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 $D = D_1 \times \cdots \times D_N$ contained in $\mathbb{R}^{Nd}$, where each set $D_i$, $i = 1, \ldots, N$, is a bounded open ball in $\mathbb{R}^d$, $d = 2, 3$.

**Keywords** Nonlinear approximation · Greedy algorithm · Fokker–Planck equation

**Mathematics Subject Classification** 65N15 · 65D15 · 41A63 · 41A25

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 [2–4, 16, 24], 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 [30]. A similar method was considered independently by Nouy [33, 34] and Nouy and Le Maître [35] 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 [38]. 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 $\Omega_x$ and $\Omega_y$ 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 [29], by drawing on connections with greedy algorithms from nonlinear approximation theory (cf. DeVore and Temlyakov [21]). In [29], the solution was represented as a sum

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

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 $H^1_0(\Omega)$ 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 [15] by Cancès, Ehrlacher 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 [29] crucially rely on the fact that the Laplace operator is self-adjoint, and as noted by the authors of [29], 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 [29] 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 aims to address: 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 \( \Omega \times D \), where \( \Omega \subset \mathbb{R}^d \), \( d = 2, 3 \), is the physical (flow) domain, and the configuration space \( D \) is the \( N \)-fold Cartesian product \( \prod_{i=1}^{N} D_i \) of sets \( D_i \subset \mathbb{R}^d \), \( i = 1, \ldots, N \), \( N \geq 2 \), 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). Proceeding as in [5–9], we rewrite the Ornstein–Uhlenbeck operator, a non-self-adjoint elliptic operator with respect to
the configuration space variable \( q \) featuring in the Fokker–Planck equation whose drift term contains an unbounded potential, acting on the probability density function \( \psi \), as a degenerate, but now self-adjoint, elliptic operator on a Maxwellian-weighted Sobolev space, acting of \( \psi/M \), where \( M \) is the associated Maxwellian that vanishes on \( \partial D \). We then perform a nonlinear approximation of the analytical solution \( \psi: (q_1, \ldots, q_N) \in D \mapsto \psi(q_1, \ldots, q_N) \) to this high-dimensional degenerate elliptic boundary-value problem on the appropriate Maxwellian-weighted Sobolev space by separated representations of the form

\[
\sum_{k=1}^{K} \prod_{i=1}^{N} \psi_{k}^{(i)}(q_i),
\]

where the factors \( \psi_{k}^{(i)} \), \( k = 1, \ldots, K \), are defined on the \( d \)-dimensional domain \( D_i \), \( i = 1, \ldots, N \). Instead of being selected from an \textit{a priori} fixed set, the factors \( \psi_{k}^{(i)} \), \( i = 1, \ldots, N \), are obtained, \( N \) at a time, for each \( k \in \{1, \ldots, K\} \), as the best approximation (in a sense to be made precise in Sect. 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 Sect. 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 \( D \). Section 3 is devoted to the description of a separated representation strategy for the problem, in the spirit of Le Bris et al. [29]. Following [29], 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 [21]. In Sect. 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 Sect. 6, we provide some conclusions and possible directions for further work.

At an abstract level, our convergence proof follows the arguments in [29]; 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 [29]. The former is mostly based on tensorizing the corresponding results for the function spaces associated with the single-spring case (i.e., the \textit{dumbbell}) and the latter relies on Hardy-type inequalities 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 Sect. 5 and Appendix, respectively.

We state the structural hypotheses restricting the class of bead–spring chain models amenable to our analysis (hypotheses A, B, C and D on pages 584, 599, 603 and 605, respectively) as they are needed in the text. Once introduced, each hypothesis is assumed to hold in the rest of the paper, except when explicitly stated otherwise.

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 \(q = (q_1, \ldots, q_N) \in D_1 \times \cdots \times D_N = \times_{i \in [N]} D_i =: D\). 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

\[
q \in D \mapsto \prod_{i \in [N]} f_i(q_i).
\]

We extend this notation in three ways. First, as the tensor-product operation is order-dependent, we will use subscripts on the \(\otimes\) and the \(\bigotimes\) signs to denote where on \(q \in D\) the function, or functions, following them act; e.g., \(\bigotimes_{i \in [N]\backslash\{j\}} f_i \otimes j f_j\) evaluated on \(q \in D\) is \(f_j(q_j) \prod_{i \in [N]\backslash\{j\}} f_i(q_i)\). Second, 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 \(\bigotimes_{i \in [N]} F_i := \{\prod_{i \in [N]} f_i : f_i \in F_i, \ i \in [N]\}\). Third, 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 \(\equiv\) 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 \(L^2_w(E)\) the Lebesgue space of square-integrable functions with respect to the weight \(w\), equipped with its usual norm,

\[
\|\varphi\|_{L^2_w(E)} := \left(\int_E |\varphi|^2 w\right)^{1/2}.
\]

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

\[
H^m_w(E) := \{\varphi \in L^1_w(E) \cap L^1_{\text{loc}}(E) : \partial^{|\alpha|} \varphi \in L^2_w(E), \ |\alpha| \leq m\},
\]

\[
\|\varphi\|_{H^m_w(E)} := \left(\sum_{|\alpha| \leq m} \|\partial^\alpha \varphi\|_{L^2_w(E)}^2\right)^{1/2} \quad \forall \varphi \in H^m_w(E).
\]

We shall suppose henceforth that \(\Omega\) is a bounded open set in \(\mathbb{R}^d\) with a sufficiently regular (say, Lipschitz continuous) boundary, and denote by \(n_x\) and \(n_{q_i}\) the unit outward normal vector defined (a.e. with respect to the surface measure) on \(\partial \Omega\) and \(\partial D_i\), \(i \in [N]\), respectively.
1.2 Fokker–Planck Equation

The spring forces in the model are given by functions \( F_i : D_i \to \mathbb{R}^d \), which have the form \( F_i(p) = U'_i(|\frac{1}{2} p|^2) \cdot p \), \( p \in D_i := B(0, \sqrt{b_i}) \subset \mathbb{R}^d \), \( b_i > 0 \), \( i \in [N] \), and the \( U_i : [0, b_i/2] \to \mathbb{R} \), the spring potentials, are such that \( U_i(s) \to +\infty \) as \( s \to b_i/2^- \). It follows that \( F_i(-p) = -F_i(p) \) for all \( p \in D_i \). Typical examples include the FENE (Finitely Extensible Nonlinear Elastic) model \([45]\) with

\[
U_i(s) = -\frac{b_i}{2} \ln \left( 1 - \frac{2s}{b_i} \right) \quad \text{and} \quad F_i(q_i) = \frac{1}{1 - |q_i|^2/b_i} q_i, \tag{1.2}
\]

where \( b_i > 0 \) is a parameter, and Cohen’s Padé approximant to the Inverse Langevin (CPAIL) model \([18]\) with

\[
U_i(s) = \frac{s}{3} - \frac{b_i}{3} \ln \left( 1 - \frac{2s}{b_i} \right) \quad \text{and} \quad F_i(q_i) = \frac{1 - |q_i|^2/(3b_i)}{1 - |q_i|^2/b_i} q_i, \tag{1.3}
\]

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 \([28]\)

\[
F_i(q_i) = \frac{\sqrt{b_i}}{3} L^{-1} \left( \frac{|q_i|}{\sqrt{b_i}} \right) q_i,
\]

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 \( \infty \), it follows that the function \( |q_i| \in [0, \sqrt{b_i}) \mapsto L^{-1}(|q_i|/\sqrt{b_i}) \in [0, \infty) \) is strictly monotonic increasing, with a vertical asymptote at \( |q_i| = \sqrt{b_i} \).

Remark 1.1 An important spring force model, which is excluded from our considerations, is the simple Hookean model described by

\[
D_i = \mathbb{R}^d, \quad U_i(s) = s \quad \text{and} \quad F_i(q_i) = q_i.
\]

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 \( \psi \) has the following form (cf. \([5–9]\)):

\[
\frac{\partial \psi}{\partial t} + \text{div}_x(u \psi) + \sum_{i=1}^N \text{div} q_i \left[ (\nabla_x u)q_i \psi - \frac{1}{4Wi} \sum_{j=1}^N A_{ij} (F_j(q_j) \psi + \nabla q_j \psi) \right]
= \frac{(l_0/L_0)^2}{4Wi(N+1)} \Delta_x \psi, \quad (x, q, t) \in \Omega \times D \times (0, T), \tag{1.4a}
\]

with initial and no-flux boundary conditions

\[
\psi(\cdot, \cdot, 0) = \psi_0, \quad (x, q) \in \Omega \times D, \tag{1.4b}
\]
\[
\frac{(l_0/L_0)^2}{4\text{Wi}(N+1)} \nabla_x \psi \cdot n_x = 0, \quad (x, q, t) \in \partial \Omega \times D \times (0, T],
\] (1.4c)

and
\[
\left[ (\nabla_x u) q_i \psi - \frac{1}{4\text{Wi}} \sum_{j=1}^{N} A_{ij} (F_j(q_j) \psi + \nabla_q_j \psi) \right] \cdot n_{q_i} = 0,
\]
i \in [N], (x, q, t) \in \Omega \times \partial D \times (0, T].
\] (1.4d)

Here, \(u : \overline{\Omega} \times [0, T] \to \mathbb{R}^d\) is the flow velocity, \(\text{Wi} := \lambda U_0/L_0\) is the (nondimensional) Weissenberg number, \(l_0\) is the characteristic length-scale of a spring, \(\lambda\) is the characteristic relaxation time of a spring and \(L_0\) and \(U_0\) are the characteristic macroscopic length and velocity, respectively (thus, \(\text{Wi}\) 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 \(\lambda_{\text{min}}\).

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 \(\partial D\).

We define the partial Maxwellians \(M_i\) and the (full) Maxwellian \(M\) by
\[
M_i(p) := Z_i^{-1} \exp \left( -U_i \left( \frac{1}{2} |p|^2 \right) \right), \quad p \in D_i, \ i \in [N];
\] (1.5)
\[
M(q) := \prod_{i=1}^{N} M_i(q_i), \quad q \in D;
\] (1.6)
that is, \(M = \bigotimes_{i \in [N]} M_i\). 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, \(\int_{D} M = 1\). We note that since \(U_i\) is assumed to tend to \(+\infty\) as \(q_i\) approaches \(\partial D_i\), the corresponding partial Maxwellian \(M_i\) tends to 0 as \(q_i\) approaches \(\partial D_i\), \(i \in [N]\); consequently, \(M\) tends to 0 as \(q\) approaches \(\partial D\). 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
\[
F_j(q_j) \psi + \nabla_{q_j} \psi = \psi \nabla_{q_j} U_j \left( \frac{1}{2} |q_j|^2 \right) + \nabla_{q_j} \psi = M \nabla_{q_j} \left( \frac{\psi}{M} \right).
\] (1.7)

Multiplying (1.4a) by \(\psi/M\), using (1.7) and (formally) integrating by parts, the corresponding weak form of (1.4a)--(1.4d) is: Find \(\psi = \psi(x, q, t)\) such that
\[
\int_{\Omega \times D} \left\{ \frac{\partial \psi}{\partial t} \frac{\phi}{M} + \text{div}_x (u \psi) \frac{\phi}{M} - \sum_{i=1}^{N} \left[ (\nabla_x u) q_i \psi - \sum_{j=1}^{N} A_{ij} \frac{4\text{Wi}}{M} \nabla_{q_j} \left( \frac{\psi}{M} \right) \right] \cdot \nabla_{q_i} \left( \frac{\phi}{M} \right) \right\} = 0
\]
\[
+ \frac{(l_0/L_0)^2}{4\text{Wi}(N+1)} \nabla_x \psi \cdot \nabla_x \phi \frac{1}{M}
\] (1.8)

for all \(\phi = \phi(x, q)\) in a suitable function space.
For the sake of convenience we define the following bilinear forms:

\[
\tilde{T}(u; \sigma, \tau) := \int_{\Omega \times D} \operatorname{div}_x(u \sigma) \tau_M, \\
\tilde{K}(\sigma, \tau) := \frac{(l_0/L_0)^2}{4\mathrm{Wi}(N + 1)} \int_{\Omega \times D} \nabla_x \sigma \cdot \nabla_x \tau_M,
\]

\[\tag{1.9}
\]

\[
T(u; \sigma, \tau) := -\int_{\Omega \times D} \sum_{i=1}^{N} (\nabla_x u) q_i \sigma \cdot \nabla q_i \left( \frac{\tau}{M} \right),
\]

\[\tag{1.10}
\]

\[
K(\sigma, \tau) := \int_{\Omega \times D} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} \frac{4\mathrm{Wi}}{M} \nabla q_i \left( \frac{\sigma}{M} \right) \cdot \nabla q_i \left( \frac{\tau}{M} \right).
\]

\[\tag{1.11}
\]

