SPECTRAL GALERKIN APPROXIMATION OF FOKKER–PLANCK EQUATIONS WITH UNBOUNDED DRIFT

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Abstract. The paper is concerned with the analysis and implementation of a spectral Galerkin method for a class of Fokker–Planck equations that arises from the kinetic theory of dilute polymers. A relevant feature of the class of equations under consideration from the viewpoint of mathematical analysis and numerical approximation is the presence of an unbounded drift coefficient, involving a smooth convex potential U that is equal to $+\infty$ along the boundary ∂D of the computational domain D. Using a symmetrization of the differential operator based on the Maxwellian M corresponding to U, which vanishes along ∂D, we remove the unbounded drift coefficient at the expense of introducing a degeneracy, through M, in the principal part of the operator. The class of admissible potentials includes the FENE (finitely extendible nonlinear elastic) model. We show the existence of weak solutions to the initial-boundary-value problem, and develop a fully discrete spectral Galerkin approximation of such degenerate Fokker–Planck equations that exhibits optimal-order convergence in the Maxwellian-weighted H^1 norm on D. The theoretical results are illustrated by numerical experiments for the FENE model in two space dimensions.

Key words. Spectral methods, Fokker–Planck equations, transport-diffusion problems

1. Introduction. This paper is concerned with the numerical approximation of the Fokker–Planck equation

$$\frac{\partial \psi}{\partial t} + \underset{\sim}{\nabla}_x \cdot (\underset{\sim}{u}(\underset{\sim}{x},t)\,\psi) + \underset{\sim}{\nabla}_q \cdot \Big((\underset{\approx}{\nabla}_x\, \underset{\sim}{u}) \underset{\sim}{q}\, \psi \Big) = \varepsilon\, \Delta_x \psi + \frac{1}{2\,\lambda}\, \underset{\sim}{\nabla}_q \cdot \Big(\underset{\sim}{\nabla}_q \psi + \underset{\sim}{F}(\underset{\sim}{q})\, \psi \Big), \tag{1.1}$$

that arises from the kinetic theory of dilute polymers [6, 7]; see also [2, 3] and references therein. Here, ε and λ are two positive parameters, referred to as *center-of-mass diffusion coefficient* and *relaxation time*, respectively, $\Omega \subset \mathbb{R}^d$ is the flow-domain of the polymer and $D \subset \mathbb{R}^d$ is the set of admissible orientation vectors of polymer chains. Typically, $D = B(\underset{\sim}{0}, \sqrt{b}\,)$, where $B(\underset{\sim}{0}, s)$ is the open ball with radius s centered at the origin in $\mathbb{R}^d$ and $b > 2$ is a nondimensional parameter that measures the maximum possible extension of polymer chains; henceforth, unless otherwise stated, D will denote $B(\underset{\sim}{0}, \sqrt{b}\,)$. The equation governs the evolution, over a nonempty closed time interval $[0, T]$, of the probability density function

$$\psi\,:\,(\underset{\sim}{x}, \underset{\sim}{q}, t) \in \Omega \times D \times [0, T] \mapsto \psi(\underset{\sim}{x}, \underset{\sim}{q}, t)$$

of a $2d$-component stochastic process, with $d \in \{2, 3\}$, which models random fluctuations of polymer molecules in a solvent due to thermal agitation. The solvent is an incompressible Newtonian fluid, with velocity $\underset{\sim}{u}$, whose motion is governed by the Navier–Stokes equation forced by the divergence of the non-Newtonian extra stress tensor, defined as the second moment of the probability density function ψ. In the simplest models of this kind, elastic effects in the polymer are captured by modelling the polymer chains as pairs of massless beads connected with an elastic spring, with spring force $\underset{\sim}{F}\,:\,D \to \mathbb{R}^d$ defined by a spring potential $U\,:\,\mathbb{R}_{\geq 0} \to \mathbb{R}$ through

$$\underset{\sim}{F}(\underset{\sim}{q}) := U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)\, \underset{\sim}{q}, \qquad \underset{\sim}{q} \in D, \tag{1.2}$$

where $U \in \mathrm{C}^\infty(D)$ is an α-convex function on D, such that the (normalized) *Maxwellian*

$$\underset{\sim}{q} \mapsto M(\underset{\sim}{q}) := \frac{1}{C(b)} \exp\Big(-U(\tfrac{1}{2}|\underset{\sim}{q}|^2)\Big) \in \mathrm{L}^1(D), \qquad \text{where } C(b) := \int_D \exp\Big(-U(\tfrac{1}{2}|\underset{\sim}{q}|^2)\Big)\, \mathrm{d}\underset{\sim}{q}.$$

