds. \square

We are now in a position to prove the existence of solutions to problems (3.3) and (3.4).

Theorem 3.2. *Given $f_{n-1} \in H(D; M)'$, each of the problems (3.3) and (3.4) has a solution.*

Proof. Since problems (3.3) and (3.4) are completely analogous, it suffices to consider one of them—say, (3.3). Then, as $(0, \dots, 0)$ is a solution of (3.3) and (3.4) when $f_{n-1} = 0$, we assume from now on that $f_{n-1} \neq 0$.

By (3.2) and the coerciveness of a , $J_{f_{n-1}}(\varphi) \geq -\frac{1}{2}a(\psi, \psi)$ for all $\varphi \in H(D; M)$, where ψ is the unique solution of (2.4) in $H(D; M)$ when $f = f_{n-1}$. As, by Lemma 2.5, the N -way tensor product of functions in $H(D_i; M_i)$, $i \in [N]$, is a subset of $H(D; M)$, $J_{f_{n-1}}$ is bounded from below over that manifold. That is,

$$\mathbf{m} := \inf_{(s^{(1)}, \dots, s^{(N)}) \in \times_{i=1}^N H(D_i; M_i)} J_{f_{n-1}} \left(\bigotimes_{i=1}^N s^{(i)} \right) > -\infty. \quad (3.8)$$

It follows from Lemma 3.1 that $\mathbf{m} < 0$. Our aim is to show that the infimum \mathbf{m} is attained at an element of the form $\bigotimes_{i=1}^N r^{(i)}$ with $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N (H(D_i; M_i) \setminus \{0\})$.

From (3.8), there exists a sequence $\left(\bigotimes_{i \in [N]} r_k^{(i)} \right)_{k \geq 1}$ of N -way tensor products of functions in $H(D_i; M_i)$, $i \in [N]$, such that

$$\lim_{k \rightarrow \infty} J_{f_{n-1}} \left(\bigotimes_{i=1}^N r_k^{(i)} \right) = \mathbf{m}.$$

On noting that, from the definition of a in (2.2), for all $\varphi \in H(D; M)$,

$$\begin{aligned} J_{f_{n-1}}(\varphi) &= \frac{1}{2} a(\varphi - \psi, \varphi - \psi) - \frac{1}{2} a(\psi, \psi) \geq \frac{1}{4} a(\varphi, \varphi) - a(\psi, \psi) \\ &\geq \frac{1}{4} \min\left(\frac{\lambda_{\min}}{4W_1}, c\right) \|\varphi\|_{H(D; M)}^2 - a(\psi, \psi), \end{aligned}$$

it follows, by setting $\varphi = \bigotimes_{i \in [N]} r_k^{(i)}$, that the sequence $\left(\bigotimes_{i \in [N]} r_k^{(i)}\right)_{k \geq 1}$ is bounded in $H(D; M)$; in other words, there exists $C > 0$ such that (cf. (2.9)):

$$\left\| \bigotimes_{i=1}^N r_k^{(i)} \right\|_{H(D; M)}^2 = \prod_{i=1}^N \|r_k^{(i)}\|_{L_{1/M_i}^2(D_i)}^2 + \sum_{j=1}^N \left(\prod_{\substack{i=1 \\ i \neq j}}^N \|r_k^{(i)}\|_{L_{1/M_i}^2(D_i)}^2 \right) \left\| \nabla(r_k^{(j)}/M_j) \right\|_{[L_{1/M_j}^2(D_j)]^d}^2 \leq C \quad (3.9)$$

for all $k \geq 1$. Since the value of $\bigotimes_{i \in [N]} r_k^{(i)}$ is unaltered by multiplying the first $N-1$ factors by positive constants $c_{1,k}, \dots, c_{N-1,k}$, respectively, and dividing the final factor by the product $c_{1,k} \cdots c_{N-1,k}$, we can assume without loss of generality that

$$\|r_k^{(i)}\|_{L_{1/M_i}^2(D_i)}^2 = 1, \quad i \in [N-1]. \quad (3.10)$$

Thus, it follows from (3.9) that

$$\left\| r_k^{(N)} \right\|_{L_{1/M_N}^2(D_N)}^2 + \left\| r_k^{(N)} \right\|_{L_{1/M_N}^2(D_N)}^2 \sum_{j=1}^{N-1} \left\| \nabla(r_k^{(j)}/M_j) \right\|_{[L_{1/M_j}^2(D_j)]^d}^2 + \left\| \nabla(r_k^{(N)}/M_N) \right\|_{[L_{1/M_N}^2(D_N)]^d}^2 \leq C. \quad (3.11)$$

Since the sequence $\left(\bigotimes_{i \in [N]} r_k^{(i)}\right)_{k \geq 1}$ is bounded in $H(D; M)$, and $H(D; M)$ is a Hilbert space, and therefore reflexive, the sequence has a weakly convergent subsequence in $H(D; M)$, denoted by $\left(\bigotimes_{i \in [N]} r_{\phi(k)}^{(i)}\right)_{k \geq 1}$; we denote its weak limit by $r \in H(D; M)$. Since $J_{f_{n-1}}$ is convex on $H(D; M)$ and continuous (and thereby also semicontinuous) in the strong topology of $H(D; M)$, it is weakly lower-semicontinuous on $H(D; M)$. Hence

$$J_{f_{n-1}}(r) \leq \liminf_{k \rightarrow \infty} J_{f_{n-1}}\left(\bigotimes_{i=1}^N r_{\phi(k)}^{(i)}\right) = \lim_{k \rightarrow \infty} J_{f_{n-1}}\left(\bigotimes_{i=1}^N r_k^{(i)}\right) = m < 0.$$

Thus we deduce that $r \neq 0$ (as $r = 0$ would imply that $J_{f_{n-1}}(r) = 0$); hence, $r \in H(D; M) \setminus \{0\}$.

According to (3.10) and (3.11) each subsequence $\left(r_{\phi(k)}^{(i)}\right)_{k \geq 1}$, is bounded in the respective space $L_{1/M_i}^2(D_i)$, for $i \in [N]$. Then, $\left(r_{\phi(k)}^{(i)}\right)_{k \geq 1}$ has a weakly convergent subsequence in $L_{1/M_i}^2(D_i)$, say $\left(r_{\phi'(k)}^{(i)}\right)_{k \geq 1}$, for $i \in [N]$; let us denote by $r^{(i)} \in L_{1/M_i}^2(D_i)$ the corresponding weak limits. As by Lemma 2.3, $C_0^\infty(D_i) \subset H(D_i; M_i) \subset L_{1/M_i}^2(D_i)$, for all $\varphi \in C_0^\infty(D_i)$ the mapping $\xi \in L_{1/M_i}^2(D_i) \mapsto \langle \varphi, \xi \rangle_{L_{1/M_i}^2(D_i)}$ defines a bounded linear functional on $L_{1/M_i}^2(D_i)$. Thus, $\left(r_{\phi'(k)}^{(i)}/M_i\right)_{k \geq 1}$ converges to $r^{(i)}/M_i$ in $\mathcal{D}'(D_i)$ for $i \in [N]$. Hence, by Lemma 2.4,

$$\lim_{k \rightarrow \infty} \bigotimes_{i=1}^N \frac{r_{\phi'(k)}^{(i)}}{M_i} = \bigotimes_{i=1}^N \frac{r^{(i)}}{M_i} = \frac{\bigotimes_{i=1}^N r^{(i)}}{M} \quad \text{in } \mathcal{D}'(D). \quad (3.12)$$

Similarly, the inclusion $C_0^\infty(D) \subset H(D; M)$ (cf. Lemma 2.3) and the fact that, for all $\varphi \in C_0^\infty(D)$, the mapping $\xi \in H(D; M) \mapsto \langle \varphi, \xi \rangle_{L_{1/M}^2(D)}$ defines a bounded linear functional on $H(D; M)$ imply

$$\lim_{k \rightarrow \infty} \bigotimes_{i=1}^N \frac{r_{\phi'(k)}^{(i)}}{M_i} = \lim_{k \rightarrow \infty} \frac{\bigotimes_{i=1}^N r_{\phi'(k)}^{(i)}}{M} = \frac{r}{M} \quad \text{in } \mathcal{D}'(D) \quad (3.13)$$

on account of r being the $H(D; \mathbf{M})$ -weak limit of the sequence $\left(\bigotimes_{i \in [N]} r_{\phi(k)}^{(i)}\right)_{k \geq 1}$. As $\mathcal{D}'(D)$ is a Hausdorff topological space, the limits in (3.12) and (3.13) have to coincide. That is,

$$\mathbf{M}^{-1}r = \mathbf{M}^{-1} \bigotimes_{i=1}^N r^{(i)} \quad \text{in } \mathcal{D}'(D).$$

Hence, $r = \bigotimes_{i=1}^N r^{(i)}$ almost everywhere. As $r \in H(D; \mathbf{M}) \setminus \{0\}$ and has a tensor-product structure, the second part of Lemma 2.5 implies that $r^{(i)} \in H(D_i; M_i) \setminus \{0\}$ for $i \in [N]$. Now,

$$J_{f_{n-1}} \left(\bigotimes_{i=1}^N r^{(i)} \right) = J_{f_{n-1}}(r) \leq \mathbf{m}.$$

Recalling the definition of \mathbf{m} from (3.8), we have thus shown that the infimum in (3.8) is attained at $\bigotimes_{i=1}^N r^{(i)}$. Thus, $(r^{(1)}, \dots, r^{(N)}) \in \times_{i=1}^N (H(D_i; M_i) \setminus \{0\})$ is a solution to problem (3.3). \square

Having proved that the minimization problems (3.3) of Algorithm 1 and (3.4) of Algorithm 2 have solutions, establishing the correctness of what is left of the algorithms is straightforward. The Galerkin problem 1.2 of Algorithm 2 is well-defined and has a unique solution for each $n \geq 1$, because it is equivalent to the minimization of a coercive quadratic form over a finite-dimensional linear space. Then, at last, the definition of the n -th residual in step 1.2 of Algorithm 1 and in step 1.3 of Algorithm 2 are correct on noting that \mathcal{A} maps $H(D; \mathbf{M})$ into $H(D; \mathbf{M})'$.

In the next section we establish the convergence of the two algorithms.

4. CONVERGENCE OF THE ALGORITHMS

4.1. Euler–Lagrange equations.

Lemma 4.1. *Local minimizers $(r_n^{(1)}, \dots, r_n^{(N)})$ of the minimization problems (3.3) or (3.4) satisfy the following Euler–Lagrange equation system: For all $(s^{(1)}, \dots, s^{(N)}) \in \times_{i \in [N]} H(D_i; M_i)$,*

$$a \left(\bigotimes_{i=1}^N r_n^{(i)}, \sum_{j=1}^N \bigotimes_{\substack{i=1 \\ i \neq j}}^N r_n^{(i)} \otimes_j s^{(j)} \right) = f_{n-1} \left(\sum_{j=1}^N \bigotimes_{\substack{i=1 \\ i \neq j}}^N r_n^{(i)} \otimes_j s^{(j)} \right). \quad (4.1)$$

From this, it follows that, for the Pure Greedy Algorithm (Algorithm 1):

$$a \left(\psi_n, \bigotimes_{i=1}^N r_n^{(i)} \right) = 0. \quad (4.2)$$

Proof. Let $(r_n^{(1)}, \dots, r_n^{(N)})$ be a solution to the minimization problem (3.3) or (3.4). Then, given any ensemble $(s^{(1)}, \dots, s^{(N)})$, (4.1) is but a way of writing that the derivative of

$$J_{f_{n-1}} \left(\bigotimes_{i=1}^N (r_n^{(i)} + \varepsilon s^{(i)}) \right)$$

with respect to ε is zero when evaluated at $\varepsilon = 0$. As, by hypothesis, $(r_n^{(1)}, \dots, r_n^{(N)})$ is a local minimizer of $J_{f_{n-1}}$ and $\varepsilon \mapsto \mathfrak{J}_n(\varepsilon) := J_{f_{n-1}} \left(\bigotimes_{i=1}^N (r_n^{(i)} + \varepsilon s^{(i)}) \right)$ is regular enough, the fact that $\mathfrak{J}_n'(0) = 0$ implies that (4.1) holds.

Setting $(s^{(1)}, \dots, s^{(N)}) = (r_n^{(1)}, \dots, r_n^{(N)})$ in (4.1), we obtain from the definition of the ψ_n that

$$a \left(\bigotimes_{i=1}^N r_n^{(i)}, \bigotimes_{i=1}^N r_n^{(i)} \right) = a \left(\psi_{n-1}, \bigotimes_{i=1}^N r_n^{(i)} \right). \quad (4.3)$$

Combining this with (3.6) we obtain (4.2). \square

Remark 4.

- (1) The above lemma only states that local minima of the minimization problem (3.3) and (3.4) satisfy the Euler–Lagrange equation (4.1). The converse may be false, of course: although the functional that is minimized is quadratic, the set over which it is minimized is nonlinear, so there is no reason why a stationary point should be a local minimum.
- (2) In what follows we make liberal use of the norm $\|\cdot\|_a := a(\cdot, \cdot)^{1/2}$ on $H(D; M)$, which, thanks to its equivalence with $\|\cdot\|_{H(D; M)}$, makes no difference when making topological statements (such as convergence).

Lemma 4.2. *Let $(r_n^{(1)}, \dots, r_n^{(N)})$ be a global minimizer for the minimization problem (3.3) of the Algorithm 1. Then,*

$$\left\| \bigotimes_{i=1}^N r_n^{(i)} \right\|_a = \frac{a\left(\psi_{n-1}, \bigotimes_{i=1}^N r_n^{(i)}\right)}{\left\| \bigotimes_{i=1}^N r_n^{(i)} \right\|_a} = \sup_{s \in \bigotimes_{i \in [N]} H(D_i; M_i) \setminus \{0\}} \frac{a(\psi_{n-1}, s)}{\|s\|_a}. \quad (4.4)$$

Proof. The first equality in (4.4) comes directly from (4.3). Now, analogously to (3.2), $J_{f_{n-1}}$ can be written as

$$J_{f_{n-1}}(\varphi) = \frac{1}{2}a(\varphi - \psi_{n-1}, \varphi - \psi_{n-1}) - \frac{1}{2}a(\psi_{n-1}, \psi_{n-1}) \quad \forall \varphi \in H(D; M).$$

Combining this representation of $J_{f_{n-1}}$ with the fact that $r_n := \bigotimes_{i \in [N]} r_n^{(i)}$ minimizes $J_{f_{n-1}}$ among the members of $\bigotimes_{i \in [N]} H(D_i; M_i)$ and the first equality of (4.4), according to which $a(\psi_{n-1}, r_n) = \|r_n\|_a^2$, we have, for all $s \in \bigotimes_{i \in [N]} H(D_i; M_i) \setminus \{0\}$, that

$$\left\| \psi_{n-1} - \frac{a(\psi_{n-1}, r_n)}{\|r_n\|_a^2} r_n \right\|_a^2 = \|\psi_{n-1} - r_n\|_a^2 \leq \left\| \psi_{n-1} - \frac{a(\psi_{n-1}, s)}{\|s\|_a^2} s \right\|_a^2.$$

Therefore,

$$\frac{a(\psi_{n-1}, r_n)^2}{a(r_n, r_n)} \geq \frac{a(\psi_{n-1}, s)^2}{a(s, s)}.$$

Taking the supremum over $s \in \bigotimes_{i \in [N]} H(D_i; M_i) \setminus \{0\}$ and noting that r_n is an admissible s we get the second equality in (4.4). \square

4.2. Convergence.

Theorem 4.3. *The Pure Greedy Algorithm (Algorithm 1) converges to the solution ψ to (2.4).*

Proof. Let $\left((r_n^{(1)}, \dots, r_n^{(N)})\right)_{n \geq 1}$ be a sequence in $\times_{i=1}^N H(D_i; M_i)$ returned by the Pure Greedy Algorithm and let us adopt the shorthand notation $r_n := \bigotimes_{i \in [N]} r_n^{(i)}$. Then, from (3.6) and (4.2) in Lemma 4.1 we obtain

$$\|\psi_{n-1}\|_a^2 = \|\psi_n + r_n\|_a^2 = \|\psi_n\|_a^2 + \|r_n\|_a^2.$$

Hence the sequence $(\|\psi_n\|_a)_{n \geq 0}$ is nonnegative and monotonic nonincreasing, and therefore converges in \mathbb{R} ; by summing the above expression over n we then deduce that

$$\sum_{n=1}^{\infty} a(r_n, r_n) < \infty. \quad (4.5)$$

Let us define the function $\phi: \mathbb{N} \rightarrow \mathbb{N}$ recursively by $\phi(1) := 1$ and

$$\phi(k) := \arg \min_{n > \phi(k-1)} \{\|r_n\|_a \leq \|r_{\phi(k-1)}\|_a\}, \quad k \geq 2.$$

From (4.5) the function ϕ is well-defined and strictly monotonic increasing. Hence, it is suitable for defining subsequences. As each $(r_n^{(1)}, \dots, r_n^{(N)})$ is a global solution to the problem (3.3) with

the instance f_{n-1} , via (3.6) and Lemma 4.2 we have, for $n \geq m \geq 1$,

$$\begin{aligned}
\|\psi_{\phi(n)-1} - \psi_{\phi(m)-1}\|_a^2 &= \|\psi_{\phi(n)-1}\|_a^2 + \|\psi_{\phi(m)-1}\|_a^2 - 2a \left(\psi_{\phi(n)-1}, \psi_{\phi(m)-1} + \sum_{k=\phi(m)}^{\phi(n)-1} r_k \right) \\
&= \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 - 2 \sum_{k=\phi(m)}^{\phi(n)-1} a(\psi_{\phi(n)-1}, r_k) \\
&\leq \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 + 2 \sum_{k=\phi(m)}^{\phi(n)-1} \|r_k\|_a \|\psi_{\phi(n)-1}\|_a \\
&\leq \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 + 2 \sum_{k=\phi(m)}^{\phi(n)-1} \|r_k\|_a^2.
\end{aligned}$$

From the convergence of $(\|\psi_{\phi(n)-1}\|_a)_{n \geq 1}$ in \mathbb{R} and (4.5), we deduce that the sequence $(\psi_{\phi(n)-1})_{n \geq 1}$ is a Cauchy sequence in $H(D; M)$ and thus converges to some $\psi_\infty \in H(D; M)$. Another consequence of the global optimality of each $(r_n^{(1)}, \dots, r_n^{(N)})$ is: For all $(s^{(1)}, \dots, s^{(N)}) \in \times_{i \in [N]} H(D_i; M_i)$ and $n \geq 1$,

$$\begin{aligned}
\frac{1}{2}a \left(\bigotimes_{i=1}^N s^{(i)}, \bigotimes_{i=1}^N s^{(i)} \right) - a \left(\psi_{\phi(n)-1}, \bigotimes_{i=1}^N s^{(i)} \right) &\geq J_{f_{\phi(n)-1}}(r_{\phi(n)}) \\
&= \frac{1}{2}a(r_{\phi(n)}, r_{\phi(n)}) - f_{\phi(n)-1}(r_{\phi(n)}) \\
&= -\frac{1}{2}a(r_{\phi(n)}, r_{\phi(n)}).
\end{aligned}$$

Taking the limit as n tends to infinity at both ends, and noting that by (4.5) the right-hand side of the last inequality converges to 0, we obtain

$$\frac{1}{2}a \left(\bigotimes_{i=1}^N s^{(i)}, \bigotimes_{i=1}^N s^{(i)} \right) - a \left(\psi_\infty, \bigotimes_{i=1}^N s^{(i)} \right) \geq 0.$$

Thus, Lemma 3.1 implies that $\psi_\infty = 0$. Hence the sequence $(\|\psi_{\phi(n)-1}\|)_{n \geq 1}$ converges to zero as $n \rightarrow \infty$. As the sequence $(\|\psi_n\|_a)_{n \geq 0}$ is monotonic nonincreasing and $(\phi(n) - 1)_{n \geq 1}$ is a monotonic increasing infinite sequence in \mathbb{N} , it follows that the full sequence $(\|\psi_n\|)_{n \geq 1}$ converges to the common limit in \mathbb{R} : $0 = \|\psi_\infty\|_a$, giving $\lim_{n \rightarrow \infty} \psi_n = 0$ in $H(D; M)$. \square

The following corollary is a direct consequence of Theorem 4.3 and will prove useful later on.