Then, (1.8) can be written concisely as

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

for all \( \varphi = \varphi(x, q) \) in a suitable function space. We note that \( \tilde{T} \) and \( \tilde{K} \) involve partial derivatives of their arguments with respect to the spatial variable \( x \) only. Analogously, \( T \) and \( K \) involve partial derivatives of their arguments with respect to the configuration space variable \( q \) 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 \( \Delta t \) be such that \( M := T/\Delta t \in \mathbb{N} \) and define \( t^n := n\Delta t \) for \( n \in \{0, \ldots, M\} \). We will consider the following alternating-direction semidiscretization of (1.8): We initialize the scheme by defining \( \psi^0 := \psi_0; \) for \( n \in \{0, \ldots, M - 1\} \) and then define the ‘intermediate’ function \( \psi^{n+1/2} \) and the approximation \( \psi^{n+1} \) to \( \psi(t^{n+1}, \cdot, \cdot), \) respectively, by

\[
\left\langle \frac{\psi^{n+1/2} - \psi^n}{\Delta t/2}, \frac{\varphi}{M} \right\rangle + \tilde{T}(u(\cdot, t^{n+1}); \psi^{n+1/2}, \varphi) + \tilde{K}(\psi^{n+1/2}, \varphi)
\]

\[= -T(u(\cdot, t^n); \psi^n, \varphi) - K(\psi^n, \varphi) \quad (1.13a)
\]

and

\[
\left\langle \frac{\psi^{n+1} - \psi^{n+1/2}}{\Delta t/2}, \frac{\varphi}{M} \right\rangle + K(\psi^{n+1}, \varphi)
\]

\[= -T(u(\cdot, t^n); \psi^n, \varphi) - \tilde{T}(u(\cdot, t^{n+1}); \psi^{n+1/2}, \varphi) - \tilde{K}(\psi^{n+1/2}, \varphi), \quad (1.13b)
\]

for all \( \varphi = \varphi(x, q) \) in a suitable function space. In (1.13a) the spatial bilinear forms \( \tilde{T} \) and \( \tilde{K} \) are treated implicitly while the configuration space bilinear forms \( T \) and \( K \) are treated explicitly. In (1.13b) the spatial bilinear forms \( \tilde{T} \) and \( \tilde{K} \) 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 $((q^{(k)}_D, w_{Q\Omega}^{(k)}), (x^{(k)}, w_{\Omega}^{(k)}))_{k \in [Q_D]}$ be $\frac{1}{M}$- and $1$-weighted quadrature rules on $D$ and $\Omega$, respectively. We then approximate (1.13a) by performing numerical integration over the configuration space, which results in

$$
\sum_{k=1}^{Q_D} w_{D}^{(k)} \int_{\Omega} \frac{\psi^{n+1/2}(\cdot, q^{(k)}) - \psi^{n}(\cdot, q^{(k)})}{\Delta t/2} \varphi(\cdot, q^{(k)})
$$

$$
+ \sum_{k=1}^{Q_D} w_{D}^{(k)} \int_{\Omega} \text{div}_{x}(u(\cdot, t^{n+1}) \psi^{n+1/2}(\cdot, q^{(k)})) \varphi(\cdot, q^{(k)})
$$

$$
+ \sum_{k=1}^{Q_D} w_{D}^{(k)} \frac{(l_0/L_0)^2}{4\text{Wi}(N + 1)} \int_{\Omega} \nabla_{x} \psi^{n+1/2}(\cdot, q^{(k)}) \cdot \nabla_{x} \varphi(\cdot, q^{(k)})
$$

$$
\approx \sum_{k=1}^{Q_D} w_{D}^{(k)} \int_{\Omega} \sum_{i=1}^{N} M(q^{(k)})(\nabla_{x} u(\cdot, t^{n})) q^{(k)}_i \psi^{n}(\cdot, q^{(k)}) \cdot \nabla_{q_i} \left(\frac{\varphi}{M}\right) \bigg|_{(\cdot, q^{(k)})}
$$

$$
- \sum_{k=1}^{Q_D} w_{D}^{(k)} \int_{\Omega} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{A_{ij}}{4\text{Wi}} M(q^{(k)}) \nabla q_j \left(\frac{\psi^{n}}{M}\right) \bigg|_{(\cdot, q^{(k)})} \cdot \nabla_{q_i} \left(\frac{\varphi}{M}\right) \bigg|_{(\cdot, q^{(k)})},
$$

for all $\varphi = \varphi(x, q)$ 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 $q \in D$ such that $\zeta_{(m)}(q^{(k)}) = \delta_{km}, k, m \in [Q_D]$, and taking successively $\varphi = \varphi_{(m)}$, where $\varphi_{(m)}(x, q) := \chi(x)\zeta_{(m)}(q)$, in the equality above, we obtain a total of $Q_D$ independent variational problems, each posed over the $d$-dimensional domain $\Omega$, of the form

$$
\frac{1}{\Delta t/2} \int_{\Omega} \psi^{n+1/2}(\cdot, q^{(m)}) \chi + \int_{\Omega} \text{div}_{x}(u(\cdot, t^{n+1}) \psi^{n+1/2}(\cdot, q^{(m)})) \chi
$$

$$
+ \frac{(l_0/L_0)^2}{4\text{Wi}(N + 1)} \int_{\Omega} \nabla_{x} \psi^{n+1/2}(\cdot, q^{(m)}) \cdot \nabla_{x} \chi
$$

$$
\approx \frac{1}{\Delta t/2} \int_{\Omega} \psi^{n}(\cdot, q^{(m)}) \chi
$$

$$
+ \frac{1}{w_{D}^{(m)}} \sum_{k=1}^{Q_D} w_{D}^{(k)} \left[ \int_{\Omega} \sum_{i=1}^{N} M(q^{(k)})(\nabla_{x} u(\cdot, t^{n})) q^{(k)}_i \right.
$$

$$
\times \psi^{n}(\cdot, q^{(k)}) \cdot \nabla_{q_i} \left(\frac{\zeta_{(m)}}{M}\right) \bigg|_{(\cdot, q^{(k)})} \chi
$$

$$
- \int_{\Omega} \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{A_{ij}}{4\text{Wi}} M(q^{(k)}) \nabla q_j \left(\frac{\psi^{n}}{M}\right) \bigg|_{(\cdot, q^{(k)})} \cdot \nabla_{q_i} \left(\frac{\zeta_{(m)}}{M}\right) \bigg|_{(\cdot, q^{(k)})} \chi
$$

$$
=: \mathcal{M}_{(m)}(\psi^{n}; \chi) \quad \forall m \in [Q_D].
$$
for all $\chi = \chi(x)$ in a suitable function space, where each $\mathcal{M}(m)(\psi^n; \cdot)$, $m \in [Q_D]$, is a linear functional. Thus, (1.14) amounts to solving $Q_D$ mutually independent linear convection-diffusion problems over $\Omega$ (see, for example, [25] for further details in this respect).

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

$$
\sum_{k=1}^{Q_D} w^{(k)}_{Q_D} \int_{D} \frac{\psi^{n+1}(x^{(k)}, \cdot) - \psi^{n+1/2}(x^{(k)}, \cdot)}{\Delta t/2} \varphi(x^{(k)}, \cdot) \text{M} \\
- \sum_{k=1}^{Q_D} w^{(k)}_{Q_D} \int_{D} \sum_{i=1}^{N} (\nabla_x u(x^{(k)}, t^n)) q_i \psi^n(x^{(k)}, \cdot) \cdot \nabla_i \left( \frac{\varphi(x^{(k)}, \cdot)}{\text{M}} \right) \\
+ \sum_{k=1}^{Q_D} w^{(k)}_{Q_D} \int_{D} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} \text{M} \nabla_j \left( \frac{\psi^{n+1}(x^{(k)}, \cdot)}{\text{M}} \right) \cdot \nabla_i \left( \frac{\varphi(x^{(k)}, \cdot)}{\text{M}} \right)
$$

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

$$
\frac{1}{\Delta t/2} \int_{D} \psi^{n+1}(x^{(m)}, \cdot) \frac{\zeta}{\text{M}} + \int_{D} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} \text{M} \nabla_j \left( \frac{\psi^{n+1}(x^{(m)}, \cdot)}{\text{M}} \right) \cdot \nabla_i \left( \frac{\zeta}{\text{M}} \right) \\
- \int_{D} \text{div}_x(u(\cdot, t^{n+1}) \psi^{n+1/2}) \left|_{(x^{(m)}, \cdot)} \frac{\zeta}{\text{M}} \right|
$$

$$
\times \psi^n(x^{(m)}, \cdot) \cdot \nabla_i \left( \frac{\zeta}{\text{M}} \right) \\
- \int_{D} \text{div}_x(u(\cdot, t^{n+1}) \psi^{n+1/2}) \left|_{(x^{(m)}, \cdot)} \frac{\zeta}{\text{M}} \right|
$$

$$
- \frac{1}{w^{(m)}_{Q_D}} \sum_{k=1}^{Q_D} w^{(k)}_{Q_D} \frac{(l_0/L_0)^2}{4\text{Wi}(N + 1)} \int_{D} \nabla_x \psi^{n+1/2} \left|_{(x^{(k)}, \cdot)} \cdot \nabla_x \chi_{(m)} \left|_{(x^{(k)}, \cdot)} \frac{\zeta}{\text{M}} \right] \\
=: \mathcal{M}_{(m)}(\psi^{n+1/2}; \zeta) \quad \forall m \in [Q_D],
$$

(1.15)
for all $\zeta = \zeta(q)$ in a suitable function space, where each $\mathfrak{H}_m(\psi^{n+1/2} \cdot), m \in [Q_\Omega]$, 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 $a(\psi, \varphi) := \int_D \sum_{i=1}^N \sum_{j=1}^N A_{ij} M \nabla q_j \left( \frac{\psi}{M} \right) \cdot \nabla q_i \left( \frac{\varphi}{M} \right) + c \int_D \frac{\psi \varphi}{M}, \quad (2.2)$

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

$$H(D; M) := \{ \varphi \in L^2_{1/M}(D) \cap M L^1_{loc}(D) : \nabla q_i (\varphi/M) \in [L^2_{M}(D)]^d \forall i \in [N] \},$$

equipped with the norm

$$\| \varphi \|_{H(D; M)} := \left( \| \varphi \|_{L^2_{1/M}(D)}^2 + \sum_{i=1}^N \| \nabla q_i (\varphi/M) \|_{[L^2_{M}(D)]^d}^2 \right)^{1/2}.$$

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

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

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

Below, 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 $H(D; M)$. That is,

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

equipped with the norm $\| \varphi \|_{H(D_i; M_i)} := (\| \varphi \|_{L^2_{1/M_i}(D_i)}^2 + \| \nabla (\varphi/M_i) \|_{[L^2_{M_i}(D_i)]^d}^2)^{1/2}.$
Remark 2.1

1. For \( i \in [N] \), \( H(D_i; M_i) \) is exactly \( H(D; M) \) if \( N = 1 \) and \( M = M_i \). None of the results involving \( H(D; M) \) appearing below depend on restrictions on \( N \) and thereby remain valid for \( H(D_i; M_i) \). Just like (2.3a), (2.3b), \( \varphi \mapsto M_i \varphi \) is an isometric isomorphism between \( L^2_{M_i}(D_i) \) and \( L^2_{1/M_i}(D_i) \) and between \( H^1_{M_i}(D_i) \) 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 \( H(D; M) \) we fully state the weak formulation of our model problem:

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

\[
\alpha(\psi, \varphi) = f(\varphi) \quad \forall \varphi \in H(D; M).
\] (2.4)

We adopt the following structural hypothesis.

**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 \( \lim_{s \to b_i/2} - U(s) = +\infty \).

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

**Remark 2.2** It is easy to check that springs obeying either of the example force models (1.2) and (1.3) comply with Hypothesis A.

**Lemma 2.3** \( L^2_M(D), H^m_M(D) \) for \( m \in \mathbb{N} \), \( L^2_{1/M}(D) \) and \( H(D; M) \) are separable Hilbert spaces.

**Proof** The operation \( \varphi \in L^2_M(D) \mapsto \varphi/\sqrt{M} \) defines an isometric isomorphism between \( L^2_M(D) \) and \( L^2(D) \). Therefore the first space inherits its separability from the latter. On noting that \( M^{-1} \in L^1_{\text{loc}}(D) \), Theorem 1.11 of [27] 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 [1, Sect. 3.5]. The spaces \( L^2_{1/M}(D) \) and \( H(D; M) \) inherit these properties via the isometric isomorphism (2.3a) and (2.3b). Finally, as their respective norms obey the parallelogram law, these spaces are Hilbert spaces.

**Lemma 2.4** The following inclusion holds: \( C^1_0(D) \subset H(D; M) \).

**Proof** The stated inclusion is a simple consequence of the fact that on any compact subset \( K \) of \( D \) the Maxwellian \( M \) is bounded above and below by positive constants (depending on \( K \)), and by noting the \( C^1 \) regularity of \( M \) on \( D \) implied by Hypothesis A.

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2.2 Properties of Tensor Products

**Lemma 2.5** Suppose that \( T \in \mathcal{D}'(D) \) is a distribution such that

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

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

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 \( \lim_{n \to \infty} R_n^{(i)} = R^{(i)} \) in \( \mathcal{D}'(D_i) \) for \( i \in [N] \), we have

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

**Proof** These are standard results from the theory of distributions, so we omit the proofs and refer the reader to Sect. 1.3.2 of the book of Vladimirov [43], for example.

**Lemma 2.6** The following statements hold:

1. For any ensemble \( r^{(i)} \in H(D_i; M_i), i \in [N], \bigotimes_{j \in [N]} r^{(i)} \in H(D; M) \).
2. Suppose that \( r^{(i)} : D_i \to \mathbb{R} \), \( i \in [N] \), 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) \( \bigotimes_{i \in [N]} r^{(i)} \in H(D; M) \setminus \{0\} \).

**Proof** (1) It is immediate from the factorization of \( M \) that \( \bigotimes_{i \in [N]} r^{(i)} \) belongs to \( L_{1/M}^{2}(D) \). Thanks to Lemma 2.5, the identity

\[
\nabla q_j \left( \frac{\bigotimes_{i=1}^{N} r^{(i)}}{M} \right) = \bigotimes_{i=1}^{N} \left( \frac{r^{(i)}}{M_i} \right) \otimes_j \nabla \left( \frac{r^{(j)}}{M_j} \right)
\]

holds in the distributional sense. Then, as \( r^{(i)}/M_i \in L_{M_i}^{1}(D_i) \) 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 \( M \) implies that, for \( j \in [N] \), \( \nabla q_j (\bigotimes_{i=1}^{N} r^{(i)}/M) \in [L_{M}^{2}(D)]^{d} \). 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 \( \bigotimes_{i=1}^{N} r^{(i)} \in H(D; M) \setminus \{0\} \); then, because of the tensor-product structure of \( M \), the positivity of \( M_i \) on compact subsets of \( D_i \) for \( i \in [N] \) and Fubini’s theorem, \( r^{(i)} \in M_i L_{1/M_i}^{1}(D_i) \cap L_{1/M_i}^{2}(D_i) \), \( i \in [N] \). Hence, each \( r^{(i)}/M_i \) defines a regular distribution in \( \mathcal{D}'(D_i) \). Again, Lemma 2.5 makes (2.5) valid and
thus,
\[
\left\| \bigotimes_{i=1}^{N} r^{(i)} \right\|_{H(D;M)}^2 = \prod_{i=1}^{N} \left\| r^{(i)} \right\|_{L^{2}_{1/M'_i}(D_i)}^2 + \sum_{j=1}^{N} \left[ \prod_{i \neq j}^{N} \left\| r^{(i)} \right\|_{L^{2}_{1/M'_i}(D_i)}^2 \right] \left\| \nabla \left( \frac{r^{(j)}}{M'_j} \right) \right\|_{[L^{2}_{M'_j}(D_j)]^d}^2.
\] (2.6)

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 (2.6) yields \( \| \nabla (r^{(i)}/M'_i) \|_{[L^{2}_{M'_i}(D_i)]^d} < \infty \) 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 \( H(D; M) \) is a Hilbert space (cf. Lemma 2.3) and \( a \) is a bounded and coercive bilinear form on \( H(D; M) \). By virtue of the Riesz representation theorem, there exists a bounded linear operator \( A : H(D; M) \to H(D; M)' \), defined by \( (A \psi)(\varphi) = a(\psi, \varphi) \) 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 [29] concerning the numerical solution of high-dimensional Poisson equations, we consider two numerical algorithms. In both algorithms \( \text{TOL} > 0 \) is a preselected tolerance.