Here, *α-convexity* of U is to be understood in the following sense: there exists $c_0 \in \mathbb{R}_{>0}$ and $\alpha \in \mathbb{R}$ such that, for each $\underset{\sim}{q} \in D$, the Hessian

$$H(\underset{\sim}{q}) := \left(\frac{\partial^2}{\partial q_i \partial q_j}\, U(\tfrac{1}{2}|\underset{\sim}{q}|^2) \right)$$

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of U satisfies $H(\underset{\sim}{q}) \geq c_0(1-|\underset{\sim}{q}|^2/b)^\alpha \,\mathrm{Id}$, where Id is the $d \times d$ identity matrix. With $\alpha < 0$ this hypothesis is in line with the physical requirement that, in order to faithfully model *finite* extension of polymer chains, the function $\underset{\sim}{q} \mapsto U'(\frac{1}{2}|\underset{\sim}{q}|^2)$ must tend to $+\infty$ as $\mathfrak{d}(\underset{\sim}{q}) := \mathrm{dist}(\underset{\sim}{q}, \partial D) \to 0$ (in other words, an applied spring force $\underset{\sim}{F}(\underset{\sim}{q})$ with *finite* intensity $|\underset{\sim}{F}(\underset{\sim}{q})|$ can only stretch a polymer chain to a length $|\underset{\sim}{q}| < \sqrt{b}$).

We shall also assume that the Maxwellian M associated with U is a *weight function of type 3* on D in the sense of Triebel [29], p.247, Definition 3.2.1.3c; i.e., there exist positive constants c_1, c_2 and λ, and a positive monotonic increasing function τ defined on the interval $(0, \lambda)$, such that $c_1\, \tau(\mathfrak{d}(\underset{\sim}{q})) \leq M(\underset{\sim}{q}) \leq c_2\, \tau(\mathfrak{d}(\underset{\sim}{q}))$ for all $\underset{\sim}{q} \in D$ such that $\mathfrak{d}(\underset{\sim}{q}) < \lambda$.

Example 1.1. *In the case of the FENE (finitely extendible nonlinear elastic) polymer model*

$$U(s) := -\frac{b}{2}\ln\left(1-\frac{2s}{b}\right), \qquad U'(s) = \frac{1}{1-\frac{2s}{b}}, \qquad s \in [0, \tfrac{b}{2}), \qquad \textit{with } b > 2.$$

It will be shown in Section 2 that the function $\underset{\sim}{q} \in B(\underset{\sim}{0}, \sqrt{b}\,) \mapsto U(\frac{1}{2}|q|^2)$ *is* α*-convex with* $\alpha = -1$ *(or, briefly,* (-1)*-convex) and* $c_0 = 1$.

Following Kolmogorov [20], the Fokker–Planck equation can be recast as follows:

$$\frac{\partial \psi}{\partial t} + \underset{\sim}{\nabla}_x \cdot (\,\underset{\sim}{u}(\underset{\sim}{x}, t)\psi) + \underset{\sim}{\nabla}_q \cdot \left(\underset{\approx}{\kappa}(\underset{\sim}{x}, t)\, \underset{\sim}{q}\, \psi\right) = \varepsilon\, \Delta_x \psi + \frac{1}{2\,\lambda}\, \underset{\sim}{\nabla}_q \cdot \left(M(\underset{\sim}{q}) \underset{\sim}{\nabla}_q \left(\frac{\psi}{M}\right)\right),$$

where $\underset{\approx}{\kappa}(\underset{\sim}{x}, t) := (\underset{\approx}{\nabla}_x\, \underset{\sim}{u})$. The probability density ψ is a function of $2d+1$ independent variables: $\underset{\sim}{x} \in \mathbb{R}^d$, $\underset{\sim}{q} \in \mathbb{R}^d$ and $t \in \mathbb{R}_{\geq 0}$. Since the dependence of the coefficients in the equation on $\underset{\sim}{x}$ and $\underset{\sim}{q}$ is separated/factorized, an efficient approach to the numerical solution of this equation in $2d+1$ variables is based on operator-splitting with respect to $(\underset{\sim}{q}, t)$ and $(\underset{\sim}{x}, t)$; see Lozinski *et al.* [12, 13, 24]. Thereby, the resulting time-dependent transport-diffusion equation with respect to $(\underset{\sim}{x}, t)$ is completely standard, $\psi_t + \nabla_x \cdot (\underset{\sim}{u}(\underset{\sim}{x}, t)\psi) = \varepsilon \Delta_x \psi$, while the transport-diffusion equation with respect to $(\underset{\sim}{q}, t)$ is

$$\frac{\partial \psi}{\partial t} + \underset{\sim}{\nabla}_q \cdot (\underset{\approx}{\kappa}\, \underset{\sim}{q} \psi) = \frac{1}{2\lambda} \underset{\sim}{\nabla}_q \cdot \left(M(\underset{\sim}{q}) \underset{\sim}{\nabla}_q \left(\frac{\psi}{M}\right)\right), \qquad (\underset{\sim}{q}, t) \in D \times (0, T]. \tag{1.3}$$