Corollary 4.4. *Let F_i be a dense subset of $H(D_i; M_i)$ for $i \in [N]$. Then, the span of $\bigotimes_{i \in [N]} F_i$ is dense in $H(D; M)$.*

Proof. Let $\tau \in H(D; M)$. Applying Theorem 4.3 to the case in which the right-hand side functional $f \in H(D; M)'$ of problem (2.4) is $\varphi \mapsto a(\tau, \varphi)$ (i.e., the $H(D; M)$ approximation problem) it follows that τ can be approximated arbitrarily closely by finite sums of the form $\sum_{m \in [M]} \bigotimes_{i \in [N]} r_m^{(i)}$, where $M \in \mathbb{N}$ and $r_m^{(i)} \in H(D_i; M_i)$ for $m \in [M]$ and $i \in [N]$. Thus, if we can show that $\bigotimes_{i \in [N]} F_i$ is dense in the manifold $\bigotimes_{i \in [N]} H(D_i; M_i)$, our desired result will stand.

Let, then, $r^{(i)} \in H(D_i; M_i)$, for $i \in [N]$. From the density of F_i in $H(D_i; M_i)$ for each $i \in [N]$, there exists a sequence $(r_n^{(i)})_{n \geq 1}$ in F_i , which converges to $r^{(i)}$ in $H(D_i; M_i)$. Now,

$$\delta_n := \bigotimes_{i=1}^N r^{(i)} - \bigotimes_{i=1}^N r_n^{(i)} = \sum_{k=1}^N \bigotimes_{i=1}^N t_{n,k}^{(i)}, \quad \text{where} \quad t_{n,k}^{(i)} := \begin{cases} r_n^{(i)} & \text{if } i > k, \\ r^{(i)} - r_n^{(i)} & \text{if } i = k, \\ r^{(i)} & \text{if } i < k. \end{cases}$$

Then, (cf. (2.9)),

$$\|\delta_n\|_{\mathbf{H}(\mathbf{D}; \mathbf{M})}^2 \leq \sum_{k=1}^N \left[\prod_{i=1}^N \|t_{n,k}^{(i)}\|_{L_{1/M_i}^2(D_i)}^2 + \sum_{j=1}^N \prod_{\substack{i=1 \\ i \neq j}}^N \|t_{n,k}^{(i)}\|_{L_{1/M_i}^2(D_i)}^2 \left\| \nabla \left(\frac{t_{n,k}^{(j)}}{M_j} \right) \right\|_{[L_{M_j}^2(D_j)]^d}^2 \right].$$

As each product term on the right-hand side above consists of $N - 1$ bounded factors and one vanishing factor as $n \rightarrow \infty$, the full expression tends to zero as n tends to infinity and, therefore, so does the left-hand side. The desired result follows. \square

Remark 5. Suppose that, for each $i \in [N]$,

$$C_0^\infty(D_i) \text{ is dense in } \mathbf{H}(D_i; M_i). \quad (4.6)$$

Then, as $\text{span} \left(\bigotimes_{i=1}^N C_0^\infty(D_i) \right) \subset C_0^\infty(\mathbf{D}) \subset \mathbf{H}(\mathbf{D}; \mathbf{M})$, we have, thanks to Corollary 4.4, that

$$C_0^\infty(\mathbf{D}) \text{ is dense in } \mathbf{H}(\mathbf{D}; \mathbf{M}). \quad (4.7)$$

Springs obeying the FENE model (1.2) comply with (4.6) under the condition $b_i \geq 2$ as is proved in Remark 3.7 of [Mas08]. Springs obeying the CPAIL model (1.3), in turn, comply with (4.6) as it is shown in Lemma A.1 in Appendix A, under the condition $b_i \geq 3$. So, in these two cases, (4.7) holds.

Interesting as (4.7) is, we make no use of it in this work and that is why we shall not adopt (4.6) as a hypothesis on a par with hypotheses A and B above or hypotheses C, D and E below. However, we do use (4.6) as an ingredient of the proof of the compliance of FENE and CPAIL spring potentials with Hypothesis C of Section 5 (cf. Corollary C.2 in Appendix C).

Theorem 4.5. *The Orthogonal Greedy Algorithm (Algorithm 2) converges to the solution ψ to problem (2.4).*

Proof. We first note that thanks to (3.6), the optimality of $\alpha^{(n)}$ in (3.5) and the optimality of $(r_n^{(1)}, \dots, r_n^{(N)})$ in (3.4) (via Lemma 4.1),

$$\|\psi_n\|_a^2 = \left\| \psi - \sum_{k=1}^n \alpha_k^{(n)} \bigotimes_{i=1}^N r_k^{(i)} \right\|_a^2 \leq \left\| \psi_{n-1} - \bigotimes_{i=1}^N r_n^{(i)} \right\|_a^2 = \|\psi_{n-1}\|_a^2 - \left\| \bigotimes_{i=1}^N r_n^{(i)} \right\|_a^2.$$

Thus, just like in the proof of Theorem 4.3, we have that the real sequence $(\|\psi_n\|_a)_{n \geq 0}$ is decreasing and thus convergent and that $\sum_{n \geq 1} a \left(\bigotimes_{i \in [N]} r_n^{(i)}, \bigotimes_{i \in [N]} r_n^{(i)} \right) < \infty$. As $(\psi_n)_{n \geq 0}$ is a bounded sequence in the Hilbert space $\mathbf{H}(\mathbf{D}; \mathbf{M})$, a weakly convergent subsequence $(\psi_{\phi(n)})_{n \geq 1}$ can be extracted and we denote the weak limit by ψ_∞ . From the optimality of $(r_{\phi(n)+1}^{(1)}, \dots, r_{\phi(n)+1}^{(N)})$ with respect to problem (3.4) we have by Lemma 4.1 that, for all $(s^{(1)}, \dots, s^{(N)}) \in \times_{i \in [N]} \mathbf{H}(D_i; M_i)$,

$$\frac{1}{2} a \left(\bigotimes_{i=1}^N s^{(i)}, \bigotimes_{i=1}^N s^{(i)} \right) - a \left(\psi_{\phi(n)}, \bigotimes_{i=1}^N s^{(i)} \right) \geq -\frac{1}{2} a \left(\bigotimes_{i=1}^N r_{\phi(n)+1}^{(i)}, \bigotimes_{i=1}^N r_{\phi(n)+1}^{(i)} \right).$$

Taking the limit $n \rightarrow \infty$ at both sides yields

$$\frac{1}{2} a \left(\bigotimes_{i=1}^N s^{(i)}, \bigotimes_{i=1}^N s^{(i)} \right) - a \left(\psi_\infty, \bigotimes_{i=1}^N s^{(i)} \right) \geq 0,$$

whence, via Lemma 3.1, $\psi_\infty = 0$. By Galerkin orthogonality for (3.5), $a(\psi - \psi_{\phi(n)}, \psi_{\phi(n)}) = 0$. That is, $\|\psi_{\phi(n)}\|_a^2 = a(\psi, \psi_{\phi(n)})$. Hence, $\lim_{n \rightarrow \infty} \|\psi_{\phi(n)}\|_a^2 = \lim_{n \rightarrow \infty} a(\psi, \psi_{\phi(n)}) = a(\psi, \psi_\infty) = 0$. As the full sequence of norms $(\|\psi_n\|_a)_{n \geq 0}$ is monotonic decreasing, the full sequence $(\psi_n)_{n \geq 0}$ converges strongly to 0 in $\mathbf{H}(\mathbf{D}; \mathbf{M})$. \square

4.3. Rate of convergence. The theory of nonlinear approximation provides us with some estimates on the rate of convergence of Algorithm 1 and Algorithm 2. Following [DT96] we introduce the space

$$\mathcal{A}_1 := \bigcup_{M>0} \overline{\mathcal{A}_1^o(M)}, \quad (4.8)$$

where

$$\mathcal{A}_1^o(M) := \left\{ \varphi \in H(\mathbf{D}; \mathbf{M}) : \varphi = \sum_{k \in \Lambda} c_k w_k, \ w_k \in \bigotimes_{i=1}^N H(D_i; M_i), \ \|w_k\|_a = 1, \right. \\ \left. |\Lambda| < \infty \text{ and } \sum_{k \in \Lambda} |c_k| \leq M \right\}, \quad (4.9)$$

together with the norm

$$\|\varphi\|_{\mathcal{A}_1} := \inf \left\{ M > 0 : \varphi \in \overline{\mathcal{A}_1^o(M)} \right\}. \quad (4.10)$$

The importance of this space becomes apparent in the light of the following two theorems.

Theorem 4.6 (Theorem 3.6 of [DT96]). *If the solution ψ of (2.4) is a member of \mathcal{A}_1 , then the n -th error ψ_n of the Pure Greedy Algorithm (Algorithm 1) satisfies*

$$\|\psi_n\|_a \leq \|\psi\|_{\mathcal{A}_1} n^{-1/6}.$$

Theorem 4.7 (Theorem 3.7 of [DT96]). *If the solution ψ of (2.4) is a member of \mathcal{A}_1 , then the n -th error ψ_n of the Orthogonal Greedy Algorithm (Algorithm 2) satisfies*

$$\|\psi_n\|_a \leq \|\psi\|_{\mathcal{A}_1} n^{-1/2}.$$

Remark 6.

- (1) Pure Greedy Algorithm-based approximations such as Algorithm 1 have been proved to obey the slightly improved rate (see [Tem08, Remark 2.3.11] and references therein)

$$\|\psi_n\|_a \leq 4 \|\psi\|_{\mathcal{A}_1} n^{-11/62}.$$

- (2) In [CEL11, Theorem 4.1] it is shown that the convergence of the Orthogonal Greedy Algorithm is exponentially fast if the factor spaces and the full ansatz space (in our setting the $H(D_i; M_i)$ and $H(\mathbf{D}; \mathbf{M})$, respectively) are finite-dimensional.

We note that \mathcal{A}_1 will remain the same space if in its definition—in (4.9), in particular—we replace the energy norm $\|\cdot\|_a$ with the standard norm of $H(\mathbf{D}; \mathbf{M})$, as these two norms are equivalent. Then, $\varphi \in H(\mathbf{D}; \mathbf{M})$ will be a member of \mathcal{A}_1 if, and only if, there exists an $M^* > 0$ such that, for all $\varepsilon > 0$, there is a $\chi_\varepsilon \in H(\mathbf{D}; \mathbf{M})$ that satisfies

$$\|\varphi - \chi_\varepsilon\|_{H(\mathbf{D}; \mathbf{M})} \leq \varepsilon, \quad \chi_\varepsilon = \sum_{k \in \Lambda^{(\varepsilon)}} c_k^{(\varepsilon)} w_k^{(\varepsilon)}, \quad |\Lambda^{(\varepsilon)}| < \infty, \quad \sum_{k \in \Lambda^{(\varepsilon)}} |c_k^{(\varepsilon)}| \leq M^*;$$

and, for $k \in \Lambda^{(\varepsilon)}$, $\|w_k^{(\varepsilon)}\|_{H(\mathbf{D}; \mathbf{M})} = 1$ and $w_k^{(\varepsilon)} \in \bigotimes_{i=1}^N H(D_i; M_i)$.

By virtue of the isometric isomorphism described in (2.3), the above relations imply that

$$\|\mathbf{M}^{-1}\varphi - \mathbf{M}^{-1}\chi_\varepsilon\|_{H_{\mathbf{M}}^1(\mathbf{D})} \leq \varepsilon, \quad \mathbf{M}^{-1}\chi_\varepsilon = \sum_{k \in \Lambda^{(\varepsilon)}} c_k^{(\varepsilon)} \mathbf{M}^{-1}w_k^{(\varepsilon)},$$

and, for $k \in \Lambda^{(\varepsilon)}$, $\|\mathbf{M}^{-1}w_k^{(\varepsilon)}\|_{H_{\mathbf{M}}^1(\mathbf{D})} = 1$ and $\mathbf{M}^{-1}w_k^{(\varepsilon)} \in \bigotimes_{i=1}^N H_{M_i}^1(D_i)$, the last relation being a consequence of the tensor-product structure of the Maxwellian \mathbf{M} . Thus we have shown that $\mathbf{M}^{-1}\varphi \in H_{\mathbf{M}}^1(\mathbf{D})$ can be approximated to within any positive tolerance ε in the norm of $H_{\mathbf{M}}^1(\mathbf{D})$ by finite linear combinations of normalized members of $\bigotimes_{i \in [N]} H_{M_i}^1(D_i)$ with the coefficients of the linear combinations having their absolute sum bounded by M^* . In other words, the membership of $\varphi \in \mathcal{A}_1$ implies the membership of $\mathbf{M}^{-1}\varphi$ in the $H_{\mathbf{M}}^1(\mathbf{D})$ -based analogue of \mathcal{A}_1 , namely,

$$\mathcal{B}_1 := \bigcup_{M>0} \overline{\mathcal{B}_1^o(M)}, \quad (4.11)$$

where

$$\mathcal{B}_1^o(M) := \left\{ \varphi \in H_M^1(D) : \varphi = \sum_{k \in \Lambda} c_k w_k, \ w_k \in \bigotimes_{i=1}^N H_{M_i}^1(D_i), \ \|w_k\|_{H_M^1(D)} = 1, \right. \\ \left. |\Lambda| < \infty \quad \text{and} \quad \sum_{k \in \Lambda} |c_k| \leq M \right\}, \quad (4.12)$$

and

$$\|\varphi\|_{\mathcal{B}_1} := \inf \left\{ M > 0 : \varphi \in \overline{\mathcal{B}_1^o(M)} \right\}. \quad (4.13)$$

In a completely analogous way, the membership of $M^{-1}\varphi$ in \mathcal{B}_1 implies the membership of φ in \mathcal{A}_1 . We then have the relations

$$\mathcal{A}_1 = M \mathcal{B}_1, \quad \|\cdot\|_{\mathcal{A}_1} = \|M^{-1}\cdot\|_{\mathcal{B}_1}, \quad (4.14)$$

where the last equality follows from the fact that the coefficients of the approximations to φ are the same as the coefficients of the corresponding approximations to $M^{-1}\varphi$.

As the definition of \mathcal{A}_1 given in (4.8) is fairly abstract, it is of interest to have conditions in terms of regularity that guarantee membership in \mathcal{A}_1 analogous to the conditions provided in [LBLM09, Remark 4] for the separated representation strategy applied to the Laplacian defined on a tensor product of one-dimensional domains. This is the theme of the next section. Because of (4.14), we can pose the problem in terms of membership in the $H_M^1(D)$ -based \mathcal{B}_1 instead with no loss of generality and substantial gain in succinctness; thus we shall henceforth phrase our results in terms of \mathcal{B}_1 rather than \mathcal{A}_1 .

5. CHARACTERIZATION OF A SUBSPACE OF RAPIDLY CONVERGING SOLUTIONS

5.1. Eigenvalues. We need the following two abstract lemmas, which state standard results (essentially, the Hilbert–Schmidt theorem and some of its corollaries). As we could not find these results in the literature in the precise form stated here, we provide brief proofs of them.

Lemma 5.1. *Let H and V be separable infinite-dimensional Hilbert spaces, with $V \subseteq H$ and $\bar{V} = H$ in the norm of H . Let $a: V \times V \rightarrow \mathbb{R}$ be a nonzero, symmetric, bounded and elliptic bilinear form. Then, there exist sequences of real numbers $(\lambda_n)_{n \in \mathbb{N}}$ and unit H -norm members of V $(e_n)_{n \in \mathbb{N}}$, which solve the following problem: Find $\lambda \in \mathbb{R}$ and $e \in H \setminus \{0\}$ such that*

$$a(e, v) = \lambda \langle e, v \rangle_H \quad \forall v \in V. \quad (5.1)$$

The λ_n , which can be assumed to be in increasing order with respect to n , are positive, bounded from below away from 0, and $\lim_{n \rightarrow \infty} \lambda_n = \infty$.

Additionally, the e_n form an H -orthonormal system whose H -closed span is H and the rescaling $e_n/\sqrt{\lambda_n}$ gives rise to an a -orthonormal system whose a -closed span is V .

Proof. This proof is an adaptation of the proof of Theorem IX.31 in [Bre83]. The Lax–Milgram lemma implies the existence of an operator $\tilde{T}: H \rightarrow V$ where, given $h \in H$, $\tilde{T}(h)$ is defined as the unique solution in V to the variational problem

$$a(\tilde{T}(h), v) = \langle h, v \rangle_H \quad \forall v \in V. \quad (5.2)$$

It also follows, via the elliptic stability estimate of the Lax–Milgram lemma and the continuity of the embedding $V \hookrightarrow H$, that \tilde{T} is bounded. Let $i: V \rightarrow H$ denote the embedding operator that maps V into H , i.e., $v \in V \mapsto i(v) = v \in H$. Then, $T := i \circ \tilde{T}$ is a bounded operator defined on H with values in H ; as $i: V \rightarrow H$ is a compact linear operator, it follows that $T: H \rightarrow H$ is a compact linear operator. Further, for all $(h, h') \in H \times H$,

$$\begin{aligned} \langle T(h), h' \rangle_H &= \langle \tilde{T}(h), h' \rangle_H = \langle h', \tilde{T}(h) \rangle_H = a(\tilde{T}(h'), \tilde{T}(h)) \\ &= a(\tilde{T}(h), \tilde{T}(h')) = \langle h, \tilde{T}(h') \rangle_H = \langle h, T(h') \rangle_H, \end{aligned}$$

whence T is self-adjoint. Thus, thanks to Theorem VI.11 in [Bre83], there exists an H -orthonormal system $(e_n)_{n \geq 1}$ of eigenvectors of T such that

$$h = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H e_n \quad \text{and} \quad \|h\|_H^2 = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H^2 \quad \forall h \in H. \quad (5.3)$$

As, for all $h \in H$, $\langle T(h), h \rangle_H = a(\tilde{T}(h), \tilde{T}(h))$ and a is V -elliptic, all the eigenvalues of T are nonnegative. Also, as T is bounded, the set of its eigenvalues is also bounded. Now, by Theorem VI.8 in [Bre83], the set of nonzero eigenvalues of T is either empty, or finite, or countable with 0 as its only accumulation point. However, on account of (5.3), the latter alternative is then the one that holds.

If 0 were an eigenvalue of T , there would exist $e \in H \setminus \{0\}$ such that $T(e) = 0$; i.e., $e \in \text{Ker}(T)$. However, from (5.2) we then have that $e \in V^{\perp_H}$. As $H = \bar{V} \oplus V^{\perp_H}$ in the norm of H and V is dense in H , $V^{\perp_H} = \{0\}$, which contradicts $e \neq 0$. Therefore, 0 is not an eigenvalue of T .

From the above, we can take the eigenvectors e_n of (5.3) as associated to positive eigenvalues μ_n bounded from above, arranged in decreasing order ($\mu_{n+1} \leq \mu_n$ for $n \geq 1$) with $\lim_{n \rightarrow \infty} \mu_n = 0$. A consequence of the absence of 0 from the spectrum of T is that all the eigenvectors of T have to be members of the smaller space V .

Assuming that $\mu \neq 0$ and $e \in V \setminus \{0\}$, $T(e) = \mu e$ if, and only if, $a(e, w) = \mu^{-1} \langle e, w \rangle_H$ for all $w \in V$. Then, all the eigenvalues of the eigenvalue problem (5.1) are reciprocals of eigenvalues of T with the possible exception of 0. However, from the V -ellipticity of a , 0 cannot be an eigenvalue of the problem (5.1). On defining $\lambda_n := \mu_n^{-1}$ and setting the e_n to be the same as in (5.3) we obtain the desired existence and distribution statements about of the eigenvalues of (5.1).