Algorithm 3.1 (Pure Greedy Algorithm)

0. Define \( f_0 := f \in H(D; M)' \).

1. For \( n \geq 1 \) do:

1.1 Find \( r^{(i)}_n \in H(D_i; M'_i), i \in [N] \), such that

\[
(r^{(1)}_n, \ldots, r^{(N)}_n) \in \arg \min_{(s^{(1)}, \ldots, s^{(N)}) \in \times_{i=1}^{N} H(D_i; M'_i)} J_{f_{n-1}} \left( \bigotimes_{i=1}^{N} s^{(i)} \right). \quad (3.3)
\]
1.2 Define \( f_n := f_{n - 1} - \mathcal{A}(\bigotimes_{i=1}^{N} r_n^{(i)}) \in H(D; M)' \).

1.3 If \( \| f_n \|_{H(D; M)'} \geq \text{TOL} \), then proceed to iteration \( n + 1 \); else, stop.

**Algorithm 3.2 (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
   \[
   (r_n^{(1)}, \ldots, r_n^{(N)}) \in \arg \min_{(s^{(1)}, \ldots, s^{(N)})} J_{f_n-1}\left(\bigotimes_{i=1}^{N} r_n^{(i)}\right). \tag{3.4}
   \]

   1.2 Minimize \( J_f \) on the span of \( \bigotimes_{i=1}^{N} r_k^{(i)} \), \( k \in [n] \); i.e., find \( \alpha^{(n)} \in \mathbb{R}^n \) such that
   \[
   \alpha^{(n)} = \arg \min_{\beta \in \mathbb{R}^n} J_f\left(\sum_{k=1}^{n} \beta_k \bigotimes_{i=1}^{N} r_k^{(i)}\right). \tag{3.5}
   \]

   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,
\[
\psi_n = \begin{cases} 
\psi_{n-1} - \bigotimes_{i=1}^{N} r_n^{(i)} & \text{for the Pure Greedy Algorithm,} \\
\psi - \sum_{k=1}^{n} \alpha_k^{(n)} \bigotimes_{i=1}^{N} r_k^{(i)} & \text{for the Orthogonal Greedy Algorithm,}
\end{cases} \tag{3.6}
\]
where \( \psi = \psi_0 \) is the unique solution of (3.1).

The proof of the correctness of Algorithm 3.1 (respectively, Algorithm 3.2) 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 2.6, 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 \( (r_n^{(1)}, \ldots, r_n^{(N)}) \) to these problems is quite another matter: it will be proved using Lemma 3.3 and Theorem 3.4 below.
Lemma 3.3 Suppose that \( f \in H(D; M)' \setminus \{0\} \) and consider the functional \( J_f \), as in (3.1). Then, there exists \((r^{(1)}, \ldots, r^{(N)})\) 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 \((r^{(1)}, \ldots, r^{(N)})\) in \( \times_{i=1}^N H(D_i; M_i) \); then,

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

Given a particular ensemble \((r^{(1)}, \ldots, r^{(N)})\) 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

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

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

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

As this is valid for any ensemble \((r^{(1)}, \ldots, r^{(N)})\) in \( \times_{i=1}^N H(D_i; M_i) \), Lemma 2.4 implies that it is valid, in particular, for any ensemble \((r^{(1)}, \ldots, r^{(N)})\) in \( \times_{i=1}^N C^\infty_0 (D_i) \), whence Lemma 2.5 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 3.4 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 \((0, \ldots, 0)\) 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 \( a \), \( J_{f_{n-1}} (\psi) \geq -\frac{1}{2} a(\psi, \psi) \) for all \( \psi \in H(D; M) \), where \( \psi \) is the unique solution of (2.4) in \( H(D; M) \) when \( f = f_{n-1} \). As, by Lemma 2.6, 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,
\[ m := \inf_{(s^{(1)}, \ldots, s^{(N)}) \in \times_{i=1}^{N} H(D_i; M_i)} J_{f_{n-1}} \left( \bigotimes_{i=1}^{N} s^{(i)} \right) > -\infty. \] (3.8)

It follows from Lemma 3.3 that \( m < 0 \). Our aim is to show that the infimum \( m \) is attained at an element of the form \( \bigotimes_{i=1}^{N} r^{(i)} \) with \( (r^{(1)}, \ldots, r^{(N)}) \in \times_{i=1}^{N} (H(D_i; M_i) \setminus \{0\}) \).

From (3.8), there exists a sequence \( \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \) of \( N \)-way tensor products of functions in \( H(D_i; M_i) \), such that

\[ \lim_{k \to \infty} J_{f_{n-1}} \left( \bigotimes_{i=1}^{N} r^{(i)}_k \right) = m. \]

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

\[ J_{f_{n-1}}(\varphi) = \frac{1}{2} a(\varphi - \psi, \varphi - \psi) - \frac{1}{2} a(\psi, \psi) \geq \frac{1}{4} a(\varphi, \varphi) - a(\psi, \psi) \]

it follows, by setting \( \varphi = \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \), that the sequence \( \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \) is bounded in \( H(D; M) \). In other words, there exists \( C > 0 \) such that (cf. (2.6))

\[ \left\| \bigotimes_{i=1}^{N} r^{(i)}_k \right\|_{H(D; M)}^2 \leq C \] (3.9)

for all \( k \geq 1 \). Since the value of \( \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \) is unaltered by multiplying the first \( N - 1 \) factors by positive constants \( c_1, k, \ldots, c_{N-1}, k \), 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

\[ \left\| r^{(i)}_k \right\|_{L^2_{1/M_i}(D_i)}^2 = 1, \quad i \in [N - 1]. \] (3.10)

Thus, it follows from (3.9) that

\[ \left\| r^{(N)}_k \right\|_{L^2_{1/M_N}(D_N)}^2 + \sum_{j=1}^{N-1} \left[ \left\| r^{(j)}_k \right\|_{L^2_{1/M_j}(D_j)}^2 \left\| \nabla \left( r^{(j)}_k \right) \right\|_{L^2_{M_j}(D_j)} \right]^2 \]

\[ = \left\| \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \right\|_{H(D; M)}^2 \leq C. \] (3.11)

Since the sequence \( \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \) 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 \( \bigotimes_{i \in \mathbb{N}} r^{(i)}_k \); 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

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

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

Thanks to (3.10) and (3.11) each subsequence $(r_{\phi(k)}^{(i)})_{k \geq 1}$ is bounded in the respective space $L_{1/M_i}^2(D_i)$, for $i \in [N]$. Then, $(r_{\phi(k)}^{(i)})_{k \geq 1}$ has a weakly convergent subsequence in $L_{1/M_i}^2(D_i)$, say $(r_{\phi(k)}^{(i)})_{k \geq 1}$, 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 2.4, $C_{0}^{\infty}(D_i) \subset H(D_i; M_i) \subset L_{1/M_i}^2(D_i)$, 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, $(r_{\phi(k)}^{(i)})_{k \geq 1}$ converges to $r^{(i)}/M_i$ in $\mathcal{D}'(D_i)$ for $i \in [N]$. Hence, by Lemma 2.5,

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

Similarly, the inclusion $C_{0}^{\infty}(D) \subset H(D; M)$ (cf. Lemma 2.4) and the fact that, for all $\varphi \in C_{0}^{\infty}(D)$, the mapping $\xi \in H(D; M) \mapsto \langle \varphi, \xi \rangle_{L_{1/M(D)}^2}$ defines a bounded linear functional on $H(D; M)$ imply that

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

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

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

Hence, $r = \bigotimes_{i=1}^{N} r_{i}^{(i)}$ almost everywhere. As $r \in H(D; M) \setminus \{0\}$ and has a tensor-product structure, the second part of Lemma 2.6 implies that $r^{(i)} \in H(D_i; M_i) \setminus \{0\}$ for $i \in [N]$. Now,

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

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

\[ \square \]
Having proved that the minimization problems (3.3) of Algorithm 3.1 and (3.4) of Algorithm 3.2 have solutions, establishing the correctness of what is left of the algorithms is straightforward. The Galerkin problem 1.2 of Algorithm 3.2 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 3.1 and in step 1.3 of Algorithm 3.2 are correct on noting that $\mathcal{A}$ maps $H(D; M)$ into $H(D; M)'$.

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 $(r_1^{(1)}, \ldots, r_N^{(N)})$ of the minimization problems (3.3) or (3.4) satisfy the following Euler–Lagrange equation system: For all $(s^{(1)}, \ldots, s^{(N)}) \in \bigotimes_{i \in [N]} H(D_i; M_i)$,

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

From this, it follows that, for the Pure Greedy Algorithm (Algorithm 3.1):

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

Proof Let $(r_1^{(1)}, \ldots, r_N^{(N)})$ be a solution to the minimization problem (3.3) or (3.4). Then, given any ensemble $(s^{(1)}, \ldots, s^{(N)})$, (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 $\varepsilon$ is zero when evaluated at $\varepsilon = 0$. As, by hypothesis, $(r_1^{(1)}, \ldots, r_N^{(N)})$ is a local minimizer of $J_{f_{n-1}}$ and $\varepsilon \mapsto J_{f_{n-1}}(\bigotimes_{i=1}^N (r_n^{(i)} + \varepsilon s^{(i)}))$ is regular enough, the fact that $J'_{f_{n-1}}(0) = 0$ implies that (4.1) holds.

Setting $(s^{(1)}, \ldots, s^{(N)}) = (r_1^{(1)}, \ldots, r_N^{(N)})$ in (4.1), we obtain from the definition of the $\psi_n$

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

Combining this with (3.6) we obtain (4.2). \qed
Remark 4.2

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 4.3 Let $(r_n^{(1)}, \ldots, r_n^{(N)})$ be a global minimizer for the minimization problem (3.3) of the Algorithm 3.1. Then,

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

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

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). \hfill \square

4.2 Convergence

Theorem 4.4 The Pure Greedy Algorithm (Algorithm 3.1) converges to the solution $\psi$ of (2.4).

Proof Let $((r_n^{(1)}, \ldots, r_n^{(N)}))_{n \geq 1}$ be a sequence in $\bigotimes_{i=1}^N H(D_i; M_i)$ 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

\[ \sum_{n=1}^{\infty} a(r_n, r_n) < \infty. \]  

(4.5)

Let us define the function \(\phi : \mathbb{N} \to \mathbb{N}\) 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 \(\phi\) is well-defined and strictly monotonic increasing. Hence, it is suitable for defining subsequences. As each \((r^{(1)}_n, \ldots, r^{(N)}_n)\) is a global solution to the problem (3.3) with the instance \(f_{n-1}\), via (3.6) and Lemma 4.3 we have for \(n \geq m \geq 1,

\[ \|\psi_{\phi(n)} - \psi_{\phi(m)} - 1\|_a^2 = \|\psi_{\phi(n)} - 1\|_a^2 + \|\psi_{\phi(m)} - 1\|_a^2 \]

\[ - 2a \left( \psi_{\phi(n)-1}, \psi_{\phi(n)-1} + \sum_{k=\phi(m)}^{\phi(n)-1} r_k \right) \]

\[ = \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 - 2 \sum_{k=\phi(m)}^{\phi(n)-1} a(\psi_{\phi(n)-1}, r_k) \]

\[ \leq \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 - 2 \sum_{k=\phi(m)}^{\phi(n)-1} \|r_k\|_a \|r_{\phi(n)}\|_a \]

\[ \leq \|\psi_{\phi(m)-1}\|_a^2 - \|\psi_{\phi(n)-1}\|_a^2 - 2 \sum_{k=\phi(m)}^{\phi(n)-1} \|r_k\|_a^2. \]

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 \((r^{(1)}_n, \ldots, r^{(N)}_n)\) is: For all \((s^{(1)}, \ldots, s^{(N)}) \in \times_{i \in [N]} H(D_i; M_i)\) and \(n \geq 1,

\[ \frac{1}{2} a \left( \bigotimes_{i=1}^{N} s^{(i)} \bigotimes_{i=1}^{N} s^{(i)} \right) - a \left( \psi_{\phi(n)-1} \bigotimes_{i=1}^{N} s^{(i)} \right) \geq J_{f_{\phi(n)-1}}(r_{\phi(n)}) \]

\[ = \frac{1}{2} a(r_{\phi(n)}, r_{\phi(n)}) - J_{f_{\phi(n)-1}}(r_{\phi(n)}) \]

\[ = -\frac{1}{2} a(r_{\phi(n)}, r_{\phi(n)}). \]
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 3.3 implies that \( \psi_{\infty} = 0 \). Hence the sequence \( (\|\psi_{\phi(n)} - 1\|)_{n \geq 1} \) converges to zero as \( n \to \infty \). As the sequence \( (\|\psi_{n}\|)_{n \geq 0} \) is monotonic nonincreasing and \( (\phi(n) - 1)_{n \geq 1} \) is a monotonic increasing infinite sequence in \( \mathbb{N} \), if follows that the full sequence \( (\|\psi_{n}\|)_{n \geq 1} \) converges to the common limit in \( \mathbb{R} : 0 = \|\psi_{\infty}\|_{a} \), giving \( \lim_{n \to \infty} \psi_{n} = 0 \) in \( H(D; M) \).