The equation (1.3) is supplemented with the following initial and boundary conditions:

$$\psi(\underset{\sim}{q}, 0) = \psi_0(\underset{\sim}{q}), \qquad \text{for all } \underset{\sim}{q} \in D, \tag{1.4}$$

$$\psi(\underset{\sim}{q}, t) = o\left(\sqrt{M(\underset{\sim}{q})}\right), \qquad \text{as } \mathfrak{d}(\underset{\sim}{q}) \to 0, \ \text{for all } t \in (0, T]. \tag{1.5}$$

Here, the initial datum ψ_0 is such that $\psi_0 \geq 0$ and $\int_D \psi_0(\underset{\sim}{q})\, \mathrm{d}\underset{\sim}{q} = 1$.

The central difficulty, from both the analytical and the computational point of view, is now the presence in (1.3) of the degenerate Maxwellian $M(\underset{\sim}{q})$, with $\lim_{\mathfrak{d}(\underset{\sim}{q}) \to 0} M(\underset{\sim}{q}) = 0$.

Example 1.2. *In the case of the FENE model,*

$$M(\underset{\sim}{q}) = \frac{1}{C(b)} \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{\frac{b}{2}}, \qquad \underset{\sim}{q} \in D = B(\underset{\sim}{0}, \sqrt{b}\,), \qquad \textit{with } b > 2.$$

Clearly, there exist positive constants c_1 *and* c_2 *such that* $c_1 \leq M(\underset{\sim}{q})/[\mathfrak{d}(\underset{\sim}{q})]^{b/2} \leq c_2$, $\underset{\sim}{q} \in D$. *Hence* M *is a weight function of type 3 on* D. *For* $b \gg 1$, M *decays very rapidly to* 0 *as* $\underset{\sim}{q}$ *approaches* ∂D. *In numerical simulations typically* $b \in [10, 100]$.

Thus we shall ignore the coupling between the Fokker–Planck equation and the Navier–Stokes system, suppress the dependence of the probability density function ψ on the variable $\underset{\sim}{x}$, assume that the $d \times d$ *stress tensor* $\underset{\approx}{\kappa} = \underset{\approx}{\nabla}_x \underset{\sim}{u}$ is independent of $\underset{\sim}{x}$, belongs to $\mathrm{C}[0,T]^{d\times d}$ and is such that $\mathrm{tr}(\underset{\approx}{\kappa})(t) = 0$ for all $t \in [0,T]$, and we focus our attention on the numerical solution of (1.3), (1.4), (1.5). For theoretical results concerning the existence of weak solutions to coupled Navier–Stokes–Fokker–Planck systems, and a detailed survey of related literature, we refer to [2–4] and [22].

The formulation (1.3) is different from that used by Lozinski *et al.* [12, 13, 24] in their work on the deterministic simulation of polymeric fluids. From the theoretical viewpoint at least the advantage of our approach is that on putting (1.3) into weak form the diffusion operator becomes symmetric (see (1.6)) which facilitates the analysis of the Fokker–Planck equation (as was done in [2–4]). Our objective here is to discretize the weak formulation of equation (1.3) using a spectral Galerkin method in the spatial variable $\underset{\sim}{q}$ coupled with a backward Euler time discretization, and to develop the convergence analysis of this method. One can, of course, consider more accurate time discretization schemes, such as an nth-order backward differentiation formula, BDFn, $n \in \{2,\dots,6\}$, for example. High-order time discretization of the problem is, however, a secondary consideration to the central theme of the paper, and we do not discuss it here.