We observe from $a(e_n, e_m) = \lambda_n \langle e_n, e_m \rangle_H$, $n \geq 1$, that $(e_n / \sqrt{\lambda_n})_{n \geq 1}$ is an a -orthonormal system in V . Let us denote the a -closure of its span by \hat{V} . Then, $v \in \hat{V}^{\perp_a}$ if, and only if, $a(v, e_n) = 0$ for all $n \geq 1$. As each e_n is an eigenfunction of the problem (5.1) associated to a nonzero eigenvalue, it follows from (5.3) that $v = 0$ and therefore $\hat{V}^{\perp_a} = \{0\}$. Thus, $V = \hat{V} \oplus \hat{V}^{\perp_a} = \hat{V}$. This, together with (5.3) itself, completes the proof. \square

Lemma 5.2. *Let the spaces H , V and the bilinear form a be as in the statement of Lemma 5.1 and let $(\lambda_n, e_n) \in \mathbb{R}_{>0} \times V$ be the eigenpairs of (5.1) obtained there. Then,*

$$h = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H e_n \quad \text{and} \quad \|h\|_H^2 = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H^2 \quad \forall h \in H, \quad (5.4)$$

and

$$v = \sum_{n=1}^{\infty} a\left(v, \frac{e_n}{\sqrt{\lambda_n}}\right) \frac{e_n}{\sqrt{\lambda_n}} \quad \text{and} \quad \|v\|_a^2 = \sum_{n=1}^{\infty} a\left(v, \frac{e_n}{\sqrt{\lambda_n}}\right)^2 \quad \forall v \in V. \quad (5.5)$$

Further,

$$h \in H \quad \text{and} \quad \sum_{n=1}^{\infty} \lambda_n \langle h, e_n \rangle_H^2 < \infty \iff h \in V. \quad (5.6)$$

Proof. The expression (5.4) is just a restatement of (5.3) in the proof of Lemma 5.1, but unlike there, here we emphasize that the e_n belong to V . The expression (5.5) comes from the identity between V and the a -closed span of the a -orthonormal set $(e_n / \sqrt{\lambda_n})_{n \geq 1}$ —part of the statement of Lemma 5.1—via, for example, Theorem VI.9 of [Bre83].

As (λ_n, e_n) is an eigenpair of (5.1), $a(v, e_n / \sqrt{\lambda_n}) = \sqrt{\lambda_n} \langle v, e_n \rangle_H$ for all $v \in V$; this and the second expression of (5.5) give the right-to-left implication in (5.6). Let us now consider an $h \in H$ that satisfies the left-hand side of (5.6). As the e_n are members of V , the partial sums

$$h_k := \sum_{n=1}^k \langle h, e_n \rangle_H e_n$$

also belong to V . The a -orthonormality of the $e_n/\sqrt{\lambda_n}$ leads to the equality, for $1 \leq k < l$,

$$\|h_l - h_k\|_a^2 = \sum_{n=k+1}^l \lambda_n \langle h, e_n \rangle_H^2.$$

As the real series $\sum_{n=1}^{\infty} \lambda_n \langle h, e_n \rangle_H^2$ is assumed to converge, the above expression tends to 0 as k and l tend to ∞ . Hence, $(h_k)_{k \geq 1}$ is a Cauchy sequence in V and thus converges to some $\hat{h} \in V$. As V is continuously embedded in H (part of being compactly embedded), the limit \hat{h} has to be the same limit the h_k have in H . That is, $h = \hat{h} \in V$. This completes the proof of (5.6). \square

The hypotheses of Lemma 5.1 and Lemma 5.2 are satisfied by the eigenvalue problems

$$\langle e^{(i)}, \varphi \rangle_{H_{M_i}^1(D_i)} = \lambda^{(i)} \langle e^{(i)}, \varphi \rangle_{L_{M_i}^2(D_i)} \quad \forall \varphi \in H_{M_i}^1(D_i), \quad (5.7)$$

(for $i \in [N]$ here and in what follows), and

$$\langle e, \varphi \rangle_{H_M^1(D)} = \lambda \langle e, \varphi \rangle_{L_M^2(D)} \quad \forall \varphi \in H_M^1(D), \quad (5.8)$$

whence their solutions do have the distribution, orthogonality and spanning properties stated in that lemma (the hypothesis $\bar{V} = H$, which is not discussed elsewhere, follows from the density of infinitely differentiable and compactly supported functions in any weighted L^2 space). In particular, they have sequences of solutions (eigenpairs) $((\lambda_n^{(i)}, e_n^{(i)}))_{n \in \mathbb{N}}$ and $((\lambda_n, e_n))_{n \in \mathbb{N}}$, respectively, with

$$\varphi \in L_{M_i}^2(D_i) \quad \text{and} \quad \sum_{n=1}^{\infty} \lambda_n^{(i)} \langle \varphi, e_n^{(i)} \rangle_{L_{M_i}^2(D_i)}^2 < \infty \iff \varphi \in H_{M_i}^1(D_i), \quad (5.9)$$

and

$$\varphi \in L_M^2(D) \quad \text{and} \quad \sum_{n=1}^{\infty} \lambda_n \langle \varphi, e_n \rangle_{L_M^2(D)}^2 < \infty \iff \varphi \in H_M^1(D). \quad (5.10)$$

Next, we exploit the special tensor-product structure of the full Maxwellian M to characterize the eigenpairs of its associated eigenvalue problem (5.8) in terms of the eigenpairs of the eigenvalue problem (5.7) associated to the partial Maxwellians M_i .

Lemma 5.3. *The net $((\lambda_n, e_n))_{\mathbf{n}=(n_1, \dots, n_N) \in \mathbb{N}^N}$ is a full system of solutions of the eigenvalue problem (5.8), where*

$$\lambda_{\mathbf{n}} := 1 + \sum_{i=1}^N (\lambda_{n_i}^{(i)} - 1) \quad \text{and} \quad e_{\mathbf{n}} := \bigotimes_{i=1}^N e_{n_i}^{(i)}. \quad (5.11)$$

Proof. Given $\tau = \bigotimes_{i \in [N]} \tau^{(i)} \in \bigotimes_{i \in [N]} C_0^\infty(D_i)$, we have that

$$\begin{aligned} \langle e_{\mathbf{n}}, \tau \rangle_{H(D; M)} &= \langle e_{\mathbf{n}}, \tau \rangle_{L_M^2(D)} + \sum_{j=1}^N \left\langle \nabla e_{n_j}^{(j)}, \nabla \tau^{(j)} \right\rangle_{[L_{M_j}^2(D_j)]^d} \prod_{\substack{i=1 \\ i \neq j}}^N \left\langle e_{n_i}^{(i)}, \tau^{(i)} \right\rangle_{L_{M_i}^2(D_i)} \\ &= \langle e_{\mathbf{n}}, \tau \rangle_{L_M^2(D)} + \sum_{j=1}^N (\lambda_{n_j}^{(j)} - 1) \left\langle e_{n_j}^{(j)}, \tau^{(j)} \right\rangle_{L_{M_j}^2(D_j)} \prod_{\substack{i=1 \\ i \neq j}}^N \left\langle e_{n_i}^{(i)}, \tau^{(i)} \right\rangle_{L_{M_i}^2(D_i)} = \lambda_{\mathbf{n}} \langle e_{\mathbf{n}}, \tau \rangle_{L_M^2(D)}. \end{aligned}$$

Since the span of $\bigotimes_{i=1}^N H(D_i; M_i)$ is dense in $H(D; M)$ (as is readily seen from Corollary 4.4 and (2.3)), the equality of the first and the last expression in the chain of equalities above is valid for all $\tau \in H(D; M)$. Hence, $(\lambda_{\mathbf{n}}, e_{\mathbf{n}})$ is an eigenpair of (5.8). Further, we deduce from the chain of equalities above that $e_{\mathbf{n}}$ is orthogonal to $e_{\mathbf{m}}$ in both $L_M^2(D)$ and $H_M^1(D)$ if $\mathbf{n} \neq \mathbf{m}$.

From (5.5) in Lemma 5.2, for $i \in [N]$, $\text{span} \left(e_n^{(i)} \right)_{n \geq 1} = H_{M_i}^1(D_i)$. Hence, by (4.4) and (2.3),

$$\overline{\bigotimes_{i=1}^N \text{span} \left(e_n^{(i)} \right)_{n \geq 1}} \subset \overline{\text{span} (e_{\mathbf{n}})_{\mathbf{n} \in \mathbb{N}^N}} = H_M^1(D).$$

Thus, $(e_{\mathbf{n}})_{\mathbf{n} \in \mathbb{N}^N}$ forms an orthogonal system that spans $H_M^1(D)$. Therefore, by Theorem VI.9 of [Bre83], all the eigenpairs of the (full) Maxwellian eigenvalue problem (5.8) have the form $(\lambda_{\mathbf{n}}, e_{\mathbf{n}})$ as given in (5.11) (modulo linear combinations of eigenfunctions belonging to the same eigenspace). \square

It follows from Lemma 5.3 that the eigenvalues and eigenfunctions of (5.8) are more naturally indexed by \mathbb{N}^N than by \mathbb{N} ; in what follows, we shall refrain from indexing *contra natura*.

5.2. Characterization via summability of Fourier coefficients. As by Lemma 5.3 the sequence $((\lambda_{\mathbf{n}}, e_{\mathbf{n}}))_{\mathbf{n} \in \mathbb{N}^N}$ is a full system of eigenpairs of (5.8), (5.5) in Lemma 5.2 ensures that, for all $\tau \in H_M^1(D)$,

$$\tau = \sum_{\mathbf{n} \in \mathbb{N}^N} \left\langle \tau, \frac{e_{\mathbf{n}}}{\sqrt{\lambda_{\mathbf{n}}}} \right\rangle_{H_M^1(D)} \frac{e_{\mathbf{n}}}{\sqrt{\lambda_{\mathbf{n}}}} = \sum_{\mathbf{n} \in \mathbb{N}^N} \sqrt{\lambda_{\mathbf{n}}} \langle \tau, e_{\mathbf{n}} \rangle_{L_M^2(D)} \frac{e_{\mathbf{n}}}{\sqrt{\lambda_{\mathbf{n}}}} \quad \text{in } H_M^1(D).$$

Hence, given the tensor-product structure of the $e_{\mathbf{n}}$ and the unit $H_M^1(D)$ -norm of the $e_{\mathbf{n}}/\sqrt{\lambda_{\mathbf{n}}}$, we can guarantee that $\tau \in \mathcal{B}_1$ (cf. (4.11)) if

$$\sum_{\mathbf{n} \in \mathbb{N}^N} \sqrt{\lambda_{\mathbf{n}}} |\langle \tau, e_{\mathbf{n}} \rangle_{L_M^2(D)}| < \infty.$$

In turn, this holds if

$$A := \sum_{\mathbf{n} \in \mathbb{N}^N} \frac{\lambda_{\mathbf{n}}}{\sigma_{\mathbf{n}}} < \infty \quad \text{and} \quad B := \sum_{\mathbf{n} \in \mathbb{N}^N} \sigma_{\mathbf{n}} \langle \tau, e_{\mathbf{n}} \rangle_{L_M^2(D)}^2 < \infty, \quad (5.12)$$

where $(\sigma_{\mathbf{n}})_{\mathbf{n} \in \mathbb{N}^N}$ is a sequence of positive real numbers that are to be chosen below. We note that the requirement of B being finite can be seen—for $\sigma_{\mathbf{n}} = \lambda_{\mathbf{n}}$, for example, this is certainly the case, as follows from (5.10)—as a regularity requirement on τ . Thus, there is a trade-off in (5.12) between the requirement that the $\sigma_{\mathbf{n}}$ grow fast enough to ensure the finiteness of A and the desirability of the $\sigma_{\mathbf{n}}$ growing slow enough to avoid demanding more regularity than necessary of the functions τ for which B is finite.

As a first step in formalizing the above we consider, given a net $\Sigma = (\sigma_{\mathbf{n}})_{\mathbf{n} \in \mathbb{N}^N}$ with entries in $\mathbb{R}_{>0}$, the space of all those $L_M^2(D)$ functions for which the term B , as defined in (5.12), is finite:

$$H_M^{\Sigma}(D) := \left\{ \varphi \in L_M^2(D) : \sum_{\mathbf{n} \in \mathbb{N}^N} \sigma_{\mathbf{n}} \langle \varphi, e_{\mathbf{n}} \rangle_{L_M^2(D)}^2 < \infty \right\}. \quad (5.13a)$$

We equip $H_M^{\Sigma}(D)$ with the norm

$$\|\varphi\|_{H_M^{\Sigma}(D)} := \left(\sum_{\mathbf{n} \in \mathbb{N}^N} \sigma_{\mathbf{n}} \langle \varphi, e_{\mathbf{n}} \rangle_{L_M^2(D)}^2 \right)^{1/2}. \quad (5.13b)$$

It is readily seen that, if there exists a $\sigma > 0$ with $\sigma_{\mathbf{n}} \geq \sigma$ for all $\mathbf{n} \in \mathbb{N}^N$, then $H_M^{\Sigma}(D)$ is a separable Hilbert space that is continuously embedded in $L_M^2(D)$. Further, if there exists a $\sigma' > 0$ such that $\sigma_{\mathbf{n}} \geq \sigma' \lambda_{\mathbf{n}}$ for all $\mathbf{n} \in \mathbb{N}^N$, then $H_M^{\Sigma}(D)$ is continuously embedded in $H_M^1(D)$ and, thanks to Lemma 2.2, it is compactly embedded in $L_M^2(D)$.

At this stage we could just choose Σ to be, e.g., $\sigma_{\mathbf{n}} = \lambda_{\mathbf{n}} \|\mathbf{n}\|_2^{\alpha}$ for some $\alpha > N$ and an application of a multiple series version of the integral test for convergence (see, for example, [GL10, Proposition 7.57]) would render the sum A in (5.12) finite. However, the resulting space $H_M^{\Sigma}(D)$ would then still have quite an abstract description. What we therefore wish to do instead is to choose each $\sigma_{\mathbf{n}}$ as a suitable polynomial function of the $(\lambda^{(1)}, \dots, \lambda^{(N)})$. Then, under certain reasonable conditions, which we will make explicit below, we shall be able to characterize the resulting space in terms of regularity properties. One of these conditions has to do with the fact that we can only know that A of (5.12) is finite, with $\sigma_{\mathbf{n}}$ as a certain polynomial function of the $\lambda_{\mathbf{n}}$, if we have some information about the asymptotic behavior of the $\lambda_{\mathbf{n}}$. Consequently, we adopt the following hypothesis.

Hypothesis C. For each $i \in [N]$ there exist positive real numbers $c_1^{(i)}$ and $c_2^{(i)}$ and $n^{(i)} \in \mathbb{N}$ such that (with d signifying the common dimension of the single-spring configuration domains D_i)

$$c_1^{(i)} n^{2/d} \leq \lambda_n^{(i)} \leq c_2^{(i)} n^{2/d} \quad \forall n \geq n^{(i)},$$

where $\lambda_n^{(i)}$ is the n -th member of the (ordered, with repetitions according to multiplicity) sequence of eigenvalues of (5.7).

Remark 7. Hypothesis C basically consists of assuming that the eigenvalues of the problem (5.7) behave like the eigenvalues of a regular elliptic operator, such as the Poisson operator. If the partial Maxwellian M_i comes from either the FENE model (1.2) or the CPAIL model (1.3) Hypothesis C holds; see Corollary C.2 in Appendix C for a proof (see also Remark 11).

Theorem 5.4. Let $\mathbf{T}^{(m)} = \left(\tau_{\mathbf{n}}^{(m)} \right)_{\mathbf{n} \in \mathbb{N}^N}$ be defined by

$$\tau_{\mathbf{n}}^{(m)} := \prod_{i=1}^N \left(\lambda_{n_i}^{(i)} \right)^m \quad \forall \mathbf{n} \in \mathbb{N}^N. \quad (5.14)$$

Then, $H_M^{\mathbf{T}^{(m)}}(\mathcal{D}) \subset \mathcal{B}_1$ if $m > \frac{d}{2} + 1$.

Proof. According to the previous discussion, the stated inclusion will hold once we have shown that the infinite sum over $\mathbf{n} \in \mathbb{N}^N$ of $\lambda_{\mathbf{n}} / \tau_{\mathbf{n}}^{(m)}$ converges; i.e., that A in (5.12) is finite. To prove this, we start by noting that, modulo a decrease of $c_1^{(i)}$ and an increase of $c_2^{(i)}$, we can take $n^{(i)} = 1$ in Hypothesis C as a consequence of all the $\lambda_n^{(i)}$ being positive; we do so from now on. This, together with (5.11) and Hypothesis C, yields that

$$\frac{\lambda_{\mathbf{n}}}{\tau_{\mathbf{n}}^{(m)}} \leq \frac{\sum_{i=1}^N \lambda_{n_i}^{(i)}}{\prod_{i=1}^N \left(\lambda_{n_i}^{(i)} \right)^m} \leq C \frac{\sum_{i=1}^N n_i^{2/d}}{\prod_{i=1}^N \left(n_i^{2/d} \right)^m} \quad (5.15)$$

for all $\mathbf{n} \in \mathbb{N}^N$ and some $C > 0$ that depends on the $c_1^{(i)}$, the $c_2^{(i)}$, N and d only. Clearly, it will be enough to show that the right-most expression in (5.15) results in a convergent series. Now,

$$\sum_{\mathbf{n}} \frac{\sum_{i=1}^N n_i^{2/d}}{\prod_{i=1}^N \left(n_i^{2/d} \right)^m} = \sum_{\mathbf{n}} \sum_{i=1}^N \frac{n_i^{2/d-2m/d}}{\prod_{j=1, j \neq i}^N n_j^{2m/d}} = \sum_{i=1}^N \left(\prod_{j=1, j \neq i}^N \sum_{n_j=1}^{\infty} n_j^{-2m/d} \right) \left(\sum_{n_i=1}^{\infty} n_i^{2/d(1-m)} \right)$$

where the constraint on m ensures that all the resulting one-dimensional sums are finite. \square

For later reference we introduce another family of weights that also produces subspaces of \mathcal{B}_1 .

Theorem 5.5. Let $\mathbf{Y}^{(m)} = \left(v_{\mathbf{n}}^{(m)} \right)_{\mathbf{n} \in \mathbb{N}^N}$ be defined by

$$v_{\mathbf{n}}^{(m)} := \left(\sum_{i=1}^N \lambda_{n_i}^{(i)} \right)^m \quad \forall \mathbf{n} \in \mathbb{N}^N. \quad (5.16)$$

Then, $H_M^{\mathbf{Y}^{(m)}}(\mathcal{D}) \subset \mathcal{B}_1$ if $m > 1 + \frac{1}{2}Nd$.

Proof. Using Hypothesis C and the already mentioned multiple series version of the integral test for convergence it can be shown that the result hinges on the finiteness of the integral $\int_{[1, \infty)^N} \left(\sum_{i=1}^N x_i^{2/d} \right)^{1-m} dx$. Thanks to the equivalence of the $2/d$ -quasinorm to the 2-norm in Euclidean space and since $[1, \infty)^N \subset \{x \in \mathbb{R}_{\geq 0}^N : \|x\|_2 \geq 1\}$, the finiteness of that integral is, in turn, implied by the finiteness of the integral

$$\int_{\{x \in \mathbb{R}_{\geq 0}^N : \|x\|_2 \geq 1\}} \|x\|_2^{\frac{2}{d}(1-m)} dx = C_N \int_1^{\infty} r^{\frac{2}{d}(1-m)+N-1} dr,$$

where C_N is the $(N-1)$ -dimensional volume of the surface $\{x \in \mathbb{R}_{\geq 0}^N : \|x\|_2 = 1\}$. As it is assumed that $m > 1 + \frac{1}{2}Nd$, the last of the above integrals is finite and the proof is completed. \square

The definition of $H_M^{T(m)}(D)$ given by (5.14) is less abstract than the definition of \mathcal{B}_1 (given in (4.11)). However, we can describe subspaces of the former space in even less abstract terms by showing that certain regularity conditions translate into summability conditions expressed in terms of Fourier coefficients, such as those that define $H_M^{T(m)}(D)$ (cf. (5.13a)). In order to understand the appropriate regularity requirements for this purpose, we need to study the regularity properties of certain degenerate elliptic operators in Maxwellian-weighted Sobolev spaces.

5.3. Characterization via membership in mixed-order weighted Sobolev spaces. We start by adopting two further hypotheses.

Hypothesis D. For $i \in [N]$ the spring potential U_i is monotonic increasing and convex.

Hypothesis E. For $i \in [N]$ there exists a distance $\gamma_i \in (0, \sqrt{b_i})$, an exponent $\alpha_i > 1$ and a function $h_i \in C^3([0, \gamma_i])$ that is positive on $[0, \gamma_i]$, such that

$$M_i(\mathbf{p}) = h_i(\mathfrak{d}_i(\mathbf{p})) \mathfrak{d}_i(\mathbf{p})^{\alpha_i}$$

for all $\mathbf{p} \in D_i$ such that $\mathfrak{d}_i(\mathbf{p}) \in (0, \gamma_i)$, where \mathfrak{d}_i is the distance-to-the-boundary function in D_i .

Remark 8. Hypothesis D can be regarded as a strengthening of Hypothesis A. It is easy to check that springs obeying the FENE model (1.2) or the CPAIL model (1.3) comply with it.