The following corollary is a direct consequence of Theorem 4.4, and it will prove useful later on.

**Corollary 4.5** 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 4.4 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 \( \tau \) 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. (2.6)),

\[
\|\delta_{n}\|_{H(D; M)}^{2} \leq \sum_{k=1}^{N} \left[ \prod_{i=1}^{N} \|t_{n,k}^{(i)}\|_{L_{1/M_{i}}(D_{i})}^{2} + \sum_{j=1}^{N} \prod_{i=1}^{N} \|t_{n,k}^{(i)}\|_{L_{1/M_{i}}(D_{i})}^{2} \|\nabla (t_{n,k}^{(i)} / M_{j})\|_{L_{2}(D_{j})}^{2} \right].
\]

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

**Remark 4.6** Suppose that, for each \( i \in [N] \),

\[
C_{0}^{\infty}(D_{i}) \text{ is dense in } H(D_{i}; M_{i}).
\]
Then, as \( \text{span}(N \bigotimes_{i=1}^{N} C_{0}^{\infty}(D_{i})) \subset C_{0}^{\infty}(D) \subset H(D; M) \), we have, thanks to Corollary 4.5,

\[
C_{0}^{\infty}(D) \text{ is dense in } H(D; M). \tag{4.7}
\]

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 [32]. Springs obeying the CPAIL model (1.3), in turn, comply with (4.6) as is shown in Lemma A.1 in Appendix A of [22], under the condition \( b_{i} \geq 3 \). So, in these two cases, (4.7) holds.

**Theorem 4.7** The Orthogonal Greedy Algorithm (Algorithm 3.2) converges to the solution \( \psi \) 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 \((r_{1}^{(n)}, \ldots, r_{N}^{(n)})\) in (3.4) (via Lemma 4.1),

\[
\| \psi_{n} \|_{a}^{2} = \| \psi - \sum_{k=1}^{n} \alpha^{(n)}_{k} \bigotimes_{i=1}^{N} r_{i}^{(n)} \|_{a}^{2} \leq \| \psi_{n-1} - \bigotimes_{i=1}^{N} r_{i}^{(n)} \|_{a}^{2} = \| \psi_{n-1} \|_{a}^{2} - \| \bigotimes_{i=1}^{N} r_{i}^{(n)} \|_{a}^{2}.
\]

Thus, just like in the proof of Theorem 4.4, we see that the real sequence \( (\| \psi_{n} \|_{a})_{n \geq 0} \) is decreasing and thus convergent and that \( \sum_{n \geq 1} a(\bigotimes_{i \in [N]} r_{i}^{(n)} , \bigotimes_{i \in [N]} r_{i}^{(n)}) < \infty \).

As \( (\psi_{n})_{n \geq 0} \) is a bounded sequence in the Hilbert space \( H(D; M) \), a weakly convergent subsequence \( (\psi_{\phi(n)})_{n \geq 1} \) can be extracted and we denote the weak limit by \( \psi_{\infty} \).

From the optimality of \( (r_{\phi(n)}^{(1)}, \ldots, r_{\phi(n)}^{(N)}) \) with respect to problem (3.4) we have by Lemma 4.1 that, for all \( (s^{(1)}, \ldots, s^{(N)}) \in \bigotimes_{i \in [N]} H(D_{i}; M_{i}) \),

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

Taking the limit \( n \to \infty \) 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 3.3, \( \psi_{\infty} = 0 \). Because of the 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, \( \lim_{n \to \infty} \| \psi_{\phi(n)} \|_{a}^{2} = \lim_{n \to \infty} a(\psi, \psi_{\phi(n)}) = a(\psi, \psi_{\infty}) = 0 \). 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 \( H(D; M) \).

\( \square \)

### 4.3 Rate of Convergence

The theory of nonlinear approximation provides us with some estimates on the rate of convergence of Algorithm 3.1 and Algorithm 3.2. Following [21], we introduce
the space
\[ \mathcal{A}_1 := \bigcup_{M > 0} \mathcal{A}^o_1(M), \] (4.8)
where
\[ \mathcal{A}^o_1(M) := \left\{ \varphi \in H(D; M) : \varphi = \sum_{k \in \Lambda} c_k w_k, \ w_k \in \bigotimes_{i=1}^N H(D_i; M_i), \ |\varphi|_a = 1, \right\} \] (4.9)
together with the norm
\[ \|\varphi\|_{\mathcal{A}_1} := \inf\{M > 0 : \varphi \in \mathcal{A}^o_1(M)\}. \] (4.10)

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

**Theorem 4.8** (Theorem 3.6 of [21]) If the solution \( \psi \) of (2.4) is a member of \( \mathcal{A}_1 \), then the \( n \)th error \( \psi_n \) of the Pure Greedy Algorithm (Algorithm 3.1) satisfies
\[ \|\psi_n\|_a \leq \|\psi\|_{\mathcal{A}_1} n^{-1/6}. \]

**Theorem 4.9** (Theorem 3.7 of [21]) If the solution \( \psi \) of (2.4) is a member of \( \mathcal{A}_1 \), then the \( n \)th error \( \psi_n \) of the Orthogonal Greedy Algorithm (Algorithm 3.2) satisfies
\[ \|\psi_n\|_a \leq \|\psi\|_{\mathcal{A}_1} n^{-1/2}. \]

**Remark 4.10**

1. Pure Greedy Algorithm-based approximations such as Algorithm 3.1 have been proved to obey the slightly improved rate (see [42, Remark 2.3.11] and references therein)
\[ \|\psi_n\|_a \leq 4\|\psi\|_{\mathcal{A}_1} n^{-11/62}. \]

2. In [15, 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 \( H(D; M) \), 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 \( H(D; M) \), as these two norms are equivalent. Then, \( \varphi \in H(D; M) \) 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 \( \chi_{\varepsilon} \in H(D; M) \) that satisfies
\[ \| \varphi - \chi^e \|_{H(D;M)} \leq \varepsilon, \quad \chi^e = \sum_{k \in A^{(e)}} c^{(e)}_k w^{(e)}_k, \]

\[ |A^{(e)}| < \infty, \quad \sum_{k \in A^{(e)}} |c^{(e)}_k| \leq M^*; \]

and, for \( k \in A^{(e)} \), \( \| w^{(e)}_k \|_{H(D;M)} = 1 \) and \( w^{(e)}_k \in \otimes_{i=1}^N H(D_i; M_i) \).

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

\[ \| M^{-1} \varphi - M^{-1} \chi^e \|_{H^1(D)} \leq \varepsilon, \quad M^{-1} \chi^e = \sum_{k \in A^{(e)}} c^{(e)}_k M^{-1} w^{(e)}_k, \]

and, for \( k \in A^{(e)} \), \( \| M^{-1} w^{(e)}_k \|_{H^1(D)} = 1 \) and \( M^{-1} w^{(e)}_k \in \otimes_{i=1}^N H^1(D_i) \), the last relation being a consequence of the tensor-product structure of the Maxwellian \( M \). Thus we have shown that \( M^{-1} \varphi \in H^1(D) \) can be approximated to within any positive tolerance \( \varepsilon \) in the norm of \( H^1(D) \) by finite linear combinations of normalized members of \( \otimes_{i=1}^{[N]} H^1(D_i) \) 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 \( M^{-1} \varphi \) in the \( H^1(D) \)-based analogue of \( \mathcal{A}_1 \), namely,

\[ \mathcal{B}_1 := \bigcup_{M > 0} \mathcal{B}^0_1(M), \quad (4.11) \]

where

\[ \mathcal{B}^0_1(M) := \left\{ \varphi \in H^1(D): \varphi = \sum_{k \in A} c_k w_k, \quad w_k \in \bigotimes_{i=1}^{[N]} H^1(D_i), \quad \| w_k \|_{H^1(D)} = 1, \quad |A| < \infty \text{ and } \sum_{k \in A} |c_k| \leq M \right\}, \quad (4.12) \]

and

\[ \| \varphi \|_{\mathcal{B}_1} := \inf\{ M > 0: \varphi \in \mathcal{B}^0_1(M) \}. \quad (4.13) \]

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

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

where the last equality follows from the fact that the coefficients of the approximations to \( \varphi \) 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 rather 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 [29, 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 $H^1_M(D)$-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 abstract lemma, which collects standard results (essentially, the Hilbert–Schmidt theorem and some of its corollaries).

Lemma 5.1 Let $H$ and $V$ be separable infinite-dimensional Hilbert spaces, with $V \subset H$ and $V = H$ in the norm of $H$. Let $a : V \times V \to \mathbb{R}$ be a nonzero, symmetric, bounded and elliptic bilinear form. Then, there exists a sequence $(\lambda_n)_{n \in \mathbb{N}}$ of real numbers and a sequence $(e_n)_{n \in \mathbb{N}}$ of unit $H$-norm members of $V$, which solve the eigenvalue 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 $\lambda_n$, which can be assumed to be in increasing order with respect to $n$, are positive, bounded from below away from 0, and $\lim_{n \to \infty} \lambda_n = +\infty$.

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 $V$, so we have

$$h = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H e_n \quad \text{and} \quad \|h\|_H^2 = \sum_{n=1}^{\infty} \langle h, e_n \rangle_H^2 \quad \forall h \in H \quad (5.2)$$

and

$$v = \sum_{n=1}^{\infty} a\left(v, \frac{e_n}{\sqrt{\lambda_n}}\right) \frac{e_n}{\sqrt{\lambda_n}} \quad \text{and} \quad \|v\|_a^2 = \sum_{n=1}^{\infty} a\left(v, \frac{e_n}{\sqrt{\lambda_n}}\right)^2 \quad \forall v \in V; \quad (5.3)$$

further,

$$h \in H \text{ and } \sum_{n=1}^{\infty} \lambda_n \langle h, e_n \rangle_H^2 < \infty \quad \iff \quad h \in V. \quad (5.4)$$

Proof The proofs of the stated results can be partially found in textbooks on functional analysis (see, for example, Theorem VI.15 in Reed and Simon [37] or Sect. 4.2 in Zeidler [46]). A version of the proof for the special case in which $V$ and $H$ are standard Sobolev spaces is contained in Sect. IX.8 of Brezis [13]; using the abstract results in Chap. VI of [13], the result in Sect. IX.8 of [13] can be easily adapted to the setting of the present theorem. For a detailed proof we refer to Lemmas 5.1 and 5.2 in the extended version of the present paper; cf. [22].

\[ Springer \]
In order to apply Lemma 5.1 in our Maxwellian-weighted context we need to adopt the following second structural hypothesis.

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

**Remark 5.2** In Step 1 of Sect. A.1 of [6] 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 of [22], under the condition $b_i \geq 3$.

**Lemma 5.3** $H^1_{M}(D)$ is compactly embedded in $L^2_{M}(D)$.

**Proof** Throughout this proof we will assume, for ease of exposition, that $N = 2$; the argument carries over to higher $N$ without difficulties. Let $u \in H^1_{M}(D)$. As, by (1.6), $M = M_1 \otimes M_2$, it follows from Fubini’s theorem that, for almost all $q_1 \in D_1$,

$$u(q_1, \cdot) \in L^2_{M_2}(D_2) \cap L^1_{\text{loc}}(D_2) \quad \text{and} \quad \partial_\alpha u(q_1, \cdot) \in L^2_{M_2}(D_2),$$

where $\alpha$ is any multi-index in $[N_0]^d$ with $0 \leq |\alpha| \leq 1$. Fubini’s theorem, again, ensures that, given $\varphi_2 \in C_0^\infty(D_2)$ and $\alpha_2 \in [N_0]^d$, $0 \leq \alpha_2 \leq 1$,

$$\left| \int_{D_1} \left[ (-1) \int_{D_2} u(q_1, \cdot) \partial_\alpha \varphi_2 \right] \varphi_1 \, dq_1 \right| = \left| \int_{D_1} \left[ \int_{D_2} \partial(0, \alpha_2) u(q_1, \cdot) \varphi_2 \right] \varphi_1 \, dq_1 \right|,$$

for all $\varphi_1 \in C_0^\infty(D_1)$. Therefore, $\partial_\alpha u(q_1, \cdot) = \partial(0, \alpha_2) u(q_1, \cdot)$ in the weak sense on $D_2$ for almost all $q_1 \in D_1$. As $\partial(0, \alpha_2) u(q_1, \cdot)$ lies in $L^2_{M_2}(D_2)$ for almost all $q_1 \in D_1$, we have

$$u(q_1, \cdot) \in H^1_{M_2}(D_2) \quad \text{for almost all } q_1 \in D_1. \quad (5.5)$$

In the same way it can be proved that $u(\cdot, q_2) \in H^1_{M_1}(D_1)$ for almost all $q_2 \in D_2$.

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

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

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 $H^1_{M_i}(D_{i,(n)})$ and $H^1(D_{i,(n)})$ and between $L^2_{M_i}(D_{i,(n)})$ and $L^2(D_{i,(n)})$. Letting, for $n \in \mathbb{N}$, $D_{(n)} := \bigcup_{i=1}^{\infty} D_{i,(n)} \subset D$, the above properties get inherited:

$$D_{(n)} \subset D_{(n+1)}, \quad n \in \mathbb{N}, \quad \bigcup_{n=1}^{\infty} D_{(n)} = D \quad \text{and} \quad H^1_{M}(D_{(n)}) \subset L^2_{M}(D_{(n)}).$$
The third statement follows from the fact that the $D_{(n)}$, being Cartesian products of bounded Lipschitz domains, are also bounded Lipschitz domains (cf. the footnote on p. 10 in [22]). Let us define $D_{1(n)} := D_{1} \setminus D_{1;n(n)}$ and $D_{(n)} := D \setminus D_{(n)}$. Thanks to [36, Theorem 17.6], the above compact embeddings on members of a nested covering imply the following characterizations (the first, for $i \in \{1, 2\}$):

$$
H^1_{M_i}(D_i) \Subset L^2_{M_i}(D_i) \iff \lim_{n \to \infty} \sup_{u \in H^1_{M_i}(D_i)} \int_{D_{i(n)}} u^2 M_i / \|u\|^2_{H^1_{M_i}(D_i)} = 0, \quad (5.6)
$$

$$
H^1_M(D) \Subset L^2_M(D) \iff \lim_{n \to \infty} \sup_{u \in H^1_M(D)} \int_{D(n)} u^2 M / \|u\|^2_{H^1_M(D)} = 0. \quad (5.7)
$$

From Hypothesis B, the left-hand side of (5.6) holds; hence, its right-hand side also holds. Using (5.5) and (5.6) 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

$$
\int_{D_1 \times D_2(n)} u^2 M = \int_{D_1} \left[ \int_{D_2(n)} u^2(q_1, \cdot) M_2(q_1) \right] M_1(q_1) dq_1
\leq \varepsilon \int_{D_1} \|u(q_1, \cdot)\|^2_{H^1_{M_2}(D_2)} M_1(q_1) dq_1
= \varepsilon \int_{D_1} \left[ \int_{D_2} \left( u^2(q_1, \cdot) + |\nabla q_2 u(q_1, \cdot)|^2 \right) M_2 \right] M_1(q_1) dq_1
\leq \varepsilon \|u\|^2_{H^1_M(D)}.
$$

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 (5.7) holds; hence, so does its left-hand side.

With the last result in hand, the hypotheses of Lemma 5.1 are satisfied by the eigenvalue problems

$$
\langle e^{(i)}, \varphi \rangle_{H^1_{M_i}(D_i)} = \lambda^{(i)} \langle e^{(i)}, \varphi \rangle_{L^2_{M_i}(D_i)} \quad \forall \varphi \in H^1_{M_i}(D_i), \quad (5.8)
$$

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

$$
\langle e, \varphi \rangle_{H^1_M(D)} = \lambda \langle e, \varphi \rangle_{L^2_M(D)} \quad \forall \varphi \in H^1_M(D), \quad (5.9)
$$

whence their solutions do have the distribution, orthogonality and spanning properties stated in that lemma (the hypothesis $V = H$, 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) $((\lambda^{(i)}_n, e^{(i)}_n))_{n \in \mathbb{N}}$ and $((\lambda_n, e_n))_{n \in \mathbb{N}}$, respectively, with
\[ \varphi \in L^2_{M_i}(D_i) \text{ and } \sum_{n=1}^{\infty} \lambda_n^{(i)} \langle \varphi, e_n^{(i)} \rangle_{L^2_{M_i}(D_i)}^2 < \infty \quad \iff \quad \varphi \in H^1_{M_i}(D_i), \quad (5.10) \]

and

\[ \varphi \in L^2_{M}(D) \text{ and } \sum_{n=1}^{\infty} \lambda_n \langle \varphi, e_n \rangle_{L^2_{M}(D)}^2 < \infty \quad \iff \quad \varphi \in H^1_{M}(D), \quad (5.11) \]

where, further, because of (5.4), the sums are equal to the corresponding weighted H^1 norms in both cases.

Next, we exploit the special tensor-product structure of the full Maxwellian M to characterize the eigenpairs of its associated eigenvalue problem (5.9) in terms of the eigenpairs of the eigenvalue problem (5.8) associated to the partial Maxwellians \( M_i \).

Lemma 5.4 The net \( ((\lambda_n, e_n))_{n=(n_1,\ldots,n_N)} \in \mathbb{N}^N \) is a full system of solutions of the eigenvalue problem (5.9), where

\[ \lambda_n := 1 + \sum_{i=1}^{N} (\lambda_n^{(i)} - 1) \quad \text{and} \quad e_n := \bigotimes_{i=1}^{N} e_n^{(i)}. \quad (5.12) \]

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

\[
\langle e_n, \tau \rangle_{H(D;M)} = \langle e_n, \tau \rangle_{L^2_{M}(D)} + \sum_{j=1}^{N} \langle \nabla e_n^{(j)}, \nabla \tau^{(j)} \rangle_{L^2_{M_j}(D_j)} \prod_{i=1}^{N} \langle e_n^{(i)}, \tau^{(i)} \rangle_{L^2_{M_i}(D_i)} \\
= \langle e_n, \tau \rangle_{L^2_{M}(D)} + \sum_{j=1}^{N} (\lambda_n^{(j)} - 1) \langle e_n^{(j)}, \tau^{(j)} \rangle_{L^2_{M_j}(D_j)} \prod_{i=1}^{N} \langle e_n^{(i)}, \tau^{(i)} \rangle_{L^2_{M_i}(D_i)} \\
= \lambda_n \langle e_n, \tau \rangle_{L^2_{M}(D)}.
\]

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 4.5 and (2.3a) and (2.3b)), 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, \( (\lambda_n, e_n) \) is an eigenpair of (5.9). Further, we deduce from the chain of equalities above that \( e_n \) is orthogonal to \( e_m \) in both \( L^2_{M}(D) \) and \( H^1_{M}(D) \) if \( n \neq m \).

From (5.3) in Lemma 5.1, for \( i \in [N] \), \( \text{span}(e_n^{(i)})_{n \geq 1} = H^1_{M_i}(D_i) \). Hence, by (4.5) and (2.3a) and (2.3b),

\[ \bigotimes_{i=1}^{N} \text{span}(e_n^{(i)})_{n \geq 1} \subset \text{span}(e_n)_{n \in \mathbb{N}^N} = H^1_{M}(D). \]

Thus, \( (e_n)_{n \in \mathbb{N}^N} \) forms an orthogonal system that spans \( H^1_{M}(D) \). Therefore, by Theorem VI.9 of [13], all the eigenpairs of the (full) Maxwellian eigenvalue problem (5.9)
have the form \((\lambda_n, e_n)\) as given in (5.12) (modulo linear combinations of eigenfunctions belonging to the same eigenspace). \(\square\)

It follows from Lemma 5.4 that the eigenvalues and eigenfunctions of (5.9) 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 5.4 the sequence \(((\lambda_n, e_n))_{n \in \mathbb{N}^N}\) is a full system of eigenpairs of (5.9), (5.3) in Lemma 5.1 ensures that, for all \(\tau \in H^1_{M}(D)\),

\[
\tau = \sum_{n \in \mathbb{N}^N} \left( \tau, \frac{e_n}{\sqrt{\lambda_n}} \right)_{H^1_{M}(D)} \frac{e_n}{\sqrt{\lambda_n}} = \sum_{n \in \mathbb{N}^N} \sqrt{\lambda_n} \langle \tau, e_n \rangle_{L^2_{M}(D)} \frac{e_n}{\sqrt{\lambda_n}} \text{ in } H^1_{M}(D).
\]

Hence, given the tensor-product structure of the \(e_n\) and the unit \(H^1_{M}(D)\)-norm of the \(e_n/\sqrt{\lambda_n}\), we can guarantee that \(\tau \in B_1\) (cf. (4.11)) if

\[
\sum_{n \in \mathbb{N}^N} \sqrt{\lambda_n} \left| \left\langle \tau, e_n \right\rangle_{L^2_{M}(D)} \right| < \infty.
\]

In turn, this holds if

\[
A := \sum_{n \in \mathbb{N}^N} \frac{\lambda_n}{\sigma_n} < \infty \quad \text{and} \quad B := \sum_{n \in \mathbb{N}^N} \sigma_n \left| \left\langle \tau, e_n \right\rangle_{L^2_{M}(D)} \right|^2 < \infty,
\]

where \((\sigma_n)_{n \in \mathbb{N}^N}\) 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 \(\sigma_n = \lambda_n\), for example, this is certainly the case, as follows from (5.11)—as a regularity requirement on \(\tau\). Thus, there is a trade-off in (5.13) between the requirement that the \(\sigma_n\) grow fast enough to ensure the finiteness of \(A\) and the desirability of the \(\sigma_n\) growing slow enough to avoid demanding more regularity than necessary of the functions \(\tau\) for which \(B\) is finite.

As a first step in formalizing the above we consider, given a net \(\Sigma = (\sigma_n)_{n \in \mathbb{N}^N}\) with entries in \(\mathbb{R}_{>0}\), the space of all those \(L^2_{M}(D)\) functions for which the term \(B\), as defined in (5.13), is finite:

\[
H^\Sigma_{M}(D) := \left\{ \varphi \in L^2_{M}(D) : \sum_{n \in \mathbb{N}^N} \sigma_n \left| \left\langle \varphi, e_n \right\rangle_{L^2_{M}(D)} \right|^2 < \infty \right\}.
\]

We equip \(H^\Sigma_{M}(D)\) with the norm

\[
\|\varphi\|_{H^\Sigma_{M}(D)} := \left( \sum_{n \in \mathbb{N}^N} \sigma_n \left| \left\langle \varphi, e_n \right\rangle_{L^2_{M}(D)} \right|^2 \right)^{1/2}.
\]

It is readily seen that, if there exists a \(\sigma > 0\) with \(\sigma_n \geq \sigma\) for all \(n \in \mathbb{N}^N\), then \(H^\Sigma_{M}(D)\) is a separable Hilbert space that is continuously embedded in \(L^2_{M}(D)\). Further, if there
exists a $\sigma' > 0$ such that $\sigma_n \geq \sigma' \lambda_n$ for all $n \in \mathbb{N}$, then $H^1_{\Sigma}(D)$ is continuously embedded in $H^1_{\Sigma}(D)$ and, thanks to Lemma 5.3, it is compactly embedded in $L^2_{\Sigma}(D)$.

At this stage we could just choose $\Sigma$ to be, e.g., $\sigma_n = \lambda_n \|n\|^{\alpha}$ for some $\alpha > N$ and an application of a multiple series version of the integral test for convergence (see, for example, [23, Proposition 7.57]) would render the sum $A$ in (5.13) finite. However, the resulting space $H^1_{\Sigma}(D)$ would then still have quite an abstract description. What we therefore wish to do instead is to choose each $\sigma_n$ as a suitable polynomial function of the $(\lambda(1), \ldots, \lambda(N))$. 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 (5.13) is finite, with $\sigma_n$ as a certain polynomial function of the $\lambda_n$, if we have some information about the asymptotic behavior of the $\lambda_n$. Consequently, we adopt the following third structural hypothesis.

**Hypothesis C** For each $i \in \mathbb{N}$ 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 (5.8).

**Remark 5.5** Hypothesis C basically amounts to assuming that the eigenvalues of the problem (5.8) behave like the eigenvalues of a regular elliptic operator, such as the Laplace operator on a bounded Lipschitz domain subject to a homogeneous Dirichlet boundary condition, for example. If the partial Maxwellian $M_i$ comes from either the FENE model (1.2) with parameter $b_1 > 2$ or the CPAIL model (1.3) with parameter $b_1 > 3$, then Hypothesis C holds; see Corollary A.3 in Appendix for a proof (see also Remark A.5).

**Theorem 5.6** Let $T^{(m)} = (\tau^{(m)}_n)_{n \in \mathbb{N}}$ be defined by

$$\tau^{(m)}_n := \prod_{i=1}^N (\lambda_n^{(i)})^m \quad \forall n \in \mathbb{N}^N.$$  \hspace{1cm} (5.15)

Then, $H_{M}^{T^{(m)}}(D) \subset \mathcal{B}_1$ 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 $n \in \mathbb{N}$ of $\lambda_n/\tau^{(m)}_n$ converges; i.e., that $A$ in (5.13) is finite. To prove this, we begin 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 (5.12) and Hypothesis C, yields
\[ \frac{\lambda_n}{\tau_n^{(m)}} \leq \frac{\sum_{i=1}^{N} \lambda_i^{(m)}}{\prod_{i=1}^{N} (\lambda_i^{(m)})^m} \leq C \frac{\sum_{i=1}^{N} n_i^{2/d}}{\prod_{i=1}^{N} (n_i^{2/d})^m} \]

(5.16)

for all \( n \in \mathbb{N}^N \) 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 (5.16) results in a convergent series. Now,

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

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

For later reference we introduce another family of weights that also produces subspaces of \( B_1 \).

**Theorem 5.7** Let \( \Upsilon^{(m)} = (\upsilon_n^{(m)})_{n \in \mathbb{N}^N} \) be defined by

\[ \upsilon_n^{(m)} := \left( \sum_{i=1}^{N} \lambda_i^{(m)} \right)^m \forall n \in \mathbb{N}^N. \]  

(5.17)

Then, \( H^{\Upsilon^{(m)}}_M(D) \subset B_1 \) if \( m > \frac{d}{2} N + 1 \).

**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 \( [1, \infty)^N \subset \{ x \in \mathbb{R}_0^N : \| x \|_2 \geq 1 \} \), the finiteness of that integral is, in turn, implied by the finiteness of the integral

\[ \int_{\{ x \in \mathbb{R}_0^N : \| x \|_2 \geq 1 \}} \| x \|_2^{\frac{2}{2}(1-m)} \, dx = C_N \int_{r=1}^{\infty} r^{\frac{2}{2}(1-m)+N-1} \, dr, \]

where \( C_N \) is the \( (N-1) \)-dimensional volume of the surface \( \{ x \in \mathbb{R}_0^N : \| x \|_2 = 1 \} \). As it is assumed that \( m > \frac{d}{2} N + 1 \), the last of the above integrals is finite and the proof is therefore complete. □

The definition of \( H^{\Upsilon^{(m)}}_M(D) \) given by (5.15) is less abstract than the definition of \( B_1 \) (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 $H^{(m)}_M(D)$ (cf. (5.14a)).

5.3 Characterization via Membership in Mixed-Order Weighted Sobolev Spaces

We begin by adopting a fourth hypothesis.

**Hypothesis D** For $i \in [N]$ there exists a distance $\gamma_i \in (0, \sqrt{b_i})$, an exponent $\alpha_i > 3$ and a function $h_i \in C^2([0, \gamma_i])$ that is positive on $[0, \gamma_i]$, such that

$$M_i(p) = h_i(\vartheta_i(p)) \vartheta_i(p)^{\alpha_i}$$

for all $p \in D_i$ such that $\vartheta_i(p) \in (0, \gamma_i)$, where $\vartheta_i$ is the distance-to-the-boundary function in $D_i$.

**Remark 5.8** With Hypothesis D 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 6 in the FENE case and greater than 9 in the CPAIL case.

**Lemma 5.9** For $i \in [N]$, the space $C_0^\infty(D_i)$ is dense in $H^{1}_{M_i}(D_i)$.

**Proof** In Proposition 9.10 of [26] the result is stated for weights that are powers greater than 1 of the distance-to-the-boundary function; the bilateral boundedness of the function $h_i$ by positive constants, implied by Hypothesis D, extends the statement to our case.