With Hypothesis E we are restricting ourselves, essentially, to power weights. The compliance of the FENE and the CPAIL models with it is also easy to check if their parameter b_i is greater than 2 in the FENE case and greater than 3 in the CPAIL case.

Lemma 5.6. For $i \in [N]$,

- (a) the space $C_0^\infty(D_i)$ is dense in $H_{M_i}^1(D_i)$;
- (b) the space $C^\infty(\overline{D_i})$ is dense in $H_{M_i}^m(D_i)$, for $m \in \mathbb{N}$.

Proof. In Proposition 9.10 (resp. Theorem 7.2) of [Kuf85] the result (a) (resp. (b)) is stated for weights that are powers greater than 1 (resp. greater or equal than 0) of the distance-to-the-boundary function; the bilateral boundedness of the function h_i by positive constants, implied by Hypothesis E, extends the statement to our case. \square

The additional requirements on the potentials U_i , $i \in [N]$, and the preceding lemma allow us to prove a first elliptic regularity result.

Lemma 5.7. Let $i \in [N]$ and suppose that $g \in L_{M_i}^2(D_i)$; then, there exists a constant $C_i > 0$, independent of g , such that the solution $z \in H_{M_i}^1(D_i)$ of

$$\langle z, \varphi \rangle_{H_{M_i}^1(D_i)} = \langle g, \varphi \rangle_{L_{M_i}^2(D_i)} \quad \forall \varphi \in H_{M_i}^1(D_i) \quad (5.17)$$

obeys the regularity estimate

$$\|z\|_{H_{M_i}^2(D_i)} + \left\| \frac{1}{M_i} \operatorname{div}(M_i \nabla z) \right\|_{L_{M_i}^2(D_i)} \leq C_i \|g\|_{L_{M_i}^2(D_i)}.$$

Proof. By Hypothesis A and Hypothesis D the function $V_i: D_i \rightarrow \mathbb{R}$ defined by $V_i := \frac{1}{2}U_i(\frac{1}{2}|\cdot|^2)$ is convex and tends to $+\infty$ as its argument approaches the boundary of D_i from within. Then, it follows from Theorem 3.4 of [DPL04] and the density of $C_0^\infty(D_i)$ in $H_{M_i}^1(D_i)$ given in part (a) of Lemma 5.6 that there exists a unique solution \tilde{z} in $\{u \in H_{M_i}^2(D_i) : \nabla V_i \cdot \nabla u \in L_{M_i}^2(D_i)\}$ to

$$\frac{1}{2}\tilde{z} - \frac{1}{2}\Delta\tilde{z} + \nabla V_i \cdot \nabla\tilde{z} = \frac{1}{2}g, \quad (5.18)$$

considered as an equation in $L^2_{M_i}(D_i)$, and it obeys the estimates

$$\|\tilde{z}\|_{L^2_{M_i}(D_i)} \leq 2 \left\| \frac{1}{2}g \right\|_{L^2_{M_i}(D_i)} = \|g\|_{L^2_{M_i}(D_i)}, \quad (5.19a)$$

$$\|\nabla \tilde{z}\|_{[L^2_{M_i}(D_i)]^d} \leq 2\sqrt{2} \left\| \frac{1}{2}g \right\|_{L^2_{M_i}(D_i)} = \sqrt{2} \|g\|_{L^2_{M_i}(D_i)}, \quad (5.19b)$$

$$\|\nabla \nabla \tilde{z}\|_{[L^2_{M_i}(D_i)]^{d \times d}} \leq 4 \left\| \frac{1}{2}g \right\|_{L^2_{M_i}(D_i)} = 2 \|g\|_{L^2_{M_i}(D_i)}. \quad (5.19c)$$

The regularity of M_i and \tilde{z} admits the use of the Leibniz formula for the product of a regular distribution and a continuously differentiable function provided in Lemma B.1 in Appendix B. We can then write $M_i \Delta \tilde{z} - 2M_i \nabla V_i \cdot \nabla \tilde{z} = \operatorname{div}(M_i \nabla \tilde{z})$ (for this we have used that M_i is proportional to $\exp(-2V_i)$ (cf. (1.5)). Plugging this into (5.18) gives

$$\left\| \frac{1}{M_i} \operatorname{div}(M_i \nabla \tilde{z}) \right\|_{L^2_{M_i}(D_i)} \leq \|g\|_{L^2_{M_i}(D_i)} + \|\tilde{z}\|_{L^2_{M_i}(D_i)} \leq 2 \|g\|_{L^2_{M_i}(D_i)}. \quad (5.20)$$

Multiplying (5.18) by $2M_i$ and using the Leibniz formula for the product of a regular distribution and a continuously differentiable function again, we find that

$$\int_{D_i} \tilde{z} \varphi M_i + \int_{D_i} \nabla \tilde{z} \cdot \nabla \varphi M_i = \int_{D_i} g \varphi$$

for all $\varphi \in C_0^\infty(D_i)$. It follows from the density of $C_0^\infty(D_i)$ in $H^1_{M_i}(D_i)$ and the uniqueness of the solution z of (5.17) that $z = \tilde{z}$ and hence (5.19) and (5.20) give the desired result. \square

In order to obtain an iterated elliptic regularity result, we need the technical lemma that follows.

Lemma 5.8 (Hardy inequalities). *Let $H > 0$. Then, there exists $C_H > 0$ such that*

$$\int_0^H \frac{1}{y^2} \left(\int_0^y f(s) \, ds \right)^2 \, dy \leq C_H \int_0^H f(s)^2 \, ds \quad \forall f \in L^1((0, H)). \quad (5.21)$$

If $\alpha > 1$, then there exists $C_{H,\alpha}$ such that

$$\int_0^H y^{\alpha-2} f(y)^2 \, dy \leq C_{H,\alpha} \int_0^H y^\alpha [f(y)^2 + f'(y)^2] \, dy \quad \forall f \in H^1_{(\cdot)^\alpha}((0, H)). \quad (5.22)$$

Proof. The inequality (5.21) follows from the standard Hardy inequality (the $H = \infty$ case); see, for example, [DiB02, Proposition VIII.18.1]. Alternatively, see [OK90, Theorem 1.14] for a very general form, which encompasses (5.21).

To prove (5.22) we will use a procedure inspired by the proof of Theorem 8.2 of [Kuf85]. The first ingredient is the inequality

$$\int_0^H y^{\alpha-2} f(y)^2 \, dy \leq C_1 \int_0^H y^\alpha f'(y)^2 \, dy$$

valid for all f in $C^1([0, H])$ such that $f(H) = 0$ (see, e.g., [OK90, Example 6.8.ii]). Let now φ_0 and φ_1 form a smooth partition of unity subordinate to the covering $H = (0, 2H/3) \cup (H/3, H)$. Then, given any $f \in C^1([0, H])$, let $f_0 := \varphi_0 f$ and $f_1 := \varphi_1 f$. Using the above inequality, the validity of (5.22) for $C^1([0, H])$ functions follows from

$$\begin{aligned} \|f\|_{L^2_{(\cdot)^{\alpha-2}}((0, H))} &\leq \|f_0\|_{L^2_{(\cdot)^{\alpha-2}}((0, 2H/3))} + \|f_1\|_{L^2_{(\cdot)^{\alpha-2}}((H/3, H))} \\ &\leq C_1^{1/2} \|f'_0\|_{L^2_{(\cdot)^\alpha}((0, 2H/3))} + \|(\cdot)^{-1} f_1\|_{L^2_{(\cdot)^\alpha}((H/3, H))} \\ &\leq C_1^{1/2} \|\varphi_0 f' + \varphi'_0 f\|_{L^2_{(\cdot)^\alpha}((0, 2H/3))} + 3/H \|f_1\|_{L^2_{(\cdot)^\alpha}((H/3, H))} \\ &\leq C_2 \|f'\|_{L^2_{(\cdot)^\alpha}((0, 2H/3))} + C_3 \|f\|_{L^2_{(\cdot)^\alpha}((0, 2H/3))} + C_4 \|f\|_{L^2_{(\cdot)^\alpha}((H/3, H))} \\ &\leq C_5 \left(\|f\|_{L^2_{(\cdot)^\alpha}((0, H))}^2 + \|f'\|_{L^2_{(\cdot)^\alpha}((0, H))}^2 \right)^{1/2}. \end{aligned}$$

The validity of the inequality for all $f \in H^1_{(\cdot),\alpha}((0, H))$ is then a consequence of the density of $C^1([0, H])$ functions in $H^1_{(\cdot),\alpha}((0, H))$, the completeness of $L^2_{(\cdot),\alpha-2}((0, H))$ and the continuity of the injection of that latter space into $L^2_{(\cdot),\alpha}((0, H))$. \square

We shall now iterate Lemma 5.7: extra regularity for g implies extra regularity for z .

Lemma 5.9. *Let $i \in [N]$ and $g \in H^2_{M_i}(D_i)$. Then, there exists a constant $C_i > 0$, independent of g , such that the solution $z \in H^1_{M_i}(D_i)$ of*

$$\langle z, \varphi \rangle_{H^1_{M_i}(D_i)} = \langle g, \varphi \rangle_{L^2_{M_i}(D_i)} \quad \forall \varphi \in H^1_{M_i}(D_i) \quad (5.23)$$

obeys the regularity estimate

$$\|z\|_{H^4_{M_i}(D_i)} \leq C_i \|g\|_{H^2_{M_i}(D_i)}.$$

Proof. The core of this proof is based on Lemmas 3.1 and 3.3 of [Fre87]. As their adaptation to our geometry is nontrivial, we give a detailed argument. Note that in this proof we shall omit the spring index i in order to avoid cluttering the notation.

Part 1: We start by describing a change of coordinates and how (5.17) transforms under it.

Given $\mathbf{p} \in \mathbb{R}^d$, let \mathbf{p}' denote $(p_1, \dots, p_{d-1}) \in \mathbb{R}^{d-1}$. Let ζ be some constant in $(0, 1)$ and let us define, for $\varepsilon \in (0, \zeta]$, the sets $\tilde{U}_\varepsilon := P'_\varepsilon \times (0, \varepsilon\gamma)$ and $U_\varepsilon := S(\tilde{U}_\varepsilon)$, where γ is the distance (with its spring index omitted) mentioned in Hypothesis E and

$$P'_\varepsilon := \begin{cases} \varepsilon(-\pi/2, \pi/2) & \text{if } d = 2, \\ \varepsilon(-1, 1) \times \varepsilon(-\pi/2, \pi/2) & \text{if } d = 3 \end{cases}$$

and $S: \tilde{U}_\zeta \rightarrow U_\zeta$ is defined by the formula

$$S(\mathbf{p}) = \begin{cases} (\sqrt{b} - p_2) (\cos(p_1), \sin(p_1)) & \text{if } d = 2, \\ (\sqrt{b} - p_3) (\sqrt{1 - p_1^2} \cos(p_2), \sqrt{1 - p_1^2} \sin(p_2), p_1) & \text{if } d = 3, \end{cases} \quad \forall \mathbf{p} \in \tilde{U}_\zeta.$$

Note that if $0 < \varepsilon_1 < \varepsilon_2 \leq \zeta$ then $U_{\varepsilon_1} \subset U_{\varepsilon_2} \subset D$ and $\tilde{U}_{\varepsilon_1} \subset \tilde{U}_{\varepsilon_2}$. Having its domain and defining formula carefully crafted for the purpose, the transformation S turns out to be invertible, orientation-preserving and $C^\infty(\tilde{U}_\zeta)$ -regular. All of this is easy to see if one takes into account that S is a variant of the polar (resp. spherical) to Cartesian coordinate transformation if $d = 2$ (resp. $d = 3$) with the radial variable being measured from the boundary of D and increasing towards its center. We denote the inverse of S by T ; it, too, has uniformly bounded derivatives of all orders.

If f is a function with domain U_ζ we will write $\tilde{f} := f \circ S$. Then, $\varphi \in C^\infty(\overline{U_\zeta}) \iff \tilde{\varphi} \in C^\infty(\overline{\tilde{U}_\zeta})$. If m is a positive integer, part (b) of Lemma 5.6 states that $C^\infty(\overline{D})$ is dense in $H^m_M(D)$; as, for any $\varepsilon \in (0, \zeta]$, U_ε is regular enough (a Lipschitz domain), $C^\infty(\overline{U_\varepsilon})$ is exactly the set of restrictions to U_ε of $C^\infty(\overline{D})$ functions, whence $C^\infty(\overline{U_\varepsilon})$ is dense in $H^m_M(U_\varepsilon)$ as well. We also have from Lemma B.3 in Appendix B, that $f \in H^m_M(U_\varepsilon) \iff \tilde{f} \in H^m_M(\tilde{U}_\varepsilon)$ and that

$$c_1(m) \|\tilde{f}\|_{H^m_M(\tilde{U}_\varepsilon)} \leq \|f\|_{H^m_M(U_\varepsilon)} \leq c_2(m) \|\tilde{f}\|_{H^m_M(\tilde{U}_\varepsilon)} \quad \forall f \in H^m_M(U_\varepsilon), \quad (5.24)$$

where the positive constants c_1 and c_2 depend on m but can be chosen to be independent of ε .

As $C^\infty(\overline{U_\zeta})$ is mapped by composition with S to $C^\infty(\overline{\tilde{U}_\zeta})$ bijectively, it follows that $C^\infty(\overline{\tilde{U}_\zeta})$ is dense in $H^1_M(\tilde{U}_\zeta)$. The rules of calculus and the density of $C^\infty(\overline{U_\zeta})$ and $C^\infty(\overline{\tilde{U}_\zeta})$ functions in $H^1_M(U_\zeta)$ and $H^1_M(\tilde{U}_\zeta)$, respectively, give the equalities

$$\int_{U_\zeta} u v M = \int_{\tilde{U}_\zeta} \tilde{u} \tilde{v} \tilde{M} a \quad \text{and} \quad \int_{U_\zeta} \nabla u \cdot \nabla v M = \int_{\tilde{U}_\zeta} \nabla \tilde{u} A \nabla \tilde{v}^T \tilde{M}, \quad (5.25a)$$

where we have used the shorthand notations

$$a = \det(\nabla S) \quad \text{and} \quad A = (\nabla S)^{-1} (\nabla S)^{-T} \det(\nabla S). \quad (5.25b)$$

The first equality in (5.25a) is valid for u and v in $L^2_M(U_\zeta)$ and the second for u and v in $H^1_M(U_\zeta)$. Direct calculations give

$$A = A^T, \quad A_{k,d} = A_{d,k} = 0 \quad \forall k \in [d-1], \quad A_{d,d} = a, \quad \text{and} \quad \partial_k a = 0 \quad \forall k \in [d-1], \quad (5.26)$$

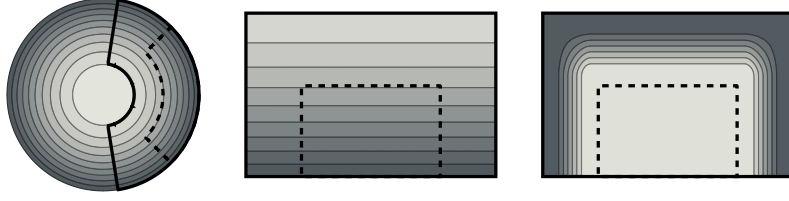


FIGURE 5.1. Illustration of the construction used in the proof of Lemma 5.9. From left to right: Contour plot of M on D with U_ζ and U_ε enclosed by the thick continuous and dashed lines, respectively; contour plot of \tilde{M} on \tilde{U}_ζ with \tilde{U}_ε enclosed by the thick dashed line; contour plot of an admissible $\tilde{\omega}$ on \tilde{U}_ζ with \tilde{U}_ε enclosed by the thick dashed line

which we will exploit later. The need for the last equality in (5.26) is the rationale behind taking of the sine of the polar angle instead of the polar angle itself as the first argument of the transformation S in the case of $d = 3$. Additionally, by construction, \tilde{M} is a function of the radial variable p_d only—namely, for all $\mathbf{p} \in \tilde{U}_\zeta$, $\tilde{M}(\mathbf{p}) = h(p_d)p_d^\alpha$, where h and α , with the spring index omitted, are those of Hypothesis E.

Let us fix $\varepsilon \in (0, \zeta)$. For localization purposes we pick a $C^\infty(U_\zeta)$ function ω with range $[0, 1]$, identically 1 in U_ε , with support bounded away from $\partial U_\zeta \setminus \partial D$ and such that $\partial_d \tilde{\omega}(\mathbf{p}) = 0$ if \mathbf{p} is within a finite distance $\gamma' > 0$ of $\partial \tilde{U}_\zeta \cap T(\partial D)$ (such a function is readily constructed as $\omega = \tilde{\omega} \circ T$ where $\tilde{\omega}(\mathbf{p}) = s(\mathbf{p}')t(p_d)$ and s and t are suitable mollified step functions). See Fig. 5.1 for a depiction of the construction so far.

Now, as every member of $C_0^\infty(\tilde{U}_\zeta)$ can be put in the form $\varphi \circ S$, where $\varphi \in C_0^\infty(U_\zeta) \subset H_M^1(U_\zeta)$, (5.23) and the equalities in (5.25) imply that \tilde{z} obeys the distributional equation

$$-\operatorname{div}(\nabla \tilde{z} A \tilde{M}) + \tilde{z} a \tilde{M} = \tilde{g} \tilde{M} a \quad \text{in } \tilde{U}_\zeta. \quad (5.27)$$

Part 2: In this part we show that the relevant derivatives of \tilde{z} in directions tangential to the radial (i.e., the d -th) coordinate possess additional regularity. The argument is a nontrivial adaptation of Lemma 3.1 of [Fre87].

Let $k \in [d - 1]$. Then, using the Leibniz formula (cf. Lemma B.1) and simple consequences of (5.26) and the fact that $\tilde{M}(\mathbf{p})$ depends on p_d only, the distributional equation (5.27) conduces to

$$\begin{aligned} & -\operatorname{div}(\nabla(\tilde{\omega} \partial_k \tilde{z}) A \tilde{M}) + \tilde{\omega} \partial_k \tilde{z} a \tilde{M} \\ &= \tilde{\omega} \partial_k \tilde{g} a \tilde{M} + \tilde{\omega} \nabla \nabla \tilde{z} : \partial_k A \tilde{M} + \tilde{\omega} \nabla \tilde{z} \cdot \operatorname{div}(\partial_k A) \tilde{M} + \tilde{\omega} \nabla \tilde{M} \cdot (\nabla \tilde{z} \partial_k A) \\ & \quad - 2 \nabla \tilde{\omega} \cdot (\nabla(\partial_k \tilde{z}) A \tilde{M}) - \partial_k \tilde{z} \operatorname{div}(\nabla \tilde{\omega} A) \tilde{M} - \partial_k \tilde{z} \nabla \tilde{M} \cdot (\nabla \tilde{\omega} A). \end{aligned} \quad (5.28)$$

We want to show that all the terms resulting above are (the linear combination of) members of the space $a \tilde{M} L_M^2(\tilde{U}_\zeta) = \tilde{M} L_M^2(\tilde{U}_\zeta)$. Of the resulting seven terms above, the first three, the fifth and the sixth pose no problem, thanks to the regularity of g and Lemma 5.7. The fourth vanishes after making full use of the equalities in (5.26) and the sole dependence of \tilde{M} on the radial variable—this is what the fourth equation in (5.26) is truly for. The membership of the seventh term in $\tilde{M} L_M^2(\tilde{U}_\zeta)$ stems from observing that

$$\begin{aligned} \left\| \partial_k \tilde{z} \nabla \tilde{M} \cdot (\nabla \tilde{\omega} A) / \tilde{M} \right\|_{L_M^2(\tilde{U}_\zeta)} &= \left\| \partial_k \tilde{z} \partial_d \tilde{M} \partial_d \tilde{\omega} a / \tilde{M} \right\|_{L_M^2(P'_\zeta \times (\gamma', \zeta \gamma))} \\ &\leq \sup_{P'_\zeta \times (\gamma', \zeta \gamma)} \left(\partial_d \tilde{M} \partial_d \tilde{\omega} a / \tilde{M} \right) \|\partial_k \tilde{z}\|_{L_M^2(\tilde{U}_\zeta)} < \infty. \end{aligned}$$

Let \hat{f} , given some function f defined on \tilde{U}_ζ , denote $f \circ T = f \circ S^{-1}$. Also, let $f_{(k)}$ denote the ratio of the right-hand side of (5.28) and $\tilde{M} a$. Then, (5.28) and the identities in (5.25) give

$$-\operatorname{div}(M \nabla \widehat{\tilde{\omega} \partial_k \tilde{z}}) + \widehat{\tilde{\omega} \partial_k \tilde{z} M} = \widehat{f_{(k)}} \quad (5.29)$$

in U_ζ , with $\widehat{f_{(k)}} \in L_M^2(U_\zeta)$. As the support of $\tilde{\omega}$ is bounded away from $\partial\tilde{U}_\zeta \setminus T(\partial D)$, we can extend $\tilde{\omega}\partial_k\tilde{z}$ and $\widehat{f_{(k)}}$ to the whole of D by zero while still satisfying (5.29). Then, Lemma 5.7 ensures that the extension of $\widehat{\tilde{\omega}\partial_k\tilde{z}}$ belongs to $H_M^2(D)$. It follows that $\tilde{\omega}\partial_k\tilde{z}$ belongs to $H_M^2(U_\zeta)$ and, consequently, $\partial_k\tilde{z} \in H_M^2(\tilde{U}_\varepsilon)$.

This procedure can be iterated. Within U_ε the identity (5.28) particularizes to

$$-\operatorname{div} \left(\nabla(\partial_k\tilde{z}) A\tilde{M} \right) + \partial_k\tilde{z} a\tilde{M} = \partial_k g a\tilde{M} + \nabla\nabla\tilde{z} : \partial_k A \tilde{M} + \nabla\tilde{z} \cdot \operatorname{div}(\partial_k A) \tilde{M}.$$

Let $g_{(k)} := \partial_k\tilde{g} + \nabla\nabla\tilde{z} : \partial_k A / a + \nabla\tilde{z} \cdot \operatorname{div}(\partial_k A)/a$ and let us redefine $\tilde{\omega}$ so that the role of \tilde{U}_ζ is now taken up by \tilde{U}_ε and the role of the latter is taken up by \tilde{U}_δ , where δ is some fixed number in $(0, \varepsilon)$. Thus, we can obtain an analogue of (5.28) for $\tilde{\omega}\partial_{l,k}\tilde{z}$, where $l, k \in [d-1]$:

$$\begin{aligned} & -\operatorname{div}(\nabla(\tilde{\omega}\partial_{l,k}\tilde{z}) A\tilde{M}) + \tilde{\omega}\partial_{l,k}\tilde{z} a\tilde{M} \\ &= \tilde{\omega}\partial_l g_{(k)} a\tilde{M} + \tilde{\omega}\nabla\nabla\partial_k\tilde{z} : \partial_l A \tilde{M} + \tilde{\omega}\nabla\partial_k\tilde{z} \cdot \operatorname{div}(\partial_l A) \tilde{M} + \tilde{\omega}\nabla\tilde{M} \cdot (\nabla(\partial_k\tilde{z}) \partial_l A) \\ & \quad - 2\nabla\tilde{\omega} \cdot (\nabla(\partial_{l,k}\tilde{z}) A\tilde{M}) - \partial_{l,k}\tilde{z} \operatorname{div}(\nabla\tilde{\omega} A) \tilde{M} - \partial_{l,k}\tilde{z} \nabla M \cdot (\nabla\tilde{\omega} A). \end{aligned}$$

Analogously to the study of the first-order tangential derivatives we need all seven terms on the right-hand side of the above equation to belong to $\tilde{M}L_M^2(\tilde{U}_\varepsilon)$ now. As, at this stage, we know that $\partial_k\tilde{z} \in H_M^2(\tilde{U}_\varepsilon)$, the second, the third, the fifth and the sixth term above pose no difficulties. The fourth term and the seventh term can be dealt with just as their counterparts in (5.28). When it comes to the first term, it is enough to show that $\partial_l g_{(k)} \in L_M^2(\tilde{U}_\varepsilon)$. Now,

$$\partial_l g_{(k)} = \partial_{l,k}\tilde{g} + \nabla\nabla\tilde{z} : \partial_l(\partial_k A / a) + \nabla\tilde{z} \cdot \partial_l(\operatorname{div}(\partial_k A)/a) + \partial_l\nabla\nabla\tilde{z} : (\partial_k A / a) + \partial_l\nabla\tilde{z} \cdot \operatorname{div}(\partial_k A)/a.$$

The first three terms above are clearly in $L_M^2(\tilde{U}_\varepsilon)$ —the first because of our hypotheses on g ; so is the fifth, for the second derivatives of \tilde{z} have the desired integrability. Finally, $\partial_l\nabla\nabla\tilde{z} \in L_M^2(\tilde{U}_\varepsilon)$ because $\partial_l\tilde{z} \in H_M^2(\tilde{U}_\varepsilon)$, as shown above. Proceeding with the argument one finds, after localization, that $\partial_{k,l}\tilde{z} \in H_M^2(\tilde{U}_\delta)$. We mention in passing that by closely following the arguments above the linear operators $g \in H_M^2(D) \mapsto \partial_l\tilde{z} \in H_M^2(\tilde{U}_\varepsilon)$ and $g \in H_M^2(D) \mapsto \partial_{k,l}\tilde{z} \in H_M^2(\tilde{U}_\delta)$ can be seen to be continuous; i.e., bounded.

Part 3: In this part we show the additional regularity of some derivatives of \tilde{z} that involve the radial direction.

Expanding and rearranging the distributional equation (5.27), noting the sole dependence of \tilde{M} on the last component of its argument and the properties of A given by (5.26) we get

$$-\frac{1}{\tilde{M}a}\partial_d(\partial_d\tilde{z} a\tilde{M}) = \tilde{g} - \tilde{z} + \frac{1}{a}\sum_{k=1}^{d-1}\sum_{j=1}^{d-1}(\partial_{j,k}\tilde{z} A_{j,k} + \partial_j\tilde{z} \partial_k A_{j,k}) =: f \quad (5.30)$$

in \tilde{U}_δ . From the previous part of the proof and our assumptions on g we have that $f \in H_M^2(\tilde{U}_\delta)$. Multiplying (5.30) by $\tilde{M}a$ and integrating with respect to the d -th variable we obtain

$$(\partial_d\tilde{z} a\tilde{M})[\mathbf{p}', p_d] - \lim_{s \rightarrow 0+} (\partial_d\tilde{z} a\tilde{M})[\mathbf{p}', s] = \int_0^{p_d} (fa\tilde{M})[\mathbf{p}', s] ds \quad (5.31)$$

for almost every \mathbf{p}' in P'_δ . We note in passing that in this part of the proof we reserve square brackets for arguments of functions. Our first task is to show that the limit on the left-hand side of (5.31) vanishes. To this end, we first observe that, for $p_d, s \in (0, \delta\gamma)$,

$$p_d^{\alpha/2}\partial_d\tilde{z}[\mathbf{p}', p_d] = s^{\alpha/2}\partial_d\tilde{z}[\mathbf{p}', s] + \int_s^{p_d} \frac{\partial}{\partial\sigma} \left(\sigma^{\alpha/2}\partial_d\tilde{z}[\mathbf{p}', \sigma] \right) d\sigma,$$

whence

$$p_d^{\alpha/2}|\partial_d\tilde{z}[\mathbf{p}', p_d]| \leq s^{\alpha/2}|\partial_d\tilde{z}[\mathbf{p}', s]| + \left| \int_s^{p_d} \frac{\alpha}{2}\sigma^{\alpha/2-1}\partial_d\tilde{z}[\mathbf{p}', \sigma] d\sigma \right| + \left| \int_s^{p_d} \sigma^{\alpha/2}\partial_{d,d}\tilde{z}[\mathbf{p}', \sigma] d\sigma \right|.$$

Furthermore,

$$\begin{aligned}
& p_d^\alpha |\partial_d \tilde{z}[\mathbf{p}', p_d]|^2 \\
& \leq 3s^\alpha |\partial_d \tilde{z}[\mathbf{p}', s]|^2 + \frac{3\alpha^2}{4} \left| \int_s^{p_d} \sigma^{\alpha/2-1} \partial_d \tilde{z}[\mathbf{p}', \sigma] d\sigma \right|^2 + 3 \left| \int_s^{p_d} \sigma^{\alpha/2} \partial_{d,d} \tilde{z}[\mathbf{p}', \sigma] d\sigma \right|^2 \\
& \leq 3s^\alpha |\partial_d \tilde{z}[\mathbf{p}', s]|^2 + \frac{3\alpha^2}{4} |p_d - s| \int_s^{p_d} \sigma^{\alpha-2} |\partial_d \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma + 3 |p_d - s| \int_s^{p_d} \sigma^\alpha |\partial_{d,d} \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma \\
& \leq 3s^\alpha |\partial_d \tilde{z}[\mathbf{p}', s]|^2 + \frac{3\alpha^2}{4} \delta\gamma \int_0^{\delta\gamma} \sigma^{\alpha-2} |\partial_d \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma + 3\delta\gamma \int_0^{\delta\gamma} \sigma^\alpha |\partial_{d,d} \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma.
\end{aligned}$$

Integrating this chain of inequalities with respect to s from 0 to $\delta\gamma$ and applying the Hardy inequality (5.22) stated in Lemma 5.8 we obtain

$$\begin{aligned}
& \delta\gamma p_d^\alpha |\partial_d \tilde{z}[\mathbf{p}', p_d]|^2 \\
& \leq 3 \int_0^{\delta\gamma} s^\alpha |\partial_d \tilde{z}[\mathbf{p}', s]|^2 ds + \frac{3\alpha^2}{4} (\delta\gamma)^2 \int_0^{\delta\gamma} \sigma^{\alpha-2} |\partial_d \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma + 3(\delta\gamma)^2 \int_0^{\delta\gamma} \sigma^\alpha |\partial_{d,d} \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma \\
& \leq 3 \int_0^{\delta\gamma} s^\alpha |\partial_d \tilde{z}[\mathbf{p}', s]|^2 ds + \frac{3\alpha^2 C_{\delta\gamma, \alpha}}{4} (\delta\gamma)^2 \int_0^{\delta\gamma} \sigma^\alpha |\partial_d \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma \\
& \quad + 3(\delta\gamma)^2 \left(\frac{\alpha^2 C_{\delta\gamma, \alpha}}{4} + 1 \right) \int_0^{\delta\gamma} \sigma^\alpha |\partial_{d,d} \tilde{z}[\mathbf{p}', \sigma]|^2 d\sigma.
\end{aligned}$$

Dividing by $\delta\gamma$, integrating with respect to \mathbf{p}' in P'_δ , using the bilateral boundedness of h and a by positive constants, and consolidating the constants, we get the trace-inequality-like bound

$$\int_{P'_\delta} p_d^\alpha |\partial_d \tilde{z}[\mathbf{p}', p_d]|^2 d\mathbf{p}' \leq C_1 \|\partial_d \tilde{z}\|_{H_M^1(\tilde{U}_\delta)}^2. \quad (5.32)$$

Thus,

$$\int_{P'_\delta} |(\partial_d \tilde{z} a \tilde{M})[\mathbf{p}', p_d]| d\mathbf{p}' \leq C_2 h[p_d]^{1/2} p_d^{\alpha/2} \left(\int_{P'_\delta} (|\partial_d \tilde{z}|^2 \tilde{M} a)[\mathbf{p}] d\mathbf{p}' \right)^{1/2} \rightarrow 0 \quad \text{as } p_d \rightarrow 0_+,$$

which implies the vanishing of the limit in (5.31).

Let us define $w: \tilde{U}_\delta \rightarrow \mathbb{R}$ by

$$w[\mathbf{p}] := \frac{\partial_d(\tilde{M}a)[\mathbf{p}]}{(\tilde{M}a)[\mathbf{p}]} \partial_d \tilde{z}[\mathbf{p}] = \frac{((ha)[p_d] p_d^\alpha)'}{(ha)[p_d]^2 p_d^{2\alpha}} \int_0^{p_d} (fa\tilde{M})[\mathbf{p}', s] ds, \quad (5.33)$$

where we have taken the liberty of treating a as an univariate function, which it is in the algebraic sense. The equality is valid for almost every $\mathbf{p} \in \tilde{U}_\delta$. Note that w is a member of $L_M^2(\tilde{U}_\delta)$ because $\nabla M \cdot \nabla z / M \in L_M^2(U_\delta)$; this, in turn, is a consequence of Lemma 5.7. We intend to show that $w \in H_M^2(U_\delta)$. Let $(f_n)_{n \in \mathbb{N}}$ be a sequence of $C^\infty(\tilde{U}_\delta)$ functions converging to f in $H_M^2(\tilde{U}_\delta)$ (its existence having been discussed in Part 1) and let

$$\begin{aligned}
w_n[\mathbf{p}] &:= \frac{((ha)[p_d] p_d^\alpha)'}{(ha)[p_d]^2 p_d^{2\alpha}} \int_0^{p_d} (f_n a \tilde{M})[\mathbf{p}', s] ds \\
&= \int_0^{p_d} \frac{(ha)'[p_d] p_d + \alpha(ha)[p_d] \left(\frac{s}{p_d}\right)^\alpha (ha f_n)[\mathbf{p}', s]}{(ha)[p_d]^2} \frac{(ha f_n)[\mathbf{p}', s]}{p_d} ds = \text{aux}[p_d] \int_0^1 \xi^\alpha (ha f_n)[\mathbf{p}', p_d \xi] d\xi
\end{aligned} \quad (5.34)$$

Here we have written $\text{aux}[p_d]$ in place of the first fraction in the second integral and denoted the function $\mathbf{p} \in \tilde{U}_\delta \mapsto h(p_d) \in \mathbb{R}$ by h as well. The second equality comes via the change of variable $\xi = s/p_d$. As the function h and the determinant a have uniform C^3 and C^∞ regularity in U_δ , the function $\text{aux} \in C^2(\tilde{U}_\delta)$ and w_n is twice continuously differentiable in the d -th direction.

Differentiating the last integral representation of w_n with respect to its d -th variable twice and then reversing the change of variable we obtain

$$\begin{aligned}\partial_{d,d}w_n[\mathbf{p}] &= \sum_{k=0}^2 \binom{2}{k} \frac{\partial^{2-k}\text{aux}}{\partial p_d^{2-k}}[p_d] \int_0^1 \partial_d^k(haf_n)[\mathbf{p}', p_d\xi] \xi^{\alpha+k} d\xi \\ &= \sum_{k=0}^2 \binom{2}{k} \frac{\partial^{2-k}\text{aux}}{\partial p_d^{2-k}}[p_d] \int_0^{p_d} \partial_d^k(haf_n)[\mathbf{p}', s] \left(\frac{s}{p_d}\right)^{\alpha+k} \frac{1}{p_d} ds,\end{aligned}$$

whence, as $s/p_d \in (0, 1)$ if $s \in (0, p_d)$,

$$\begin{aligned}p_d^{\alpha/2} |\partial_{d,d}w_n[\mathbf{p}]| &\leq \frac{1}{p_d} \int_0^{p_d} \left(\sum_{k=0}^2 \binom{2}{k} \left| \frac{\partial^{2-k}\text{aux}}{\partial p_d^{2-k}}[p_d] \partial_d^k(haf_n)[\mathbf{p}', s] \right| \left(\frac{s}{p_d}\right)^{\alpha/2+k} \right) s^{\alpha/2} ds \\ &\leq \frac{1}{p_d} \int_0^{p_d} \left(\sum_{k=0}^2 \binom{2}{k} \left| \frac{\partial^{2-k}\text{aux}}{\partial p_d^{2-k}}[p_d] \partial_d^k(haf_n)[\mathbf{p}', s] \right| \right) s^{\alpha/2} ds \\ &\leq \frac{C_3}{p_d} \int_0^{p_d} \left(|(haf_n)|^2 + |\partial_d(haf_n)|^2 + |\partial_{d,d}(haf_n)|^2 \right)^{1/2} [\mathbf{p}', s] s^{\alpha/2} ds\end{aligned}$$

for some $C_3 > 0$ independent of $\mathbf{p} = (\mathbf{p}', p_d)$. We square the resulting inequality, integrate it with respect to p_d from 0 to $\delta\gamma$, use the Hardy inequality (5.21) in Lemma 5.8 and note yet again the bilateral boundedness of h and a by positive constants to obtain

$$\begin{aligned}\int_0^{\delta\gamma} p_d^\alpha (ha)[p_d] |\partial_{d,d}w_n[\mathbf{p}]|^2 dp_d \\ \leq C_4 \int_0^{\delta\gamma} \left(|(haf_n)|^2 + |\partial_d(haf_n)|^2 + |\partial_{d,d}(haf_n)|^2 \right) [\mathbf{p}] s^\alpha (ha)[p_d] dp_d,\end{aligned}$$

where C_4 is still independent of $\mathbf{p}' \in P'_\delta$. Integrating this with respect to $\mathbf{p}' \in P'_\delta$, using the regularity of h and a and taking into account that $(\tilde{M}a)[\mathbf{p}] = (ha)[p_d]p_d^\alpha$ for all $\mathbf{p} \in \tilde{U}_\delta$ one gets

$$\|\partial_{d,d}w_n\|_{L^2_M(\tilde{U}_\delta)} \leq C_5 \|f_n\|_{H^2_M(\tilde{U}_\delta)}.$$

This argument can be carried over to all derivatives of order less than or equal to two of w_n (including zeroth order derivatives of w_n , meaning w_n itself). The result is

$$\|w_n\|_{H^2_M(\tilde{U}_\delta)} \leq C_6 \|f_n\|_{H^2_M(\tilde{U}_\delta)}.$$

As $H^2_M(\tilde{U}_\delta)$ is a Hilbert space, there exists a subsequence $(w_{\phi(n)})_{n \geq 1}$ with a weak limit $w^* \in H^2_M(\tilde{U}_\delta)$. By the continuity of the injection of $H^2_M(\tilde{U}_\delta)$ into $L^2_M(\tilde{U}_\delta)$, w^* is also the weak limit of the $w_{\phi(n)}$ in $L^2_M(\tilde{U}_\delta)$.

Now, given any $\chi \in L^2_M(\tilde{U}_\delta)$,

$$\begin{aligned}\int_{\tilde{U}_\delta} \left(\frac{\text{aux}[p_d]}{p_d} \int_0^{p_d} \left(\frac{s}{p_d}\right)^\alpha (ha\chi)[\mathbf{p}', s] ds \right)^2 \tilde{M}[\mathbf{p}] d\mathbf{p} \\ = \int_{\tilde{U}_\delta} \frac{\text{aux}[p_d]^2}{p_d^2} \left(\int_0^{p_d} \left(\frac{s}{p_d}\right)^{\alpha/2} s^{\alpha/2} (ha\chi)[\mathbf{p}', s] ds \right)^2 h[p_d] d\mathbf{p} \\ \leq C_7 \int_{P'_\delta} \int_0^{\delta\gamma} \frac{1}{p_d^2} \left(\int_0^{p_d} s^{\alpha/2} (ha\chi)[\mathbf{p}', s] ds \right)^2 dp_d d\mathbf{p}' \\ \leq C_8 \int_{P'_\delta} \int_0^{\delta\gamma} s^\alpha |(ha\chi)[\mathbf{p}', s]|^2 ds d\mathbf{p}' \\ \leq C_9 \|\chi\|_{L^2_M(\tilde{U}_\delta)}^2.\end{aligned}$$

Hence, the operation that defines w (resp. w_n) in terms of f (resp. f_n) in (5.33) (resp. (5.34)) is a bounded map from $L^2_M(\tilde{U}_\delta)$ to itself. Therefore, $\lim_{n \rightarrow \infty} f_n = f$ in $L^2_M(\tilde{U}_\delta)$ implies $\lim_{n \rightarrow \infty} w_n = w$ in the same space. Thus, w and the weak limit w^* have to be the same measurable function and so $w \in H^2_M(\tilde{U}_\delta)$. We get the bound $\|w\|_{H^2_M(\tilde{U}_\delta)} \leq \liminf_{n \rightarrow \infty} \|w_{\phi(n)}\|_{H^2_M(\tilde{U}_\delta)} \leq C_6 \|f_{\phi(n)}\|_{H^2_M(\tilde{U}_\delta)}$. As (with no loss of generality) we can assume that the f_n are scaled so that their $H^2_M(\tilde{U}_\delta)$ norm is identically equal to the same norm of f , it follows that

$$\|w\|_{H^2_M(\tilde{U}_\delta)} \leq C_6 \|f\|_{H^2_M(\tilde{U}_\delta)}.$$

From (5.30) and (5.33),

$$-\partial_{d,d}\tilde{z} = f + \frac{\partial_d(\tilde{M}a)}{\tilde{M}a} \partial_d \tilde{z} = f + w,$$

whence $\|\partial_{d,d}\tilde{z}\|_{H^2_M(\tilde{U}_\delta)} \leq (1 + C_6) \|f\|_{H^2_M(\tilde{U}_\delta)} \leq C_{10} \|\tilde{g}\|_{H^2_M(\tilde{U}_\delta)}$. We know from the previous part that all second derivatives of \tilde{z} that do not involve the d -th direction have $H^2_M(\tilde{U}_\delta)$ norms bounded by the $H^2_M(\tilde{U}_\delta)$ norm of \tilde{g} . This and the corresponding result for $\partial_{d,d}\tilde{z}$ is enough to be able to bound all derivatives of \tilde{z} of order less than or equal to four, and thus deduce that

$$\|\tilde{z}\|_{H^4_M(\tilde{U}_\delta)} \leq C_{11} \|g\|_{H^2_M(D)}$$

or, equivalently in the light of (5.24), that

$$\|z\|_{H^4_M(U_\delta)} \leq C_{12} \|g\|_{H^2_M(U_\delta)}. \quad (5.35)$$

Part 4: By modifying the transformation S one can get a localized bound of the form (5.35) for any origin-centered rotation of U_δ . It follows that (5.35) remains valid (with some other constant C_{12}) if we replace U_δ by the annulus/spherical shell $\{\mathbf{p} \in D : |\mathbf{p}| > \sqrt{b} - \delta\gamma\}$.