Our goal is to relate the regularity of a function as measured in a scale of weighted Sobolev spaces to the weighted summability of its squared Fourier coefficients (i.e., to its membership in a space of the form (5.14a), (5.14b)). Roughly speaking, this is accomplished by first showing that the image of $\varphi$ under the action of the second-order operator associated with (5.8) lies in $L^2_{M_i}(D_i)$ if $\varphi \in H^2_{M_i}(D_i)$—this is not trivial and requires the introduction of the Hardy-type inequalities presented below—and then showing that the application of one such operator to a function is paralleled by the multiplication of each coefficient of its eigenfunction expansion by the corresponding eigenvalue; the details of the argument presented in compressed form here are given in Lemma 5.11 below.

**Lemma 5.10** (Hardy inequalities) For $i \in [N]$, there exist $\tilde{C}_i > 0$ and $\hat{C}_i > 0$ such that

$$\left\| \frac{\nabla M_i}{M_i} \cdot \nabla f \right\|_{L^2_{M_i}(D_i)} \leq \tilde{C}_i \| f \|_{H^2_{M_i}(D_i)} \quad \forall f \in H^2_{M_i}(D_i)$$

(5.18)

and

$$\left\| \frac{\nabla M_i}{M_i} \cdot \nabla f \right\|_{H^1_{M_i}(D_i)} \leq \hat{C}_i \| f \|_{H^3_{M_i}(D_i)} \quad \forall f \in H^3_{M_i}(D_i).$$

(5.19)
Proof We will first prove the following inequality: If $H, \beta > 1$, then there exists $C_{H, \beta} > 0$ such that

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

(5.20)

To prove (5.20) we will use a procedure inspired by the proof of Theorem 8.2 of [26]. The first ingredient is the inequality

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

valid for all $f$ in $C^1((0,H))$, $H > 0$, such that $f(H) = 0$ (see, e.g., [36, Example 6.8.ii]). Let now $\varphi_0$ and $\varphi_1$ 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 (5.20) for $C^1([0,H])$ functions follows from

$$
\| f \|_{L^2_{\psi, \beta}((0,H))} \leq \| f_0 \|_{L^2_{\psi, \beta}((0,2H/3))} + \| f_1 \|_{L^2_{\psi, \beta}((H/3,H))}
$$

$$
\leq C_1^{1/2} \| f'_0 \|_{L^2_{\psi, \beta}((0,2H/3))} + \| (\cdot)^{-1} f_1 \|_{L^2_{\psi, \beta}((0,2H/3))}
$$

$$
\leq C_1^{1/2} \| \varphi_0 f' + \varphi'_0 f \|_{L^2_{\psi, \beta}((0,2H/3))} + 3/H \| f_1 \|_{L^2_{\psi, \beta}((H/3,H))}
$$

$$
\leq C_2 \| f'_0 \|_{L^2_{\psi, \beta}((0,2H/3))} + C_3 \| f \|_{L^2_{\psi, \beta}((0,2H/3))} + C_4 \| f \|_{L^2_{\psi, \beta}((H/3,H))}
$$

$$
\leq C_5 \left( \| f \|_{L^2_{\psi, \beta}((0,H))}^2 + \| f' \|_{L^2_{\psi, \beta}((0,H))}^2 \right)^{1/2}.
$$

The validity of the inequality for all $f \in H^1_{\psi}((0, H))$ is then a consequence of the density of $C^1([0,H])$ functions in $H^1_{\psi}((0, H))$ (cf. [26, Theorem 7.2]), the completeness of $L^2_{\psi, \beta-2}((0,H))$ and the uniqueness of the distributional limit of a sequence in $\mathcal{D}'((0,H))$.

We will prove (5.18) in the $d = 2$ case; the $d = 3$ case is analogous. Also, we will omit the spring index $i$ in order to avoid cluttering the notation. First of all, as the Maxwellian weight $M$ is regular enough and it can be bounded from below in $D^{(0)} := B(0, \sqrt{b} - \gamma/2) \subset D$, it is clear that for some $C_6 > 0$

$$
\left\| \frac{\nabla M}{M} \cdot \nabla f \right\|_{L^2_{\psi, M}(D_0)} \leq C_6 \| f \|_{H^2_{\psi, M}(D_0)} \leq C_6 \| f \|_{H^2_{\psi, M}(D)}.
$$

(5.21)

Let $E := \{ p = (p_1, p_2) \in D : |p| > \sqrt{b} - \gamma \}$; i.e., a piece of the annulus $\{ p \in D : |p| > \sqrt{b} - \gamma \}$. Let also $\tilde{E} := (0, \pi) \times (0, \gamma)$ and let $S : \tilde{E} \to E$ be the polar-to-Cartesian coordinate transformation defined by $S(\theta, \rho) = (\sqrt{b} - \rho)(\cos(\theta), \sin(\theta))$. 

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which was modified so that the radial variable grows inwards from the boundary of $D$. The transformation $S$ is smooth, orientation-preserving and its Jacobian determinant is positive and bounded away from zero. Also,

$$((\nabla S)^{-1}(\nabla S)^{-T})(\theta, \rho) = \text{diag}((\sqrt{b} - \rho)^{-2}, 1).$$

Let $\tilde{M} := M \circ S$. Then, $g \in H^m_M(E)$ if and only if $g \circ S \in H^m_{\tilde{M}}(\tilde{E})$ and, for some positive constants $c_m$ and $C_m$,

$$c_m \|g\|_{H^m_M(E)} \leq \|g \circ S\|_{H^m_{\tilde{M}}(\tilde{E})} \leq C_m \|g\|_{H^m_M(E)}. \quad (5.22)$$

Indeed, the proof for the unweighted case in Theorem 3.41 in [1] is readily adapted to our Maxwellian-weighted setting by noting that the density of $C^\infty(\tilde{E})$ in $H^m_M(E)$ and the density of $C^\infty(\tilde{E})$ in $H^m_{\tilde{M}}(\tilde{E})$, which are necessary in that proof, are consequences of Proposition 7.6 of [26] thanks to the power-like behavior of the Maxwellian weight assumed in Hypothesis D. An alternative proof, which does not rely on a density argument, can be found in Lemma B.3 of the extended version of the present paper; cf. [22].

As $M$ is radially symmetric, $\tilde{M}$ depends only on its second variable. Therefore, adopting the convention of gradients being row vectors,

$$\left(\frac{\nabla M}{M} \cdot \nabla f\right) \circ S = \frac{\nabla \tilde{M}}{\tilde{M}}(\nabla S)^{-1}(\nabla S)^{-T}(\nabla \tilde{f})^T \circ S = \frac{\partial_2 \tilde{M}}{\tilde{M}} \partial_2 \tilde{f} = \frac{h'(\cdot_2)}{h(\cdot_2)} \partial_2 \tilde{f} + \alpha(\cdot_2)^{-1} \partial_2 \tilde{f},$$

where we have used the fact that $\tilde{M}(\theta, \rho) = h(\rho)\rho^\alpha$ (cf. Hypothesis D) and have denoted $\tilde{f} = f \circ S$. We will now show that the last expression in the above chain of equalities is bounded in $L^2_{\tilde{M}}(\tilde{E})$ by $\|\tilde{f}\|_{H^2_{\tilde{M}}(\tilde{E})}$. It is immediate that this is the case for the first of its terms, on account of $h$ being regular enough and bounded away from zero. For the second term we have

$$\|\cdot_2^{-1} \partial_2 \tilde{f}\|_{L^2_{\tilde{M}}(\tilde{E})}^2 \leq C_7 \int_0^\pi \int_0^\gamma \rho^\alpha \rho^{-2} |\partial_2 \tilde{f}(\theta, \rho)|^2 \rho \rho \text{d}\theta$$

$$\leq C_8 \int_0^\pi \int_0^\gamma \rho^\alpha (|\partial_2 \tilde{f}(\theta, \rho)|^2 + |\partial_2, 2 \tilde{f}(\theta, \rho)|^2) \rho \rho \text{d}\theta$$

$$\leq C_9 \|\tilde{f}\|_{H^2_{\tilde{M}}(\tilde{E})}^2, \quad (5.23)$$

where first and third inequalities are consequences of the bilateral boundedness of $h$ and the second comes from (5.20) with $H = \gamma$ and $\beta = \alpha$ in the $\rho$-direction, which can be used for almost every $\theta \in (0, \pi)$ by virtue of Fubini’s theorem. We can then use (5.22) and deduce that

$$\left\|\frac{\nabla M}{M} \cdot \nabla f\right\|_{L^2_{\tilde{M}}(\tilde{E})} \leq C_{10} \|f\|_{H^2_M(E)}. \quad (5.24)$$
By varying the transformation \( S \) and the sets \( E \) and \( \tilde{E} \), we can get bounds analogous to (5.24) for each member of a finite open covering of the annulus \( \{ p \in D : |p| > \sqrt{b - \gamma} \} \). Combining those bounds with (5.21) we obtain (5.18).

The proof of (5.19) is completely analogous to the proof of (5.18) but for the fact that now, after performing the same localization and change of variable, it is also necessary to prove that

\[
\nabla \left( \frac{\partial_2 \tilde{M}}{M} \partial_2 \tilde{f} \right) = \nabla \left( \frac{h'(\cdot)}{h(\cdot)} \partial_2 \tilde{f} + \alpha(\cdot)^{-1} \partial_2 \tilde{f} \right) \in [L^2_m(E)]^d.
\]

Bounding the first angular derivative of \( \partial_2 \tilde{M} / \tilde{M} \partial_2 \tilde{f} \) in \( L^2_m(\tilde{E}) \) poses no new problems, as \( \tilde{M} \) depends only on the radial variable. However, doing the same with its first radial derivative brings forth a constant multiple of the term \( (\cdot)^{-2} \partial_2 \tilde{f} \), which is handled according to (cf. (5.23))

\[
\| \partial_2 (\cdot)^{-2} \partial_2 \tilde{f} \|_{L^2_m(\tilde{E})}^2 \leq C_{11} \int_0^\pi \int_0^\gamma \rho^{\alpha-4} \left| \partial_2 \tilde{f}(\theta, \rho) \right|^2 d\rho d\theta
\]

\[
\leq C_{12} \int_0^\pi \int_0^\gamma \rho^{\alpha} \sum_{k=1}^3 \partial_2^k \tilde{f}(\theta, \rho) d\rho d\theta
\]

\[
\leq C_{13} \| \tilde{f} \|_{H^3_m(\tilde{E})}^2,
\]

where the inequality (5.20) was used twice, once with \( \beta = \alpha - 2 \) and then with \( \beta = \alpha \)—the former explaining the need for demanding that \( \alpha > 3 \) in Hypothesis D. This forms the core of the proof of (5.19). \( \square \)

We now introduce, for each \( m = (m_1, \ldots, m_N) \in \mathbb{N}_0^N \), the Hilbert space (with corresponding norm)

\[
H^m_M(D) := \{ \varphi \in L^2_M(D) : \partial_{(\alpha_1,\ldots,\alpha_N)} \varphi \in L^2_M(D), \ |\alpha_i| \leq m_i, \ i \in [N] \},
\]

\[
\| \varphi \|_{H^m_M(D)} := \sum_{(\alpha_1,\ldots,\alpha_N) \in \mathbb{N}^d_0} \| \partial_{(\alpha_1,\ldots,\alpha_N)} \varphi \|_{L^2_M(D)}^2.
\]

In particular, \( H^{(0,\ldots,0)}_M(D) = L^2_M(D) \). The crucial property of these spaces we are going to use is that, given a multi-index \( \alpha \in \mathbb{N}^d_0 \) and a function \( \varphi \in H^m_M(D) \), where \( m_i \geq |\alpha| \) for some particular \( i \in [N] \),

\[
\partial_{(0,\ldots,0,\alpha_i,\ldots,0,\ldots,0)} \varphi \in H^{m'_i}_M(D), \text{ where } m'_j := \begin{cases} m_i & \text{if } i \neq j, \\ m_i - |\alpha| & \text{if } i = j. \end{cases}
\]

The following lemma holds.

**Lemma 5.11** For \( m \in \{2, 3\} \), \( H^{(m,\ldots,m)}_M(D) \subset H^{(m)}_M(D) \) with continuous embedding.
Proof We recall that, by Lemma 5.4, \((\lambda_n, e_n)_{n \in \mathbb{N}}\) as defined in (5.12) is a complete set of solutions of the \(M\)-weighted eigenvalue problem (5.9) and that the \(e_n\) have tensor-product structure. Also, by the definitions in (5.14a) and (5.14b) and (5.15), \(H_M^{(em)}(D)\) is the space of \(L^2_M(D)\) functions whose squared Fourier coefficients, weighted with the coefficients defined by

\[
\tau_n^{(m)} = \prod_{i=1}^N (\lambda_{n_i})^m \quad \forall n \in \mathbb{N}^N,
\]

have finite sum.