Let D_0 be the ball $B(0, \sqrt{b} - \delta\gamma/2) \Subset D$. As $C_0^\infty(D_0) \subset C_0^\infty(D)$, we have that

$$\langle z, \varphi \rangle_{H^1_M(D_0)} = \langle g, \varphi \rangle_{L^2_M(D_0)} \quad \forall \varphi \in C_0^\infty(D_0).$$

The existence of a positive infimum of M in D_0 implies that z is the weak solution to a regular (i.e., uniformly) elliptic problem in D_0 with $H^2(D_0)$ right-hand side. It follows, via the $C^{2,1}(D_0)$ regularity of M (see, e.g., [GT01, Theorem 8.10]), that for some $C_{13} > 0$,

$$\|z\|_{H^4_M(D'_0)} \leq C_{13} \|g\|_{H^2_M(D_0)} \leq C_{13} \|g\|_{H^2_M(D)},$$

with $D'_0 := B(0, \sqrt{n} - 3\delta\gamma/4) \Subset D_0$.

Combining this last estimate with the result in the annulus/spherical shell mentioned above (which in union with D'_0 covers D), we obtain the desired global bound. \square

The next lemma is an almost trivial corollary of Lemma 5.9, yet it is a true iterate of Lemma 5.7 in the sense that the hypothesis on the right-hand side function is the thesis on the solution in Lemma 5.7. This makes it suitable for the arguments that will be used in the proof of Lemma 5.11.

Lemma 5.10. *Let $i \in [N]$ and suppose that $g \in H^2_{M_i}(D_i)$ and that $M_i^{-1} \operatorname{div}(M_i \nabla g) \in L^2_{M_i}(D_i)$. Then, there exists a constant $C_i > 0$, independent of g_i , such that the solution $z \in H^1_{M_i}(D_i)$ of*

$$\langle z, \varphi \rangle_{H^1_{M_i}(D_i)} = \langle g, \varphi \rangle_{L^2_{M_i}(D_i)} \quad \forall \varphi \in H^1_{M_i}(D_i)$$

obeys the regularity estimate

$$\begin{aligned} \|z\|_{H^4_{M_i}(D_i)} + \left\| \frac{1}{M_i} \operatorname{div}(M_i \nabla z) \right\|_{H^2_{M_i}(D_i)} + \left\| \frac{1}{M_i} \operatorname{div} \left(M_i \nabla \left[\frac{1}{M_i} \operatorname{div}(M_i \nabla z) \right] \right) \right\|_{L^2_{M_i}(D_i)} \\ \leq C_i \left(\|g\|_{H^2_{M_i}(D_i)} + \left\| \frac{1}{M_i} \operatorname{div}(M_i \nabla g) \right\|_{L^2_{M_i}(D_i)} \right). \end{aligned}$$

Proof. This follows directly from Lemma 5.9 on noting that $M_i^{-1} \operatorname{div}(M_i \nabla z) = g - z$ in the distributional sense first, and then in the sense of measurable functions. \square

Lemma 5.11. *Let $i \in [N]$. The following statements of equivalence hold:*

$$\begin{aligned} \tau \in \mathbf{H}_{M_i}^2(D_i) \quad \text{and} \quad \frac{1}{M_i} \operatorname{div}(M_i \nabla \tau) \in \mathbf{L}_{M_i}^2(D_i) \\ \iff \tau \in \mathbf{L}_{M_i}^2(D_i) \quad \text{and} \quad \sum_{n=1}^{\infty} (\lambda_n^{(i)})^2 \langle \tau, e_n^{(i)} \rangle_{\mathbf{L}_{M_i}^2(D_i)}^2 < \infty; \end{aligned} \quad (5.36)$$

and

$$\begin{aligned} \tau \in \mathbf{H}_{M_i}^4(D_i), \quad \frac{1}{M_i} \operatorname{div}(M_i \nabla \tau) \in \mathbf{H}_{M_i}^2(D_i) \quad \text{and} \quad \frac{1}{M_i} \operatorname{div} \left(M_i \nabla \left[\frac{1}{M_i} \operatorname{div}(M_i \nabla \tau) \right] \right) \in \mathbf{L}_{M_i}^2(D_i) \\ \iff \tau \in \mathbf{L}_{M_i}^2(D_i) \quad \text{and} \quad \sum_{n=1}^{\infty} (\lambda_n^{(i)})^4 \langle \tau, e_n^{(i)} \rangle_{\mathbf{L}_{M_i}^2(D_i)}^2 < \infty. \end{aligned} \quad (5.37)$$

Proof. We will omit the spring index when proving (5.36) and (5.37). We start by denoting by L the operator that associates each $\varphi \in W_{\text{loc}}^{2,1}(D)$ with the distribution $M^{-1} \operatorname{div}(M \nabla \varphi)$ (this is a well-defined distribution because of the regularity of φ and M ; cf. Lemma B.1 in Appendix B). We also write $\hat{L} := -L + I$ where I is the operator that associates each distribution with itself. Let us define the Hilbert spaces (and associated norms)

$$\tilde{\mathbf{H}}_M^2(D) := \{ \varphi \in \mathbf{H}_M^2(D) : L(\varphi) \in \mathbf{L}_M^2(D) \}, \quad (5.38a)$$

$$\| \varphi \|_{\tilde{\mathbf{H}}_M^2(D)}^2 := \| \varphi \|_{\mathbf{H}_M^2(D)}^2 + \| L(\varphi) \|_{\mathbf{L}_M^2(D)}^2 \quad (5.38b)$$

and

$$\tilde{\mathbf{H}}_M^4(D) := \{ \varphi \in \mathbf{H}_M^4(D) : L(\varphi) \in \tilde{\mathbf{H}}_M^2(D) \}, \quad (5.39a)$$

$$\| \varphi \|_{\tilde{\mathbf{H}}_M^4(D)}^2 := \| \varphi \|_{\mathbf{H}_M^4(D)}^2 + \| L(\varphi) \|_{\tilde{\mathbf{H}}_M^2(D)}^2. \quad (5.39b)$$

Because of the definition of $\tilde{\mathbf{H}}_M^2(D)$, $\hat{L} : \mathbf{H}_M^2(D) \rightarrow \mathbf{L}_M^2(D)$ is a bounded linear operator. As for every $\varphi \in \mathbf{L}_M^2(D)$ the solution $z \in \mathbf{H}_M^1(D)$ to

$$\langle z, \psi \rangle_{\mathbf{H}_M^1(D)} = \langle f, \psi \rangle_{\mathbf{L}_M^2(D)} \quad \forall \psi \in \mathbf{H}_M^1(D)$$

exists and, thanks to Lemma 5.7, is bounded in $\tilde{\mathbf{H}}_M^2(D)$, $\hat{L}^{-1} : \mathbf{L}_M^2(D) \rightarrow \tilde{\mathbf{H}}_M^2(D)$ is well-defined and bounded. Similarly, by the definition of $\tilde{\mathbf{H}}_M^4(D)$ and Lemma 5.10, $\hat{L}^2 : \tilde{\mathbf{H}}_M^4(D) \rightarrow \mathbf{L}_M^2(D)$ is a bounded linear operator with a bounded inverse.

Let $\tau \in \tilde{\mathbf{H}}_M^2(D)$; i.e., τ complies with the left-hand side of (5.36). It then follows that $f_\tau := -L(\tau) + \tau \in \mathbf{L}_M^2(D)$ and Parseval's identity thus yields

$$\infty > \| f_\tau \|_{\mathbf{L}_M^2(D)}^2 = \sum_{n \geq 1} \langle f_\tau, e_n \rangle_{\mathbf{L}_M^2(D)}^2 = \sum_{n \geq 1} \langle \tau, e_n \rangle_{\mathbf{H}_M^1(D)}^2 = \sum_{n \geq 1} \lambda_n^2 \langle \tau, e_n \rangle_{\mathbf{L}_M^2(D)}^2,$$

where $\langle f_\tau, e_n \rangle_{\mathbf{L}_M^2(D)} = \langle \tau, e_n \rangle_{\mathbf{H}_M^1(D)}$ follows by the density of $\mathbf{C}_0^\infty(D)$ in $\mathbf{H}_M^1(D)$.

To prove the converse, note that the eigenfunctions e_n of (5.7) are solutions of $e_n = \hat{L}^{-1}(\lambda_n e_n)$, whence $\| e_n \|_{\tilde{\mathbf{H}}_M^2(D)} \leq C \| \lambda_n e_n \|_{\mathbf{L}_M^2(D)} = C \lambda_n$. Consequently, the partial sums

$$\tau_k := \sum_{n=1}^k \langle \tau, e_n \rangle_{\mathbf{L}_M^2(D)} e_n$$

are members of $\tilde{\mathbf{H}}_M^2(D)$. Then, if $k \leq l$, the $\mathbf{L}_M^2(D)$ -orthonormality of the e_n yields that

$$\left\| \hat{L}(\tau_l) - \hat{L}(\tau_k) \right\|_{\mathbf{L}_M^2(D)}^2 = \left\| \sum_{n=k+1}^l \langle \tau, e_n \rangle_{\mathbf{L}_M^2(D)} \hat{L}(e_n) \right\|_{\mathbf{L}_M^2(D)}^2 = \sum_{n=k+1}^l \lambda_n^2 \langle \tau, e_n \rangle_{\mathbf{L}_M^2(D)}^2.$$

As the sum $\sum_{n \geq 1} \lambda_n^2 \langle \tau, e_n \rangle_{\mathbf{L}_M^2(D)}^2$ is assumed to converge, the sequence $\left(\hat{L}(\tau_k) \right)_{k \geq 1}$ is a Cauchy sequence in $\mathbf{L}_M^2(D)$ and hence it converges to some $f^* \in \mathbf{L}_M^2(D)$. The continuity of \hat{L}^{-1} implies

that the sequence $(\tau_k)_{k \geq 1}$ converges in $\tilde{H}_M^2(D)$ to $\hat{L}^{-1}(f^*)$. The same sequence converges in $L_M^2(D)$ to τ . The continuity of the injection of $H_M^2(D)$ into $L_M^2(D)$ then implies that $\tau = \hat{L}^{-1}(f^*) \in \tilde{H}_M^2(D)$. This completes the proof of (5.36).

Let us suppose now that τ in $\tilde{H}_M^4(D)$; i.e., τ complies with the left-hand side of (5.37). It follows that $f_\tau := -L(\tau) + \tau \in \tilde{H}_M^2(D)$ and $g_\tau := -L(f_\tau) + f_\tau \in L_M^2(D)$. Parseval's identity gives

$$\begin{aligned} \infty > \|g_\tau\|_{L_M^2(D)}^2 &= \sum_{n \geq 1} \langle g_\tau, e_n \rangle_{L_M^2(D)}^2 = \sum_{n \geq 1} \langle f_\tau, e_n \rangle_{H_M^1(D)}^2 \\ &= \sum_{n \geq 1} \lambda_n^2 \langle f_\tau, e_n \rangle_{L_M^2(D)}^2 = \sum_{n \geq 1} \lambda_n^4 \langle \tau, e_n \rangle_{L_M^2(D)}^2, \end{aligned}$$

where the second equality follows, similarly as above, by the density of $C_0^\infty(D)$ in $H_M^1(D)$ thanks to the boosted regularity of f_τ . The latter also allows the use of (5.7) to obtain the third equality.

To prove the converse we first note that each e_n is a solution of $e_n = \hat{L}^{-2}(\lambda_n^2 e_n)$, whence $\|e_n\|_{\tilde{H}_M^4(D)} \leq C \|\lambda_n e_n\|_{L_M^2(D)} = C \lambda_n$. Thus, the partial sums τ_k are members of $\tilde{H}_M^4(D)$; hence, if $k \leq l$,

$$\left\| \hat{L}^2(\tau_l) - \hat{L}^2(\tau_k) \right\|_{L_M^2(D)}^2 = \left\| \sum_{n=k+1}^l \langle \tau, e_n \rangle_{L_M^2(D)} \hat{L}^2(e_n) \right\|_{L_M^2(D)}^2 = \sum_{n=k+1}^l \lambda_n^4 \langle \tau, e_n \rangle_{L_M^2(D)}^2.$$

The finiteness of the sum $\sum_{n \geq 1} \lambda_n^4 \langle \tau, e_n \rangle_{L_M^2(D)}^2$ thus implies that $(\hat{L}^2(\tau_k))_{k \geq 1}$ is a Cauchy sequence, which by virtue of the completeness of $L_M^2(D)$ converges to some $g^* \in L_M^2(D)$. The continuity of \hat{L}^{-2} implies that the τ_k converge to $\hat{L}^{-2}g^*$ in $\tilde{H}_M^4(D)$. As the partial sums converge in $L_M^2(D)$ to τ , $\tau = \hat{L}^{-2}g^* \in \tilde{H}_M^4(D)$. We have thus proved (5.37). \square

We intend to exploit the previous single-domain results in order to say something about the multi-domain case. To this end, we define, for $i \in [N]$, the distributional operators $L_i: \{\varphi \in L_{\text{loc}}^1(D): \nabla_{\mathbf{q}_i} \varphi \in [W_{\text{loc}}^{1,1}(D)]^d\} \rightarrow \mathcal{D}'(D)$ by

$$L_i(\varphi) := M_i^{-1} \text{div}_{\mathbf{q}_i}(M_i \nabla_{\mathbf{q}_i} \varphi).$$

We also define $\hat{L}_i := -L_i + I$, where I is the identity operator mapping $\mathcal{D}'(D)$ onto itself. An easily verifiable and important property of these operators is that, as long as their composition is well-defined, they commute with respect to their spring index. Hence, we can naturally use multi-indices in \mathbb{N}_0^N to denote the repeated application of distinct L_i or \hat{L}_i :

$$L_\beta := L_1^{\beta_1} \circ \dots \circ L_N^{\beta_N}, \quad \hat{L}_\beta := \hat{L}_1^{\beta_1} \circ \dots \circ \hat{L}_N^{\beta_N},$$

where any zero among the β_i is assumed to give rise to the identity operator. For these multi-indices we define the function $|\beta|_\infty := \max_{i \in [N]} \beta_i$. Now, for derivatives in $\mathcal{D}'(D)$, the multi-indices belong to \mathbb{N}_0^{Nd} and come naturally grouped in N length- d sub-multi-indices (one for each factor of the Cartesian product $D = D_1 \times \dots \times D_N$). Thus we define the function $|\cdot|_{\infty,1}: \mathbb{N}_0^{Nd} \rightarrow \mathbb{N}_0$ by

$$|\alpha|_{\infty,1} = |(\alpha_1, \dots, \alpha_N)|_{\infty,1} := \max_{i \in [N]} |\alpha_i|_1 = \max_{i \in [N]} |\alpha_i|;$$

that is, the maximal order among the component single-domain multi-indices.

With this compact notation, we now define the Hilbert spaces (with corresponding norms)

$$\tilde{H}_M^{2,\text{mix}}(D) := \left\{ \varphi \in L_M^2(D): \partial_\alpha \varphi \in L_M^2(D), |\alpha|_{\infty,1} \leq 2; L_\beta(\varphi) \in L_M^2(D), |\beta|_\infty = 1 \right\}, \quad (5.40a)$$

$$\|\varphi\|_{\tilde{H}_M^{2,\text{mix}}(D)}^2 := \sum_{\substack{\alpha \in \mathbb{N}_0^{Nd} \\ |\alpha|_{\infty,1} \leq 2}} \|\partial_\alpha \varphi\|_{L_M^2(D)}^2 + \sum_{\substack{\beta \in \mathbb{N}_0^d \\ |\beta|_\infty = 1}} \|L_\beta(\varphi)\|_{L_M^2(D)}^2 \quad (5.40b)$$

and

$$\tilde{H}_M^{4,\text{mix}}(\mathcal{D}) := \left\{ \varphi \in L_M^2(\mathcal{D}) : \partial_{\alpha} \varphi \in L_M^2(\mathcal{D}), |\alpha|_{\infty,1} \leq 4; \right. \\ \left. L_{\beta}(\varphi) \in H_M^2(\mathcal{D}), |\beta|_{\infty} = 1; L_{\beta}(\varphi) \in L_M^2(\mathcal{D}), |\beta|_{\infty} = 2 \right\}, \quad (5.41a)$$

$$\|\varphi\|_{\tilde{H}_M^{4,\text{mix}}(\mathcal{D})}^2 := \sum_{\substack{\alpha \in \mathbb{N}_0^{Nd} \\ |\alpha|_{\infty,1} \leq 4}} \|\partial_{\alpha} \varphi\|_{L_M^2(\mathcal{D})}^2 + \sum_{\substack{\beta \in \mathbb{N}_0^d \\ |\beta|_{\infty} = 1}} \|L_{\beta}(\varphi)\|_{H_M^2(\mathcal{D})}^2 + \sum_{\substack{\beta \in \mathbb{N}_0^d \\ |\beta|_{\infty} = 2}} \|L_{\beta}(\varphi)\|_{L_M^2(\mathcal{D})}^2. \quad (5.41b)$$

The following lemma holds.

Lemma 5.12. *For $m \in \{2, 4\}$, $\tilde{H}_M^{m,\text{mix}}(\mathcal{D}) \subset H_M^{\mathbf{T}^{(m)}}(\mathcal{D})$.*

Proof. We recall that, by Lemma 5.3, $((\lambda_{\mathbf{n}}, e_{\mathbf{n}}))_{\mathbf{n} \in \mathbb{N}^N}$ as defined in (5.11) is a complete set of solutions of the M -weighted eigenvalue problem (5.8) and that the latter have tensor-product structure. Also, by the definitions in (5.13) and (5.14), $H_M^{\mathbf{T}^{(m)}}(\mathcal{D})$ is the space of $L_M^2(\mathcal{D})$ functions whose squared Fourier coefficients, weighted with the coefficients defined by

$$\tau_{\mathbf{n}}^{(m)} = \prod_{i=1}^N \left(\lambda_{n_i}^{(i)} \right)^m \quad \forall \mathbf{n} \in \mathbb{N}^N,$$

have finite sum.

If $\varphi \in \tilde{H}_M^{m,\text{mix}}(\mathcal{D})$, one can apply to it each operator \hat{L}_i a total of $m/2$ times *cumulatively* and the result will lie in $L_M^2(\mathcal{D})$; i.e., $\hat{L}_{(m/2, \dots, m/2)}(\varphi) \in L_M^2(\mathcal{D})$. By Parseval's identity,

$$\infty > \left\| \hat{L}_{(m/2, \dots, m/2)} \varphi \right\|_{L_M^2(\mathcal{D})}^2 = \sum_{\mathbf{n} \in \mathbb{N}^N} \left\langle \hat{L}_{(m/2, \dots, m/2)}(\varphi), e_{\mathbf{n}} \right\rangle_{L_M^2(\mathcal{D})}^2 = \sum_{\mathbf{n} \in \mathbb{N}^N} \prod_{i=1}^N \left(\lambda_{n_i}^{(i)} \right)^m \langle \varphi, e_{\mathbf{n}} \rangle_{L_M^2(\mathcal{D})}^2, \quad (5.42)$$

where the second equality is justified by the density of $C_0^\infty(\mathcal{D})$ functions in $H_M^1(\mathcal{D})$, the regularity of φ and the Cartesian product form of the domain \mathcal{D} and the tensor-product form of the Maxwellian weight function M . As the finiteness of the last expression in (5.42) is exactly the condition for membership in $H_M^{\mathbf{T}^{(m)}}(\mathcal{D})$, we obtain the desired result. \square

We recall that Theorem 5.4 gives a condition on the parameter of the space $H_M^{\mathbf{T}^{(m)}}(\mathcal{D})$ under which it becomes a subspace of the abstract space \mathcal{B}_1 , which in turn is connected by (4.14) to the space \mathcal{A}_1 of fast convergence of the greedy algorithms (cf. Theorem 4.6 and Theorem 4.7). Then, from Lemma 5.12 it is apparent that the arguably less abstract space $\tilde{H}_M^{m,\text{mix}}(\mathcal{D})$ will be a subspace of \mathcal{B}_1 for a suitable choice of the parameter. We shall now make this statement more precise.

Theorem 5.13. *Let $H_M^{\mathbf{T}^{(4)}}(\mathcal{D})$ be defined according to (5.14), where $d \in \{2, 3\}$, as elsewhere, is the common dimensionality of the Cartesian factors that make up \mathcal{D} ; then,*

$$\tilde{H}_M^{4,\text{mix}}(\mathcal{D}) \subset H_M^{\mathbf{T}^{(4)}}(\mathcal{D}) \subset \mathcal{B}_1.$$

Proof. Lemma 5.12 gives that $\tilde{H}_M^{4,\text{mix}}(\mathcal{D}) \subset H_M^{\mathbf{T}^{(4)}}(\mathcal{D})$. As 4 is greater than $1 + \frac{d}{2}$ for both $d = 2$ and $d = 3$, Theorem 5.4 gives that $H_M^{\mathbf{T}^{(4)}}(\mathcal{D}) \subset \mathcal{B}_1$. \square

Remark 9. If the hypotheses we have been making throughout this work (i.e., Hypotheses A, B, C, D and E) are met, nothing in our arguments essentially restricts the results to the physically relevant cases $d = 2$ and $d = 3$. In particular, in the case of $d = 1$, the combination of Theorem 5.4 with Lemma 5.12 and the fact that $2 > 1 + \frac{1}{2}$ yields that

$$\tilde{H}_M^{2,\text{mix}}(\mathcal{D}) \subset H_M^{\mathbf{T}^{(2)}}(\mathcal{D}) \subset \mathcal{B}_1.$$

Sobolev spaces of dominating mixed smoothness akin to $\tilde{H}_M^{2,\text{mix}}(\mathcal{D})$ can also be shown to be subspaces of the regularity class \mathcal{B}_1 in the case of the classical Poisson problem studied in [LBLM09]:

Find $\psi \in H_0^1(D)$ (with the standard meaning of the Sobolev space $H_0^1(D)$; i.e., the set of all elements of $H^1(D)$ that have zero trace on ∂D —not a zero-weighted Sobolev space!) such that

$$\langle \psi, \varphi \rangle_{H_0^1(D)} = \langle f, \varphi \rangle_{L^2(D)} \quad \forall \varphi \in H_0^1(D),$$

where $D = D_1 \otimes \cdots \otimes D_N$ and each D_i , $i \in [N]$, is an open interval. The corresponding greedy algorithms seek approximations that are linear combinations of $\bigotimes_{i \in [N]} H_0^1(D_i)$ functions. The argument of Theorem 5.4 above holds in this case without any change, and so, given that the n -th eigenvalue of the corresponding analogue to the partial-domain eigenvalue problem (5.7) is proportional to n^2 , we have that

$$\left\{ \varphi \in L^2(D) : \sum_{\mathbf{n} \in \mathbb{N}^N} \left[\left(\sum_{i=1}^N n_i^2 \right)^2 + \prod_{i=1}^N (n_i^2)^2 \right] \langle \varphi, e_{\mathbf{n}} \rangle_{L^2(D)}^2 < \infty \right\} \subset \mathcal{B}_1.$$

In this non-degenerate setting it is possible to identify the space on the left-hand side of the above expression with

$$H^{2,\text{mix}}(D) \cap H_0^1(D) := \left\{ \varphi \in H_0^1 : \partial_\alpha \varphi \in L^2(D), |\alpha|_\infty = \max_{1 \leq i \leq N} \alpha_i \leq 2 \right\}.$$

This characterization should be contrasted with the condition for membership in \mathcal{A}_1 (which is identical to \mathcal{B}_1 in this unweighted setting) derived in [LBLM09, Remark 4], which demands, instead, that the true solution belongs to $H^m(D) \cap H_0^1(D)$, with $m > 1 + N/2$. In fact the characterization given in [LBLM09, Remark 4] can be generalized to the requirement that the exact solution belongs to $H^m(D) \cap H_0^1(D)$, with $m > 1 + Nd/2$, when the factor domains are no longer one-dimensional but d -dimensional; and, thanks to Theorem 5.5, such a characterization in terms of standard Sobolev spaces (rather than spaces of dominating mixed smoothness) also has a counterpart in our degenerate setting.

An attractive feature of spaces of dominating mixed smoothness is that their regularity index is independent of N and such spaces are therefore more naturally suited to (high-dimensional) tensor-product settings such as ours. We note in this respect that we conjecture that the reverse of the inclusion stated in Lemma 5.12 also holds, implying equality of the two spaces there—just as in Lemma 5.11 for the single-domain spaces. We suspect that the proof of this would involve tensorizing the statements of Lemma 5.7 and Lemma 5.10. However, even if Lemma 5.12 held with an equality of spaces, there would still be some slack between the discussed mixed smoothness levels and the lower bound of the admissible parameter m such that $H_M^{T(m)}(D) \subset \mathcal{B}_1$. The reason is that we have gone about obtaining elliptic regularity results by two integer degrees of differentiation at a time. Consequently, we have not defined anything we could label $\tilde{H}_{M_i}^m(D_i)$ or $\tilde{H}_M^{m,\text{mix}}(D)$ with $m \notin \{2, 4\}$ while being consistent with the definitions we have given for the single-spring spaces $\tilde{H}_{M_i}^2(D_i)$ in (5.38) and $\tilde{H}_{M_i}^4(D_i)$ in (5.39), and with the multi-spring spaces $\tilde{H}_M^{2,\text{mix}}(D)$ in (5.40) and $\tilde{H}_M^{4,\text{mix}}(D)$ in (5.41). Given the presence of the second-order operators of the form $M_i^{-1} \text{div}(M_i \nabla \cdot)$ and $M^{-1} \text{div}(M \nabla \cdot)$ in the definition of these even-indexed spaces, it is not immediately clear what a suitable explicit definition of the analogous odd-indexed—let alone non-integer-indexed—spaces might be. We shall address this question by using function space interpolation.

We start with the fact that, given two nets of positive weights $\Sigma^{(i)} = \left(\sigma_{\mathbf{n}}^{(i)} \right)_{\mathbf{n} \in \mathbb{N}^N}$, $i \in \{1, 2\}$, one can show that for $\theta \in (0, 1)$ the (real) $(\theta, 2)$ -interpolation space between them obeys

$$\left[H_M^{\Sigma^{(1)}}(D), H_M^{\Sigma^{(2)}}(D) \right]_{\theta, 2} = H_M^{\tilde{\Sigma}}(D),$$

where $\tilde{\Sigma} = (\tilde{\sigma}_{\mathbf{n}})_{\mathbf{n} \in \mathbb{N}^N}$ and $\tilde{\sigma}_{\mathbf{n}} := \left(\sigma_{\mathbf{n}}^{(1)} \right)^{1-\theta} \left(\sigma_{\mathbf{n}}^{(2)} \right)^{\theta}$ for all $\mathbf{n} \in \mathbb{N}^N$, with equivalence of norms (the proof is a simple modification of the argument given in [Tar07, Chapter 23]). As, according to the definition in (5.14),

$$\tau_{\mathbf{n}}^{(2\theta)} = \left(\tau_{\mathbf{n}}^{(0)} \right)^{1-\theta} \left(\tau_{\mathbf{n}}^{(2)} \right)^{\theta} \quad \text{and} \quad \tau_{\mathbf{n}}^{(2+2\theta)} = \left(\tau_{\mathbf{n}}^{(2)} \right)^{1-\theta} \left(\tau_{\mathbf{n}}^{(4)} \right)^{\theta}$$

for all $\theta \in (0, 1)$ and \mathbf{n} in \mathbb{N}^N , it follows that

$$H_M^{T(2\theta)}(D) = \left[H_M^{T(0)}(D), H_M^{T(2)}(D) \right]_{\theta,2} \quad \text{and} \quad H_M^{T(2+2\theta)}(D) = \left[H_M^{T(2)}(D), H_M^{T(4)}(D) \right]_{\theta,2},$$

with equivalence of norms. Given that the inclusions in Lemma 5.12 are actually continuous embeddings and $H_M^{T(0)}(D) = L_M^2(D)$, it follows that

$$\left[L_M^2(D), \tilde{H}_M^{2,\text{mix}}(D) \right]_{\theta,2} \subset H^{T(2\theta)} \quad \text{and} \quad \left[\tilde{H}_M^{2,\text{mix}}(D), \tilde{H}_M^{4,\text{mix}}(D) \right]_{\theta,2} \subset H_M^{T(2+2\theta)}(D),$$

with continuous embedding. Since whenever $m > 1 + \frac{d}{2}$ we have that $H_M^{T(m)}(D) \subset \mathcal{B}_1$, defining $\tilde{H}_M^{m,\text{mix}}(D)$ as the interpolation space appearing on the left-hand side of the corresponding inclusion above if $m \in (0, 2)$ or $m \in (2, 4)$ and as $L_M^2(D)$ if $m = 0$ is an appealing idea, for then we can simply state that

$$m > 1 + \frac{2}{d} \implies \tilde{H}_M^{m,\text{mix}}(D) \subset \mathcal{B}_1.$$

6. CONCLUSIONS AND DIRECTIONS FOR FUTURE WORK

We proved the well-posedness (Theorem 3.2) and convergence (Theorem 4.3 and Theorem 4.5) of two greedy algorithms, which seek approximations to solutions of high-dimensional and degenerate Fokker–Planck equations using a separated representation procedure. We then gave sufficient conditions on the true solution of the equation for the fast-convergence of the approximations given by those algorithms; first, in terms of summability of Fourier coefficients (Theorem 5.4), and then, in terms of regularity (Theorem 5.13). In the process of proving these main results, a number of auxiliary results were proved, some of which are of interest in their own right; e.g., function spaces with tensor-product weights inherit compact embedding (Lemma 2.2) and density (Corollary 4.4) properties from the spaces corresponding to the weights that appear as factors of the tensor product weight; the existence of elliptic regularity results for single-spring degenerate elliptic problems (particularly Lemma 5.10); and eigenvalue asymptotics in the same degenerate setting (Lemma C.3 in Appendix C).

The greedy algorithms described in Section 3 are abstract. They entail obtaining the true minima of functionals in nonlinear manifolds embedded in infinite-dimensional function spaces (cf. (3.3) and (3.4)). Any practical implementation of the separated representation strategy must then introduce a discretization (e.g., by a finite element method or a spectral method) and a procedure for the approximation of those minima in the resulting discretized manifolds (e.g., an alternating direction scheme, Newton iteration, etc.). The mathematical analysis of the effects of the discretization and the use of approximate minimization algorithms on the convergence of the greedy algorithms is the subject of ongoing research. On a related note, we are also interested in the implementation of the combination of the separated representation strategy and the alternating direction scheme described in (1.14) and (1.15) in order to approximate the full Fokker–Planck equation (1.4). Further up in model complexity is the coupling between the full Fokker–Planck equation and the Navier–Stokes equations for the velocity and pressure of an incompressible solvent, which is also of interest to us. The Navier–Stokes–Fokker–Planck system is a fully coupled macro-micro system, since the configuration probability density function given by the Fokker–Planck equation feeds into the Navier–Stokes equations a contribution to the extra-stress tensor while the Navier–Stokes velocity field enters in the Fokker–Planck equation (cf. [BCAH87, §15.2]). An important property of the full Fokker–Planck equation is that its solution is almost everywhere nonnegative and has unit integral over the configuration space D (i.e., it is a probability density function) at almost every point in time t and space \mathbf{x} if the initial condition has those properties. It is of interest to learn whether the separated representation strategy can be adapted to give approximations that also preserve the property of being a probability density function.

The generalization of our results to other tensor-product-based high-dimensional PDEs is also of interest. In particular, the adaptation of the separated representation strategy to the Fokker–Planck equations for the configuration of *bead-rod* polymer chains (see, e.g., [BCAH87, §11.3]) is of relevance; these models are not covered by our arguments, at least not in their present form.

APPENDIX A. BASIC RESULTS FOR SOBOLEV SPACES WEIGHTED WITH CPAIL MAXWELLIANS

We shall derive some key properties of the function spaces associated with the CPAIL force model (1.3), with parameter $b \geq 3$, using the corresponding properties of the function spaces associated with the FENE force model (1.2), with parameter $2b/3$.

Let $b \geq 3$. It follows from (1.2), (1.3) and (1.5) that the Maxwellian M_C associated to a spring obeying the CPAIL model with parameter b and the Maxwellian M_F associated to a spring obeying the FENE model with parameter $2b/3$ are, respectively,

$$M_C(\mathbf{p}) = Z_C \exp(-|\mathbf{p}|^2/6) \left(1 - \frac{|\mathbf{p}|^2}{b}\right)^{b/3}, \quad \mathbf{p} \in D_C = B(0, \sqrt{b}) \subset \mathbb{R}^d$$

and

$$M_F(\mathbf{p}) = Z_F \left(1 - \frac{|\mathbf{p}|^2}{2b/3}\right)^{b/3}, \quad \mathbf{p} \in D_F = B(0, \sqrt{2b/3}) \subset \mathbb{R}^d,$$

where Z_C and Z_F are positive constants whose specific values are of no particular relevance below. Let us denote by T the invertible map $\mathbf{p} \in D_C \mapsto \sqrt{2/3}\mathbf{p} \in D_F$. On defining $\tilde{M}: D_C \rightarrow \mathbb{R}$ via $\tilde{M} := M_F \circ T$ we find that there exist positive constants c_1 and c_2 such that $c_1 \tilde{M} \leq M_C \leq c_2 \tilde{M}$. This implies that $H_{M_C}^1(D_C)$ and $H_{\tilde{M}}^1(D_C)$ (the latter is well-defined since \tilde{M}^{-1} inherits from M_C^{-1} its $L_{\text{loc}}^1(D_C)$ regularity—thereby falling under the hypotheses of [KO84, Theorem 1.11]) are algebraically and topologically the same space. The same is true of the pairs of spaces given by $L_{M_C}^2(D_C)$ and $L_{\tilde{M}}^2(D_C)$ and $H(M_C; D_C)$ and $H(\tilde{M}; D_C)$.

Now, T and T^{-1} are $[C^\infty(\overline{D_C})]^d$ and $[C^\infty(\overline{D_F})]^d$ functions, respectively. Then, an argument analogous to Lemma B.3 leads to the fact that the composition with T^{-1} is a well-defined, invertible, linear and bounded operator between $H_{\tilde{M}}^1(D_C)$ and $H_{M_F}^1(D_F)$ and also between $L_{\tilde{M}}^2(D_C)$ and $L_{M_F}^2(D_F)$, and its inverse is the composition with T . By (2.3), composition with T^{-1} is also such an operator between $H(D_C; \tilde{M})$ and $H(D_F; M_F)$ having as its inverse the composition with T .

We can thus use the connection between the M_F -weighted spaces and the \tilde{M} -weighted spaces and the connection between the latter and the M_C -weighted spaces to state that

$$H_{M_F}^1(D_F) \Subset L_{M_F}^2(D_F) \implies H_{M_C}^1(D_C) \Subset L_{M_C}^2(D_C)$$

and

$$\overline{C_0^\infty(D_F)}^{H(D_F; M_F)} = H(D_F; M_F) \implies \overline{\{f \circ T: f \in C_0^\infty(D_F)\}}^{H(D_C; M_C)} = H(D_C; M_C).$$

As $2b/3 \geq 2$, the statements on the left-hand side of the above implications hold (as noted in Remark 3 and Remark 5); consequently, so do the statements on each right-hand side. By noting that, on account of its infinite differentiability, the composition with T maps $C_0^\infty(D_F)$ into $C_0^\infty(D_C)$ and that M_C itself is a $C^\infty(D_C)$ function, we have proved the following lemma.

Lemma A.1. *Let $M: D \rightarrow \mathbb{R}$ be the Maxwellian associated to a spring obeying the CPAIL force model (1.3) with parameter $b \geq 3$. Then, the compact embedding $H_M^1(D) \Subset L_M^2(D)$ holds; and the set $C_0^\infty(D)$ is dense in $H(D; M)$.*

APPENDIX B. SOME RESULTS ON DISTRIBUTIONS

Throughout this section Ω will denote an open subset of \mathbb{R}^d .

Lemma B.1. *Let $\alpha \in \mathbb{N}_0^d$ and let $f \in L_{\text{loc}}^1(\Omega)$ and $g \in C(\Omega)$ be such that $\partial_\beta f \in L_{\text{loc}}^1(\Omega)$ and $\partial_\beta g \in C(\Omega)$ for all $\beta \leq \alpha$. Then, $\partial_\alpha(fg) \in L_{\text{loc}}^1(\Omega)$ and*

$$\partial_\alpha(fg) = \sum_{\beta \leq \alpha} \frac{\alpha!}{\beta!(\alpha - \beta)!} \partial_\beta f \partial_{\alpha - \beta} g, \quad (\text{B.1})$$

where the convention $\gamma! = \prod_{i \in [d]} \gamma_i!$ for all $\gamma \in \mathbb{N}_0^d$ has been followed.

Proof. The result is obviously true for $\alpha = (0, \dots, 0)$. Then, in the $|\alpha| = 1$ case, the result is stated under the assumption of $f, g, \partial_\alpha f, \partial_\alpha g, fg$ and $f\partial_\alpha g + g\partial_\alpha f$ being members of $L^1_{\text{loc}}(\Omega)$ (which is clearly implied by our hypotheses) in the discussion that follows Theorem 7.4 of [GT01]. The final result follows from standard combinatorial arguments and an induction procedure. \square

The purpose of the following lemma is to formulate a result analogous to Theorem 3.41 of [AF03] for weighted Sobolev spaces without resorting to density arguments, which may be unavailable for one or both of the weighted Sobolev spaces being connected.

Lemma B.2. *Let T be an invertible $C^\infty(\bar{\Omega})$ transformation with codomain $\tilde{\Omega}$ and let $f \in L^1_{\text{loc}}(\Omega)$ be such that its distributional derivatives are in $L^1_{\text{loc}}(\Omega)$ up to the order $\alpha \in \mathbb{N}^d$. Then,*

$$\partial_\alpha(f \circ T^{-1}) = \sum_{1 \leq |\beta| \leq |\alpha|} M_{\alpha,\beta}(\partial_\beta f \circ T^{-1}) \in L^1_{\text{loc}}(\tilde{\Omega}), \quad (\text{B.2})$$

where $M_{\alpha,\beta}$ is a polynomial of degree not exceeding $|\beta|$ in derivatives of orders not exceeding $|\alpha|$ of the various components of T^{-1} .

Proof. Let S denote the inverse of T and let S_k denote the its k -th component. From Theorem 6.1.2 in [Hör83] and the remark that follows it we know, first, that there exists a unique continuous linear map $S^*: \mathcal{D}'(\Omega) \rightarrow \mathcal{D}'(\tilde{\Omega})$ whose restriction to $C(\Omega)$ is $u \mapsto u \circ S$ and, second, that the chain rule,

$$\partial_j S^* u = \sum_{k=1}^d \partial_j S_k S^* \partial_k u$$

holds in $\mathcal{D}'(\tilde{\Omega})$. It is easy to see (either directly or from the proof of Theorem 6.1.2 of [Hör83]) that $S^* u$ has the explicit form

$$S^* u(\varphi) = u((\varphi \circ T) |\det(\nabla T)|) \quad \forall \varphi \in C_0^\infty(\tilde{\Omega}).$$

For a regular distribution such as f the above characterization and the change of variable formula for integrable functions (see, e.g., [Bog07, Theorem 3.7.1]) makes $S^* f$ precisely the regular distribution associated with the $L^1_{\text{loc}}(\tilde{\Omega})$ function $f \circ S$. Similarly, $S^* \partial_k f$ will be the regular distribution associated with the $L^1_{\text{loc}}(\tilde{\Omega})$ function $\partial_k f \circ S$. Hence, $\partial_j(f \circ T^{-1}) = \sum_{k=1}^d \partial_j S_k \partial_k f \circ S$ and (B.2) is proved for $|\alpha| = 1$. An induction argument then establishes (B.2) in the general case. \square

Lemma B.3. *Let $\tilde{\Omega}$ and T be as in Lemma B.2 and let w be a weight function defined on Ω . Then, $f \in H_w^m(\Omega)$ if, and only if, $f \circ T^{-1} \in H_w^m(\tilde{\Omega})$ and there exist positive constants $c_1(m)$ and $c_2(m)$ such that*

$$c_1 \|f \circ T^{-1}\|_{H_w^m(\tilde{\Omega})} \leq \|f\|_{H_w^m(\Omega)} \leq c_2 \|f \circ T^{-1}\|_{H_w^m(\tilde{\Omega})},$$

where $\tilde{w} = w \circ T^{-1}$.