Let us introduce, for \(i \in [N]\), the directional operators \(L_i : \{\varphi \in L^1_{\text{loc}}(D) : \nabla q_i \varphi \in [W^1_{\text{loc}}(D)]\} \rightarrow \mathcal{D}'(D)\) defined as

\[
L_i(\varphi) := -\frac{1}{M} \text{div}_{q_i}(M \nabla q_i \varphi) + \varphi = -\Delta q_i \varphi - \frac{\nabla M_i}{M_i} \cdot \nabla q_i \varphi + \varphi.
\]  

(5.27)

Let us also introduce the abbreviations

\[
q' = (q_2, \ldots, q_N), \quad M' = \bigotimes_{i=2}^N M_i, \quad D' = \bigotimes_{i=2}^N D_i,
\]

\[
n' = (n_2, \ldots, n_N), \quad \text{and} \quad e_{n'} = \bigotimes_{i=2}^N e_{n_i}^{(i)}.
\]  

(5.28)

Suppose that \(\varphi \in H_M^{(2,0,\ldots,0)}(D)\). Repeated application of Fubini’s theorem, the equality \(\partial_\alpha [\varphi(\cdot, q')] = \partial(\alpha, 0, \ldots, 0) \varphi(\cdot, q')\) (a.e. with respect to \(q' \in D'\)) and the inequality (5.18) of Lemma 5.10 give

\[
\left\| \frac{\nabla M_1}{M_1} \cdot \nabla q_1 \varphi \right\|_{L^2_M(D)}^2 = \int_{D'} \left[ \int_{D_1} \left| \frac{\nabla M_1}{M_1} \cdot \nabla \varphi(\cdot, q') \right|^2 M_1(q') \, dq' \right] M'(q') \, dq' \leq C \int_{D'} \left[ \sum_{|\alpha| \leq 2} \| \partial_\alpha (\varphi(\cdot, q')) \|_{L^2_{M_1}(D_1)}^2 \right] M'(q') \, dq' = C \sum_{|\alpha| \leq 2} \| \partial(\alpha, 0, \ldots, 0) \varphi \|_{L^2_M(D)}^2.
\]

(5.29)

As \(q \mapsto M_1(q_1)\) is a function of \(q_1\) only,

\[
\left\| \partial(0, \beta_2, \ldots, \beta_N) \left[ \nabla M_1 \cdot \nabla q_1 \varphi \right] \right\|_{L^2_M(D)}^2 \leq C \sum_{|\alpha| \leq 2} \| \partial(0, \beta_2, \ldots, \beta_N) \varphi \|_{L^2_M(D)}^2
\]

whenever \(\partial(\beta_1, \ldots, \beta_N) \varphi \in H_M^{(2,0,\ldots,0)}(D)\), which, together with the corresponding (and straightforward) result for the operator \(\Delta q_1\) and (5.27), results in

\[
\left\| L_1(\varphi) \right\|_{H_M^{(0,2,\ldots,2)}(D)} \leq C \| \varphi \|_{H_M^{(2,\ldots,2)}(D)} \quad \forall \varphi \in H_M^{(2,\ldots,2)}(D).
\]

(5.30)
The argument leading to (5.30) can be adapted for the other directional operators $L_i$ of (5.27), so that in general we have, for $i \in [N]$,

$$
\| L_i(\varphi) \|_{H^g(i) - 2e(i)(D)} \leq C \| \varphi \|_{H^g(i)(D)} \quad \forall \varphi \in H^g(i)(D),
$$

(5.31)

where $g^{(i)} \in \mathbb{N}^N$ and $e^{(i)} \in \mathbb{N}^N$ are defined as

$$
g^{(i)} := (0, \ldots, 0, 2_{i}^{\text{th entry}}, 2, \ldots, 2) \quad \text{and} \quad e^{(i)} := (0, \ldots, 0, 1_{i}^{\text{th entry}}, 0, \ldots, 0).
$$

Therefore, as $g^{(i)} - 2e^{(i)} = g^{(i+1)}$ for $i \in [N - 1]$ and $g^{(N)} - 2e^{(N)} = (0, \ldots, 0)$, the estimates given in (5.31) can be combined to give

$$
\| (L_N \circ L_{N-1} \circ \cdots \circ L_1)(\varphi) \|_{L^2(D)} \leq C \| \varphi \|_{H^{(2,\ldots,2)}(D)} \quad \forall \varphi \in H^{(2,\ldots,2)}(D).
$$

(5.32)

Now, as the eigenfunctions $e_n$ are tensor products of eigenfunctions of the single-domain eigenvalue problems (5.8) (cf. (5.12)), Fubini’s theorem and Lemma 5.9 (which allows for safely conflating the weak derivatives of the definitions of the eigenfunctions in (5.8) and the distributional derivatives in $D_i$ induced by the operator $L_i$) yield

$$
\varphi \in H^{2e(i)}(D) \implies \langle L_i(\varphi), e_n \rangle_{L^2(D)} = \lambda^{(i)}_{n_i} \langle \varphi, e_n \rangle_{L^2(D)} \quad \forall n \in \mathbb{N}^N.
$$

(5.33)

By (5.32), Parseval’s identity and (5.33), for all $\varphi \in H^{(2,\ldots,2)}(D)$,

$$
C \| \varphi \|_{H^{(2,\ldots,2)}(D)} \geq \| (L_N \circ L_{N-1} \circ \cdots \circ L_1)(\varphi) \|_{L^2(D)}^2
= \sum_{n \in \mathbb{N}^N} \| (L_N \circ L_{N-1} \circ \cdots \circ L_1)(\varphi), e_n \|_{L^2(D)}^2
= \sum_{n \in \mathbb{N}^N} (\lambda^{(N)}_{n_N})^2 \| (L_{N-1} \circ \cdots \circ L_1)(\varphi), e_n \|_{L^2(D)}^2
= \cdots
= \sum_{n \in \mathbb{N}^N} \left[ \prod_{i=1}^N (\lambda^{(i)}_{n_i})^2 \right] \langle \varphi, e_n \rangle_{L^2(D)}^2.
$$

(5.34)

As the finiteness of the last expression in (5.34) is exactly the condition for membership in $H^{(2)}(D)$, we obtain the desired result in the case of $m = 2$.

We now turn to the case of $m = 3$. We will continue to use the abbreviations introduced in (5.28) plus $q''$, $M''$, $D''$, $n''$ and $e_{n''}$ being their analogues, with the concatenation/product considered with indices in $\{3, \ldots, N\}$ this time; thus, for example, $q'' = (q_3, \ldots, q_N)$. Further, we introduce the following abbreviations for sets of multi-indices suitable for functions defined on $D \subset (\mathbb{R}^d)^N$, $D' \subset (\mathbb{R}^d)^{N-1}$, 

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D'' ⊂ (\mathbb{R}^d)^{N-2} and their further analogues:

\[ A_j := \{ (\alpha_j, \ldots, \alpha_N) \in (\mathbb{N}^d)^{N-j+1} : 0 \leq |\alpha_i| \leq 1 \text{ } \forall i \in \{j, \ldots, N\} \} \quad \forall j \in [N]. \]  

(5.35)

Let \( \psi \) be an arbitrary member of \( H_{\hat{M}}^{[1,\ldots,1]}(D) \). Adopting, just for the rest of this proof, the convention \( \psi_\alpha = \partial_\alpha \psi \), \( \psi_{(0,\alpha')} = \partial_{(0,\alpha')} \psi \), etc., we obtain

\[ \mathcal{J}(\psi) := \sum_{\alpha \in A_1} \|\psi_\alpha\|^2_{L^2_{M_1}(D)} = \sum_{\alpha' \in A_2} \sum_{0 \leq |\alpha_1| \leq 1} \|\partial_{(\alpha_1,0,\ldots,0)} \psi_{(0,\alpha')}\|^2_{L^2_{M_1}(D)} \]

\[ = \sum_{\alpha' \in A_2} \int_D \|\psi_{(0,\alpha')}\|_{H^1_{M_1}(D_1)}^2 \|q'\|_{M'(\mathbb{R}^d)} \, dq' \]

\[ = \sum_{\alpha' \in A_2} \sum_{n_1=1}^{\infty} \lambda_{n_1}^{(1)} \int_D \|\psi_{(0,\alpha')}\|_{H^1_{M_1}(D_1)}^2 \|q'\|_{M'(\mathbb{R}^d)} \, dq' \]

\[ = \sum_{\alpha'' \in A_3} \sum_{n_1=1}^{\infty} \lambda_{n_1}^{(1)} \sum_{0 \leq |\alpha_2| \leq 1} \int_D \|\psi_{(0,\alpha_2,\alpha'')}\|_{H^1_{M_1}(D_1)}^2 \|q'\|_{M'(\mathbb{R}^d)} \, dq', \]

(5.36)

where the third equality uses the expansion property (5.10) of the eigenvalue problem (5.8) and Lebesgue’s monotone convergence theorem to turn the \( H_{\hat{M}}^{[1]}(D_1) \) norm into a sum of squared inner products and to interchange the latter and the integral with respect to \( D' \). The fourth equality is a consequence of the definition of the index sets \( A_j \) (cf. (5.35)). It is not difficult to check that for every \( n_1 \in \mathbb{N} \) and almost every \( q'' \in D'' \),

\[ \{\psi_{(0,\alpha_2,\alpha'')} : (\cdot, q''') \}^2_{L^2_{M_1}(D_1)} \]

i.e., derivatives in the \( q_2 \) direction are interchangeable with the \( L^2_{M_1}(D_1) \) inner product with \( e_{n_1}^{(1)} \). Thus, \( \mathcal{J}(\psi) \), the starting point of (5.36), is equal to

\[ \sum_{\alpha'' \in A_3} \sum_{n_1=1}^{\infty} \lambda_{n_1}^{(1)} \int_{D''} \|\psi_{(0,0,\alpha'')}\|_{L^2_{M_1}(D_1)}^2 \|q''\|_{M''(\mathbb{R}^d)} \, dq''. \]

Expanding the \( H^2_{M_2}(D_2) \) norm above according to (5.10) results, after a number of Fubini’s theorem-based rearrangements of the underlying integrals, in \( \mathcal{J}(\psi) \) being equal to

\[ \sum_{\alpha'' \in A_3} \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \lambda_{n_1}^{(1)} \lambda_{n_2}^{(2)} \int_{D''} \|\psi_{(0,0,\alpha'')}\|_{L^2_{M_1}(D_1)}^2 \|q''\|_{M''(\mathbb{R}^d)} \, dq''. \]

The process leading from the third line of (5.36) to the above expression can be repeated: \( \mathcal{J}(\psi) \) is shown to be equal to expressions like the one above with progressively smaller outermost sum index sets, more sums over \( \mathbb{N} \), lower-dimensional
integrals of higher-dimensional weighted $L^2$ inner products and involving products of more eigenvalues of the problems in (5.8). This process finally leads to

$$\sum_{n \in \mathbb{N}} \left[ \prod_{i=1}^{N} \lambda_{n_i}^{(i)} \right] \langle \psi, e_n \rangle^2_{L^2_M(D)} = \mathcal{S}(\psi) \leq C \| \psi \|^2_{H^{(1,\ldots,1)}_M(D)} \quad \forall \psi \in H^{(1,\ldots,1)}_M(D).$$

(5.37)

Now, let $\varphi \in H^{(3,\ldots,3)}_M(D)$. An argument analogous to the one presented for the case of $m = 2$, with (5.19) in place of (5.18) in (5.29), yields

$$\| (L_N \circ L_{N_1} \circ \cdots \circ L_1)(\varphi) \|_{H^{(1,\ldots,1)}_M(D)} \leq C \| \varphi \|_{H^{(3,\ldots,3)}_M(D)}.$$ Combining the above bound with (5.37) with $\psi$ chosen as $(L_N \circ L_{N_1} \circ \cdots \circ L_1)(\varphi)$, we obtain

$$\| \varphi \|_{H^{(3,\ldots,3)}_M(D)} \geq C \sum_{n \in \mathbb{N}} \left[ \prod_{i=1}^{N} (\lambda_{n_i}^{(i)})^3 \right] \langle (L_N \circ L_{N_1} \circ \cdots \circ L_1)(\varphi), e_n \rangle^2_{L^2_M(D)},$$

where the factor $\prod_{i=1}^{N} (\lambda_{n_i}^{(i)})^2$, gained in the second inequality, is obtained as in the case of $m = 2$ (cf. (5.33) and (5.34)). This completes the proof. \hfill \Box

**Remark 5.12** In the course of proving Lemma 5.11 we have also proved the continuous embedding of $H^{(1,\ldots,1)}_M(D)$ into $H^{(1)}_M(D)$. Neither this result nor the continuous embedding of $H^{(2,\ldots,2)}_M(D)$ into $H^{(2)}_M(D)$ require the full force of Hypothesis D; they remain valid if, for example, $h_i \in C^1([0, \gamma_i])$ and $\alpha_i > 1$. A close read of the proof of Lemma 5.11 reveals that, under the above relaxed conditions, we have the weaker but still useful result

$$\{ \varphi \in H^{(3,\ldots,3)}_M(D) : (L_N \circ L_{N_1} \circ \cdots \circ L_2 \circ L_1)(\varphi) \in L^2_M(D) \} \subset H^{(3)}_M(D)$$

with continuous embedding upon introducing a suitable norm for the space on the left-hand side of this inclusion.

We recall that Theorem 5.6 gives a condition on the parameter of the space $H^{(m)}_M(D)$ under which it becomes a subspace of the 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 4.8 and Theorem 4.9). Then, from Lemma 5.11 it is apparent that the space $H^{(m,\ldots,m)}_M(D)$ will be a subspace of $\mathcal{B}_1$ for a suitable choice of the parameter $m$. We shall now make this statement more precise.

**Theorem 5.13** Let $H^{(3)}_M(D)$ be defined according to (5.15), where $d \in \{2, 3\}$, as elsewhere, is the common dimensionality of the Cartesian factors that make up $D$; then,

$$H^{(3,\ldots,3)}_M(D) \subset H^{(3)}_M(D) \subset \mathcal{B}_1.$$
Lemma 5.11 gives $H_{M}^{(3,\ldots,3)}(D) \subset H_{M}^{T(3)}(D)$. As 3 is greater than $1 + \frac{d}{2}$ for both $d = 2$ and $d = 3$, Theorem 5.6 gives $H_{M}^{T(3)}(D) \subset B_{1}$. □

Remark 5.14 If the hypotheses we have been making throughout this work (i.e., Hypotheses A, B, C, and D) 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 5.6 with Lemma 5.11 and the fact that $2 > 1 + \frac{1}{2}$ yields

$H_{M}^{(2,\ldots,2)}(D) \subset H_{M}^{T(2)}(D) \subset B_{1}$.

Sobolev spaces of dominating mixed smoothness akin to $H_{M}^{(2,\ldots,2)}(D)$ can also be shown to be subspaces of the regularity class $B_{1}$ in the case of the classical Poisson problem studied in [29]: 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 $\partial D$—not a zero-weighted Sobolev space!) such that

$\langle \psi, \varphi \rangle_{H_{0}^{1}(D)} = \langle f, \varphi \rangle_{L_{2}(D)} \forall \varphi \in H_{0}^{1}(D)$,

where $D = D_{1} \otimes \ldots \otimes D_{N}$ and each $D_{i}$, $i \in [N]$, is an open interval. The corresponding greedy algorithms seek approximations that are linear combinations of $\otimes_{i \in [N]} H_{0}^{1}(D_{i})$ functions. The argument of Theorem 5.6 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 (5.8) is proportional to $n^{2}$, we have

$\left\{ \varphi \in L_{2}(D) : \sum_{n \in \mathbb{N}^{N}} \left[ \prod_{i=1}^{N} (n_{i}^{2})^{2} \right] \langle \varphi, e_{n} \rangle_{L_{2}(D)}^{2} < \infty \right\} \subset B_{1}$.