Proof. We use Lemma B.2 to replace the first part of the proof of Theorem 3.41 of [AF03]. Then, the rest of that proof, *mutatis mutandis*, carries over to our case. \square

APPENDIX C. EIGENVALUE ASYMPTOTICS FOR ORNSTEIN-UHLENBECK OPERATORS WITH FENE AND CPAIL POTENTIALS VIA THE LIOUVILLE TRANSFORMATION

Lemma C.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded and convex domain of class C^3 and let $w \in C^2(\Omega)$ be a positive function such that $C_0^2(\Omega)$ is dense in $H_w^1(\Omega)$ and $H_w^1(\Omega) \Subset L_w^2(\Omega)$. We further assume that*

- (1) $\inf_{\mathbf{p} \in \Omega} Q_1(\mathbf{p}) > -\infty$, or
- (2) there exists a $\Theta > 0$ such that $\gamma_\Theta := \inf_{\mathbf{p} \in \Omega} \mathfrak{d}(\mathbf{p})^2 Q_\Theta(\mathbf{p}) \in (-1/4, 0]$,

where $Q_\Theta := \Theta - w^{-1/2} \operatorname{div}(w \nabla w^{-1/2})$ and \mathfrak{d} is the distance-to-the-boundary function in Ω .

Let $(\lambda_n)_{n \in \mathbb{N}}$ be the (ordered, with repetitions according to multiplicity) sequence of eigenvalues of the problem: Find $\lambda \in \mathbb{R}$ and $u \in H_w^1(\Omega) \setminus \{0\}$ such that

$$\langle u, v \rangle_{H_w^1(\Omega)} = \lambda \langle u, v \rangle_{L_w^2(\Omega)} \quad \forall v \in H_w^1(\Omega). \quad (\text{C.1})$$

Then, there exist positive numbers c_1 and c_2 and a natural number n_0 such that

$$n \geq n_0 \implies c_1 n^{2/d} \leq \lambda_n \leq c_2 n^{2/d}. \quad (\text{C.2})$$

Proof. Let, for $\Theta > 0$, $(\lambda_{\Theta,n})_{n \in \mathbb{N}}$ be the (ordered, with repetitions according to multiplicity) sequence of eigenvalues of the shifted problem: Find $\lambda^\Theta \in \mathbb{R}$ and $u \in H_w^1(\Omega) \setminus \{0\}$ such that

$$\langle u, v \rangle_{H_w^1(\Omega), \Theta} := \langle \nabla u, \nabla v \rangle_{[L_w^2(\Omega)]^d} + \Theta \langle u, v \rangle_{L_w^2(\Omega)} = \lambda^\Theta \langle u, v \rangle_{L_w^2(\Omega)} \quad \forall v \in H_w^1(\Omega). \quad (\text{C.3})$$

By the hypotheses of the lemma the existence and the accumulation at ∞ only of the $\lambda_{\Theta,n}$ is guaranteed via Lemma 5.1. It further follows from the spectral theory of self-adjoint compact operators that $\lambda_{\Theta,n}$ can be characterized by the Courant–Fischer–Weyl min-max principle:

$$\lambda_{\Theta,n} = \min_{\substack{\dim(S)=n \\ S \subset H_w^1(\Omega)}} \max_{z \in S \setminus \{0\}} \frac{\langle z, z \rangle_{H_w^1(\Omega), \Theta}}{\langle z, z \rangle_{L_w^2(\Omega)}} = \inf_{\substack{\dim(S)=n \\ S \subset C_0^2(\Omega)}} \sup_{z \in S \setminus \{0\}} \frac{\langle z, z \rangle_{H_w^1(\Omega), \Theta}}{\langle z, z \rangle_{L_w^2(\Omega)}}, \quad (\text{C.4})$$

the second equality being a consequence of the density of $C_0^2(\Omega)$ in $H_w^1(\Omega)$ (cf. [Dav95, Theorem 4.5.3]). Note that when $\Theta = 1$ the problem (C.3) and the problem (C.1) coincide (and so do the sequences $(\lambda_{\Theta,n})_{n \in \mathbb{N}}$ and $(\lambda_n)_{n \in \mathbb{N}}$).

Let $L := w^{-1/2} \in C^2(\Omega)$, let z be an arbitrary $C_0^2(\Omega)$ function and let $y := L^{-1}z$. Then,

$$\begin{aligned} \|z\|_{H_w^1(\Omega), \Theta}^2 &= \int_{\Omega} \left(|\nabla(Ly)|^2 + \Theta(Ly)^2 \right) L^{-2} \\ &= \int_{\Omega} |\nabla y|^2 + \int_{\Omega} \left(\Theta + L^{-2} |\nabla L|^2 \right) y^2 + \int_{\Omega} L^{-1} \nabla L \cdot \nabla(y^2) \\ &= \int_{\Omega} |\nabla y|^2 + \int_{\Omega} \left(\Theta + L^{-2} |\nabla L|^2 \right) y^2 - \int_{\Omega} \operatorname{div}(L^{-1} \nabla L) y^2 \\ &= \int_{\Omega} |\nabla y|^2 + \int_{\Omega} [\Theta - L \operatorname{div}(L^{-2} \nabla L)] y^2 \\ &= \int_{\Omega} |\nabla y|^2 + \int_{\Omega} Q_\Theta y^2. \end{aligned}$$

Similarly, $\|z\|_{L_w^2(\Omega)}^2 = \|y\|_{L^2(\Omega)}^2$. As $z \in C_0^2(\Omega)$ is arbitrary and $z \mapsto L^{-1}z$ is a bijection of $C_0^2(\Omega)$ into itself, (C.4) begets

$$\lambda_{\Theta,n} = \inf_{\substack{\dim(S)=n \\ S \subset C_0^2(\Omega)}} \sup_{y \in S \setminus \{0\}} \frac{\|\nabla y\|_{[L^2(\Omega)]^d}^2 + \int_{\Omega} Q_\Theta y^2}{\|y\|_{L^2(\Omega)}^2}.$$

If condition (1) holds, there must exist a $\Theta > 0$ such that $Q_\Theta \geq 0$ in Ω . For such a Θ , of course, $\int_{\Omega} Q_\Theta y^2 \geq 0$. On the other hand, if condition (2) is met, then with the particular Θ given in the condition we have that

$$\int_{\Omega} Q_\Theta y^2 \geq \gamma_\Theta \int_{\Omega} \frac{y^2}{\mathfrak{d}^2} \geq \frac{\gamma_\Theta}{4} \|\nabla y\|_{[L_w^2(\Omega)]^d}^2,$$

the last inequality being a multi-dimensional Hardy inequality (see, e.g., [MMP98, Theorem 11], bearing in mind that γ_Θ has been assumed to be nonpositive). In either case, we can write

$$\lambda_{\Theta,n} \geq \inf_{\substack{\dim(S)=n \\ S \subset C_0^2(\Omega)}} \sup_{y \in S \setminus \{0\}} \frac{\alpha \|\nabla y\|_{[L^2(\Omega)]^d}^2}{\|y\|_{L^2(\Omega)}^2}, \quad (\text{C.5})$$

where

$$0 < \alpha := \begin{cases} 1 & \text{if condition (1) holds,} \\ (1 + \gamma_\Theta/4) & \text{if condition (2) holds.} \end{cases}$$

The C^3 regularity of $\partial\Omega$ implies the existence of an $\varepsilon_0 \in (0, 1)$ such that for each $\varepsilon \in (0, \varepsilon_0)$ there exists a subdomain $\Omega_\varepsilon \Subset \Omega$ that is also of class C^3 and has measure $(1 - \varepsilon)|\Omega|$. Fixing $\varepsilon \in (0, \varepsilon_0)$, the fact that the extensions by zero of functions in $C_0^2(\Omega_\varepsilon)$ form a subspace of $C_0^2(\Omega)$ and (C.4) imply that the eigenvalues of the unshifted problem (C.1) can be bounded from above according to

$$\lambda_n \leq \inf_{\substack{\dim(S)=n \\ S \subset C_0^2(\Omega_\varepsilon)}} \sup_{z \in S \setminus \{0\}} \frac{\langle z, z \rangle_{H_w^1(\Omega_\varepsilon)}}{\langle z, z \rangle_{L_w^2(\Omega_\varepsilon)}}. \quad (\text{C.6})$$

Now, the right-hand side of (C.5) and the right-hand side of (C.6) are precisely the n -th eigenvalue associated with the (variational form of the) problem

$$-\alpha \Delta y = \mu y \quad \text{in } \Omega, \quad y = 0 \quad \text{on } \partial\Omega$$

and the problem

$$-\operatorname{div}(w \nabla y) + w y = \nu w y \quad \text{in } \Omega_\varepsilon, \quad y = 0 \quad \text{on } \partial\Omega_\varepsilon,$$

respectively. These standard eigenvalue problems obey Weyl's law (this results from the fairly general Theorem 2.4 of [Cla67] with input from the regularity result in [Bro61, Theorem 2.4]—alternatively, see [CH53, §VI.4.4]); that is,

$$\lim_{\mu \rightarrow \infty} \frac{\#\{n \in \mathbb{N} : \mu_n \leq \mu\}}{\mu^{d/2}} = \frac{\alpha^{-d/2} |\Omega|}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} = \alpha^{-d/2} C > 0, \quad (\text{C.7a})$$

$$\lim_{\nu \rightarrow \infty} \frac{\#\{n \in \mathbb{N} : \nu_n \leq \nu\}}{\nu^{d/2}} = \frac{|\Omega_\varepsilon|}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} = (1 - \varepsilon) C > 0, \quad (\text{C.7b})$$

where $C := |\Omega| ((2\sqrt{\pi})^d \Gamma(1 + d/2))^{-1}$. Particularizing these limits to $\mu = \mu_n$ and $\nu = \nu_n$ they turn into statements about the rate of growth of the eigenvalues themselves, as opposed to the counting functions. That is,

$$\lim_{n \rightarrow \infty} \mu_n / n^{2/d} = \alpha C^{-2/d} \quad \text{and} \quad \lim_{n \rightarrow \infty} \nu_n / n^{2/d} = (1 - \varepsilon)^{-2/d} C^{-2/d}.$$

From the definition of the shifted eigenvalue problem (C.3), for any Θ , it is immediate that $\lambda_{\Theta, n} = \lambda_n + \Theta - 1$ for all $n \in \mathbb{N}$. We then deduce, via the inequalities (C.5) and (C.6), that the asymptotic bounds (C.2) hold. \square

Remark 10.

- (1) It follows from the proof of Lemma C.1 that, if condition (1) holds, the constants c_1 and c_2 of (C.2) can be taken arbitrarily close to $C^{-2/d}$ and, consequently, to each other.
- (2) One might relax the condition of convexity of the domain in Lemma C.1 at the possible cost of having a stricter lower bound for γ_Θ in condition (2), as the constant for the Hardy inequality might deteriorate. The C^3 regularity condition on the domain can be drastically relaxed (see, for example [BS70]); however, the literature tends to force one to choose at most two among readability, the size of the class of problems covered, and frugality in terms of hypotheses. For our purposes, the statement in Lemma C.1 suffices.

Corollary C.2. *The eigenvalues of the eigenvalue problem (5.7) associated with both the FENE model (1.2) and the CPAIL model (1.3) obey (C.2) if their parameter b_i is greater than 2 and 3, respectively.*

Proof. We shall apply Lemma C.1. For both the FENE and CPAIL models the domains (being balls) and their associated Maxwellian weights are regular enough. The compact embedding and density hypotheses are satisfied in the parameter ranges under consideration (cf. Hypothesis B, Remark 3, Remark 5 and (2.3)). It only remains to prove condition (1) or condition (2).

From (1.2) and (1.5) it follows that the Maxwellian associated to the FENE potential is

$$M_i(\mathbf{p}) = Z_i^{-1} (1 - |\mathbf{p}|^2/b_i)^{b_i/2}, \quad \mathbf{p} \in B(0, \sqrt{b_i}), \quad (\text{C.8})$$

where Z_i is a positive constant. A direct calculation returns that with this weight Q_Θ is

$$Q_\Theta(\mathbf{p}) = \Theta + \left(\frac{1}{4} - \frac{1}{b_i}\right) |\mathbf{p}|^2 \left(1 - \frac{|\mathbf{p}|^2}{b_i}\right)^{-2} - \frac{d}{2} \left(1 - \frac{|\mathbf{p}|^2}{b_i}\right)^{-1}.$$

In this form, it is readily apparent that Q_1 is bounded from below in its domain $B(0, \sqrt{b_i})$ (i.e., (1) holds) if $b_i > 4$. From the fact that $\mathfrak{d}(\mathbf{p}) = \sqrt{b_i} - |\mathbf{p}|$ for all \mathbf{p} in the domain under consideration it is easy to see that $\mathfrak{d}^2 Q_\Theta$ is always bounded from below and uniformly continuous up to the boundary. If $b_i \in (2, 4]$, Q_Θ is never bounded from below, so it takes negative values and thus the infimum of $\mathfrak{d}^2 Q_\Theta$ is strictly less than zero. As \mathfrak{d}^2 is continuous and positive within the domain yet zero at its boundary, the existence of a Θ that makes case (2) hold is equivalent to demanding that

$$\lim_{|\mathbf{p}| \rightarrow \sqrt{b_i}-} \mathfrak{d}(\mathbf{p})^2 Q_1(\mathbf{p}) \in (-1/4, 0].$$

As in the range $b_i \in (2, 4]$ that limit is $b_i(b_i/4 - 1)/4$ we see that the condition (2) holds there.

Analogously, (1.3) and (1.5) imply that the Maxwellian associated to the CPAIL potential is

$$M_i(\mathbf{p}) = Z_i^{-1} \exp(-|\mathbf{p}|^2/6) (1 - |\mathbf{p}|^2/b_i)^{b_i/3}, \quad \mathbf{p} \in B(0, \sqrt{b_i}), \quad (\text{C.9})$$

with Z_i a positive constant. Again, a direct calculation yields

$$Q_\Theta(\mathbf{p}) = \Theta - \frac{d}{6} + \frac{|\mathbf{p}|^2}{36} + \left(\frac{1}{9} - \frac{2}{3b_i}\right) |\mathbf{p}|^2 \left(1 - \frac{|\mathbf{p}|^2}{b_i}\right)^{-2} - \left(\frac{d}{3} - \frac{|\mathbf{p}|^2}{9}\right) \left(1 - \frac{|\mathbf{p}|^2}{b_i}\right)^{-1}.$$

By arguments similar to those given when considering the FENE potential, we have that condition (1) holds if $b_i > 6$ or if $b_i = 6$ and $d = 2$; and that condition (2) holds if $b_i \in (3, 6]$. \square

If two weights w and \tilde{w} defined on a domain Ω are comparable—that is, there exist two positive constants c_1 and c_2 such that $c_1 w \leq \tilde{w} \leq c_2 w$ —a number of consequences follow immediately. As discussed elsewhere, $L_w^2(\Omega)$ and $L_{\tilde{w}}^2(\Omega)$ on the one hand and $H_w^1(\Omega)$ and $H_{\tilde{w}}^1(\Omega)$ on the other will be one and the same algebraically and topologically. In particular, the hypotheses of Lemma 5.1 will be met by the eigenvalue problem

$$\langle e, v \rangle_{H_w^1(\Omega)} = \lambda \langle e, v \rangle_{L_w^2(\Omega)} \quad \forall v \in H_w^1(\Omega)$$

if, and only if, they are met by the eigenvalue problem

$$\langle e, v \rangle_{H_{\tilde{w}}^1(\Omega)} = \tilde{\lambda} \langle e, v \rangle_{L_{\tilde{w}}^2(\Omega)} \quad \forall v \in H_{\tilde{w}}^1(\Omega).$$

The inf-sup characterization (cf. (C.4)) of the successive eigenvalues of both problems allow for the bounds

$$\frac{c_1}{c_2} \lambda_n \leq \tilde{\lambda}_n \leq \frac{c_2}{c_1} \lambda_n.$$

That is, the bounds (C.2) will hold for one set of eigenvalues if, and only if, they hold for the other. This allows for establishing the following sufficiency condition for weights defined on two- or three-dimensional balls, which is in most cases much easier to test than the conditions of Lemma C.1.

Lemma C.3. *Let Ω be an open ball in two or three dimensions and let w be a positive and continuous weight defined on Ω with the property*

$$\sigma_1 \mathfrak{d}(\mathbf{p})^\alpha \leq w(\mathbf{p}) \leq \sigma_2 \mathfrak{d}(\mathbf{p})^\alpha$$

for all $\mathbf{p} \in \Omega$ such that $\mathfrak{d}(\mathbf{p}) < \delta$, for some exponent $\alpha > 1$, for some margin $\delta > 0$ and some positive constants σ_1 and σ_2 .

Then, the eigenvalues of the problem

$$\langle e, v \rangle_{H_w^1(\Omega)} = \lambda \langle e, v \rangle_{L_w^2(\Omega)} \quad \forall v \in H_w^1(\Omega)$$

obey the two-sided bounds (C.2).

Proof. If the radius of the ball happens to be $\sqrt{2\alpha}$ the conditions on w force it to be comparable to the FENE Maxwellian (C.8) and so the result follows from the above discussion. Otherwise, one just needs to rescale the domain; this will effect a fixed linear transformation on the eigenvalues, but will not affect the validity of the bounds (C.2) (the constants involved will change, though). \square

Remark 11. The eigenvalue problem (5.7) associated with either the FENE or the CPAIL model falls within what is called *weak degeneracy* case in the Russian spectral theory literature; i.e., problems of the form: Given $\Omega \subset \mathbb{R}^d$, find $(\lambda, u) \in \mathbb{R} \times (H_{\mathfrak{D}\alpha}^1(\Omega) \setminus \{0\})$ such that

$$\int_{\Omega} (A \nabla u \cdot \nabla v + h u v) \mathfrak{D}^\alpha = \lambda \int_{\Omega} b u v \mathfrak{D}^\beta \quad \forall v \in H_{\mathfrak{D}\alpha}^1(\Omega), \quad (\text{C.10})$$

where $\alpha - \beta < 2/d$ (see [VS74, §1] for the precise statement, which includes additional conditions on Ω , A , h , b , α and β). As, in the FENE and CPAIL versions of (5.7), the same weight (the associated Maxwellian) appears in both the left- and right-hand side bilinear forms, and, in both cases, that weight is bounded from above and below by powers of \mathfrak{D} (cf. (C.8), (C.9)), it turns out that our problem is equivalent to a problem of the form (C.10) with $\alpha - \beta = 0$.

The result, according to [VS74, Theorem 1.1] and assuming that $b \geq 0$ is that

$$\lim_{\lambda \rightarrow \infty} \lambda^{-d/2} \#\{n \in \mathbb{N} : \lambda_n < \lambda\} = \frac{1}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} \int_{\Omega} \frac{\mathfrak{D}^{-(\alpha-\beta)d/2} b^{d/2}}{\sqrt{\det(A)}} \quad (\text{C.11})$$

(compare this with (C.7); note also that in [VS74] the statement is made in terms of what in our notation is $1/\lambda$). The problem with this particular source is that, for a proof, it remits the reader to either one of two publications. The first, [BS72] proves related yet not directly applicable results—there is a gap that needs to be bridged by means, perhaps elementary, that are unknown to us. We have not been able to get hold of the second, [Taš75] by G. M. Taščijan (also romanized as Tashchiyan). However, the latter is also cited in [Taš81, Theorem 1], where a generalization of (C.11) is proved, under the condition (in our notation) $d > 2$.

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