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

$H^{(2,\ldots,2)}(D) \cap H_{0}^{1}(D) = \left\{ \varphi \in L_{2}(D) : \partial_{\alpha} \varphi \in L_{2}(D), \ |\alpha|_{\infty} \leq 2 \right\} \cap H_{0}^{1}(D)$.

This characterization should be contrasted with the condition for membership in $A_{1}$ (which is identical to $B_{1}$ in this unweighted setting) derived in [29, 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 [29, Remark 4] can be generalized to the requirement that the exact solution belongs to $H^{m}(D) \cap H_{0}^{1}(D)$, with $m > 1 + N d/2$, when the factor domains are no longer one-dimensional but $d$-dimensional; and, thanks to Theorem 5.7, 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 inclusions stated in Lemma 5.11 also hold,
implying equality of the two spaces there. This is indeed the case for \( m = 2 \) in the single-domain (i.e., \( N = 1 \)) case, as it stems from the combination of Lemma 5.11 of [22] and Lemma 5.11. However, even if Lemma 5.11 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 \( H^{T(m)}_M(D) \subset \mathcal{B}_1 \). The reason is that the methods used in Lemma 5.11 to prove the continuous embeddings of spaces of the form \( H^{(m,...,m)}_M(D) \) into \( H^{T(m)}_M(D) \) are only appropriate for integer values of the parameter \( m \); indeed, we have not even defined \( H^{(m,...,m)}_M(D) \) for non-integer \( m \).

We shall address this question by using function space interpolation. We start with the fact that, given two nets of positive weights \( \Sigma^{(i)} = (\sigma^{(i)}_n)_{n \in \mathbb{N}} \), \( i \in \{1, 2\} \), one can show that for \( \theta \in (0, 1) \) the (real) \((\theta, 2)\)-interpolation space between them obeys

\[
[H^{\Sigma^{(1)}}_M(D), H^{\Sigma^{(2)}}_M(D)]_{\theta, 2} = H^{\tilde{\Sigma}}_M(D),
\]

where \( \tilde{\Sigma} = (\tilde{\sigma}_n)_{n \in \mathbb{N}} \) and \( \tilde{\sigma}_n := (\sigma^{(1)}_n)^{1-\theta}(\sigma^{(2)}_n)^{\theta} \) for all \( n \in \mathbb{N} \), with equivalence of norms (the proof is a simple modification of the argument given in [39, Chap. 23]).

As, according to the definition in (5.15),

\[
\tau^{(k+\theta)}_n = (\tau^{(k)}_n)^{1-\theta}(\tau^{(k+1)}_n)^{\theta}
\]

for all \( k \in \mathbb{N}_0, \theta \in (0, 1) \) and \( n \) in \( \mathbb{N} \), it follows that

\[
H^{T(k+\theta)}_M(D) = [H^{T(k)}_M(D), H^{T(k+1)}_M(D)]_{\theta, 2},
\]

with equivalence of norms. From Lemma 5.11 and the fact that, because of the definitions in (5.15) and (5.26a), (5.26b) \( H^{T(0)}_M(D) = H^{(0,...,0)}_M(D) = L^2_M(D) \), it follows that for \( k \in \{0, 1, 2\} \) and \( \theta \in (0, 1) \),

\[
[H^{(k,...,k)}_M(D), H^{(k+1,...,k+1)}_M(D)]_{\theta, 2} \subset H^{T(k+\theta)}_M(D),
\]

with continuous embedding. Since whenever \( m > 1 + \frac{d}{2} \) we have \( H^{T(m)}_M(D) \subset \mathcal{B}_1 \), defining \( H^{(m,...,m)}_M(D) \) as the interpolation space appearing on the left-hand side of the above inclusion if \( m \in (1, 2) \cup (2, 3) \) is an appealing idea, for then we can simply state that

\[
m > 1 + \frac{d}{2} \implies H^{(m,...,m)}_M(D) \subset \mathcal{B}_1.
\]

6 Conclusions and Directions for Future Work

We have proved the correctness (Theorem 3.4) and convergence (Theorem 4.4 and Theorem 4.7) 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 5.6), 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 5.3) and density (Corollary 4.5) properties from the spaces corresponding to the weights that appear as factors of the tensor-product weight; and eigenvalue asymptotics in the same degenerate setting (Lemma A.4 in Appendix).

The greedy algorithms described in Sect. 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 (1.4a)–(1.4d). 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. [10, §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 $\mathcal{D}$ (i.e., it is a probability density function) at almost every point in time $t$ and space $x$ 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., [10, §11.3]) is of relevance; these models are not covered by our arguments, at least not in their present form.

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Lemma A.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 $C^2_0(\Omega)$ is dense in $H^1_w(\Omega)$ and $H^1_w(\Omega) \subseteq L^2_w(\Omega)$. We further assume that

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

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

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 $u \in H^1_w(\Omega) \setminus \{0\}$ such that

$$\langle u, v \rangle_{H^1_w(\Omega)} = \lambda \langle u, v \rangle_{L^2_w(\Omega)} \quad \forall v \in H^1_w(\Omega). \quad (A.1)$$

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

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

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 $u \in H^1_w(\Omega) \setminus \{0\}$ such that

$$\langle u, v \rangle_{H^1_w(\Omega),\Theta} := \langle \nabla u, \nabla v \rangle_{L^2_w(\Omega)}^d + \Theta \langle u, v \rangle_{L^2_w(\Omega)} = \lambda_{\Theta} \langle u, v \rangle_{L^2_w(\Omega)} \quad \forall v \in H^1_w(\Omega). \quad (A.3)$$

By the hypotheses of the lemma the existence and the accumulation at $\infty$ 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:

$$\lambda_{\Theta,n} = \min_{\dim(S)=n} \max_{z \in S \setminus \{0\}} \langle z, z \rangle_{H^1_w(\Omega),\Theta} = \inf_{\dim(S)=n} \sup_{z \in S \setminus \{0\}} \langle z, z \rangle_{L^2_w(\Omega)}, \quad (A.4)$$

the second equality being a consequence of the density of $C^2_0(\Omega)$ in $H^1_w(\Omega)$ (cf. [20, Theorem 4.5.3]). Note that when $\Theta = 1$ the problem (A.3) and the problem (A.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 $C^2_0(\Omega)$ function and let $y := L^{-1} z$. Then,

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

Similarly, \( \|z\|^2_{L^2_w(\Omega)} = \|y\|^2_{L^2_w(\Omega)} \). As \( z \in C^2_0(\Omega) \) is arbitrary and \( z \mapsto L^{-1}z \) is a bijection of \( C^2_0(\Omega) \) into itself, (A.4) begets

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

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

\[
\int_{\Omega} Q_\Theta y^2 \geq \gamma_\Theta \int_{\Omega} y^2 \frac{\partial^2}{\partial z^2} \geq \frac{\gamma_\Theta}{4} \|\nabla y\|^2_{L^2_w(\Omega)}
\]

the last inequality being a multi-dimensional Hardy inequality (see, e.g., [31, Theorem 11], bearing in mind that \( \gamma_\Theta \) has been assumed to be nonpositive). In either case, we can write

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

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 \( \Omega_\varepsilon \subseteq \Omega \) 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 \( C^2_0(\Omega_\varepsilon) \) form a subspace of \( C^2_0(\Omega) \) and (A.4) imply that the eigenvalues of the unshifted problem (A.1) can be bounded from above according to

\[
\lambda_n \leq \inf_{\text{dim}(S)=n} \sup_{z \in S \setminus \{0\}} \frac{\langle z, z \rangle_{H^1_w(\Omega_\varepsilon)}}{\langle z, z \rangle_{L^2_w(\Omega_\varepsilon)}} \quad (A.6)
\]

Now, the right-hand side of (A.5) and the right-hand side of (A.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

\[
-\text{div}(w \nabla y) + wy = vw y \quad \text{in} \; \Omega_\varepsilon, \quad y = 0 \quad \text{on} \; \partial \Omega_\varepsilon.
\]
respectively. These standard eigenvalue problems obey Weyl’s law (this results from
the general Theorem 2.4 of [17] with input from the regularity result in [14, Theo-
rem 2.4]—alternatively, see [19, § VI.4.4]); that is,
\[
\lim_{\mu \to \infty} \frac{\#\{n \in \mathbb{N} : \mu_n \leq \mu\}}{\mu^{d/2}} = \frac{\alpha^{-d/2}|\Omega|}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} = \alpha^{-d/2}C > 0, \\
\lim_{\nu \to \infty} \frac{\#\{n \in \mathbb{N} : \nu_n \leq \nu\}}{\nu^{d/2}} = \frac{|\Omega_\epsilon|}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} = (1 - \epsilon)C > 0,
\]
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,
\[
\lim_{n \to \infty} \frac{\mu_n}{n^{2/d}} = \alpha C^{-2/d} \quad \text{and} \quad \lim_{n \to \infty} \frac{\nu_n}{n^{2/d}} = (1 - \epsilon)^{-2/d}C^{-2/d}.
\]
From the definition of the shifted eigenvalue problem (A.3), for any \( \Theta \), it is immediate that \( \lambda_{\Theta,n} = \lambda_n + \Theta - 1 \) for all \( n \in \mathbb{N} \). We then deduce, via the inequalities (A.5) and (A.6), that the asymptotic bounds (A.2) hold.

Remark A.2
1. It follows from the proof of Lemma A.1 that, if condition (1) holds, the constants \( c_1 \) and \( c_2 \) of (A.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 A.1 at the possible cost of having a stricter lower bound for \( \gamma_\Theta \) 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 [11]); 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 A.1 suffices.

Corollary A.3 The eigenvalues of the eigenvalue problem (5.8) associated with both the FENE model (1.2) and the CPAIL model (1.3) obey (A.2) if their parameter \( b_i \) is greater than 2 and 3, respectively.

Proof We shall apply Lemma A.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 5.2, Remark 4.6 and (2.3a) and (2.3b)). 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
\[
M_i(p) = Z_i^{-1} \left(1 - \frac{|p|^2}{b_i}\right)^{b_i/2}, \quad p \in B(0, \sqrt{b_i}),
\]
where $Z_i$ is a positive constant. A direct calculation returns that with this weight $Q_{\Theta}$ is

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

In this form, it is 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 $\phi(p) = \sqrt{b} - |p|$ for all $p$ in the domain under consideration it is easy to see that $\nabla^2 Q_{\Theta}$ is always bounded from below and uniformly continuous up to the boundary. If $b_i \in (2, 4)$, $Q_{\Theta}$ is never bounded from below, so it takes negative values and thus the infimum of $\nabla^2 Q_{\Theta}$ is strictly less than zero. As $\nabla^2$ is continuous and positive within the domain yet zero at its boundary, the existence of a $\Theta$ that makes case (2) hold is equivalent to demanding that

$$\lim_{|p| \to \sqrt{b_i}} \phi(p)^2 Q_1(p) \in (-1/4, 0].$$

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

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

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

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

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

If two weights $w$ and $\tilde{w}$ defined on a domain $\Omega$ 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, $L^2_w(\Omega)$ and $L^2_{\tilde{w}}(\Omega)$ on the one hand and $H^1_w(\Omega)$ and $H^1_{\tilde{w}}(\Omega)$ 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

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

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

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

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The inf-sup characterization (cf. (A.4)) of the successive eigenvalues of the two problems results in 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 (A.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 A.1.

**Lemma A.4** Let \( \Omega \) be an open ball in two or three dimensions and let \( w \) be a positive and continuous weight defined on \( \Omega \) with the property
\[ \sigma_1 \vartheta(p)^\alpha \leq w(p) \leq \sigma_2 \vartheta(p)^\alpha \]
for all \( p \in \Omega \) such that \( \vartheta(p) < \delta \), for some exponent \( \alpha > 1 \), for some margin \( \delta > 0 \) and some positive constants \( \sigma_1 \) and \( \sigma_2 \).

Then, the eigenvalues of the problem
\[ \langle e, v \rangle_{H_0^1(\Omega)} = \lambda \langle e, v \rangle_{L^2_w(\Omega)} \quad \forall v \in H_0^1(\Omega) \]
obey the two-sided bounds (A.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 (A.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 (A.2) (the constants involved will change, though). \( \square \)

**Remark A.5** The eigenvalue problem (5.8) 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 \( (\lambda, u) \in \mathbb{R} \times (H_0^1(\Omega) \setminus \{0\}) \) such that
\[ \int_{\Omega} (A \nabla u \cdot \nabla v + huv) \vartheta^\alpha = \lambda \int_{\Omega} buv \vartheta^\beta \quad \forall v \in H_0^1(\Omega), \quad (A.10) \]
where \( \alpha - \beta < 2/d \) (see [44, § 1] for the precise statement, which includes additional conditions on \( \Omega, A, h, b, \alpha \) and \( \beta \)). As, in the FENE and CPAIL versions of (5.8), 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 \( \vartheta \) (cf. (A.8), (A.9)), it turns out that our problem is equivalent to a problem of the form (A.10) with \( \alpha - \beta = 0 \).

The result, according to [44, Theorem 1.1] and assuming that \( b \geq 0 \) is that
\[ \lim_{\lambda \to \infty} \lambda^{-d/2} \#\{n \in \mathbb{N} : \lambda_n < \lambda\} = \frac{1}{(2\sqrt{\pi})^d \Gamma(1 + d/2)} \int_{\Omega} \frac{\vartheta^{-(\alpha-\beta)d/2}b^{d/2}}{\sqrt{\det(A)}} \quad (A.11) \]
(compare this with (A.7a), (A.7b); note also that in [44] 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, [12] 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, [40] by G.M. Taščijan (also romanized as Taschchiyan). However, the latter is also cited in [41, Theorem 1], where a generalization of (A.11) is proved, under the condition (in our notation) $d > 2$.

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