Let

$$\mathfrak{H} := \left\{ \varphi \in \mathrm{L}^2_{\mathrm{loc}}(D) \,:\, \int_D \left(\frac{\varphi}{\sqrt{M}}\right)^2 \mathrm{d}\underset{\sim}{q} < \infty \right\},$$

$$\mathfrak{K} := \left\{ \varphi \in \mathfrak{H} \,:\, \int_D \left(\left(\frac{\varphi}{\sqrt{M}}\right)^2 + \left|\sqrt{M}\,\underset{\sim}{\nabla}_q\Big(\frac{\varphi}{M}\Big)\right|^2 \right) \mathrm{d}\underset{\sim}{q} < \infty, \quad \frac{\varphi}{\sqrt{M}}\bigg|_{\partial D} = 0 \right\}.$$

Taking our test functions as φ/M with $\varphi \in \mathfrak{K}$, we obtain the following weak formulation of the initial-boundary-value problem (1.3).

Given $\psi_0 \in \mathfrak{H}$, find $\psi \in \mathrm{L}^\infty(0,T;\mathfrak{H}) \cap \mathrm{L}^2(0,T;\mathfrak{K})$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_D \frac{\psi\,\varphi}{M}\,\mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}\,\underset{\sim}{q})\frac{\psi}{\sqrt{M}}\cdot\sqrt{M}\,\underset{\sim}{\nabla}_q\Big(\frac{\varphi}{M}\Big)\,\mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda}\int_D \sqrt{M}\,\underset{\sim}{\nabla}_q\left(\frac{\psi}{M}\right)\cdot\sqrt{M}\,\underset{\sim}{\nabla}_q\Big(\frac{\varphi}{M}\Big)\,\mathrm{d}\underset{\sim}{q} = 0 \quad \forall \varphi \in \mathfrak{K}, \tag{1.6}$$

in the sense of distributions on $(0,T)$, and $\psi(\cdot,0) = \psi_0(\cdot)$.

Now, by introducing the notation

$$\hat{\varphi} := \frac{\varphi}{\sqrt{M}} \quad \text{and} \quad \underset{\sim}{\nabla}_M \hat{\varphi} := \sqrt{M}\,\underset{\sim}{\nabla}_q\left(\frac{\hat{\varphi}}{\sqrt{M}}\right)$$

we can reformulate (1.6) by observing that from the definition of $\mathfrak{K}$ we have

$$\varphi \in \mathfrak{K} \quad \Leftrightarrow \quad \hat{\varphi} \in \mathrm{H}^1_0(D;M) := \{\zeta \in \mathrm{H}^1(D;M) \,:\, \zeta|_{\partial D} = 0\},$$

where

$$\mathrm{H}^1(D;M) := \left\{ \zeta \in \mathrm{L}^2(D) : \|\zeta\|^2_{\mathrm{H}^1(D;M)} := \int_D \left(|\zeta|^2 + |\underset{\sim}{\nabla}_M \zeta|^2\right) \mathrm{d}\underset{\sim}{q} < \infty \right\}.$$

When applied to an element of $\mathrm{H}^1_0(D;M)$ the norm $\|\cdot\|_{\mathrm{H}^1(D;M)}$ will be written $\|\cdot\|_{\mathrm{H}^1_0(D;M)}$.

We note in passing that the substitution $\hat{\varphi} = \varphi/\sqrt{M}$ also appears in the recent paper by Du, Lu and Yu [16], though the operator $\underset{\sim}{\nabla}_M$ does not. With this notation, (1.6) has the following form.

Given $\hat{\psi}_0 := \psi_0/\sqrt{M} \in \mathrm{L}^2(D)$, find $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_D \hat{\psi}\,\hat{\varphi}\,\mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}\,\underset{\sim}{q})\hat{\psi}\cdot\underset{\sim}{\nabla}_M\hat{\varphi}\,\mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda}\int_D \underset{\sim}{\nabla}_M\hat{\psi}\cdot\underset{\sim}{\nabla}_M\hat{\varphi}\,\mathrm{d}\underset{\sim}{q} = 0 \quad \forall \hat{\varphi} \in \mathrm{H}^1_0(D;M), \tag{1.7}$$

in the sense of distributions on $(0,T)$, and $\hat{\psi}(\cdot,0) = \hat{\psi}_0(\cdot)$.

The function space $\mathrm{H}^1(D;M)$ may seem exotic; we shall see, however, that this is not so: in Section 2, we shall apply the Brascamp–Lieb inequality, with a probability measure based on the Maxwellian, to show that, when U is (-1)-convex, $\mathrm{H}^1(D;M) \cap \mathrm{C}^1(\overline{D}) = \mathrm{H}^1_0(D) \cap \mathrm{C}^1(\overline{D})$; thus, loosely speaking, from the viewpoint of $\mathrm{C}^1(\overline{D})$, $\mathrm{H}^1(D;M)$ and $\mathrm{H}^1_0(D)$ are indistinguishable. This may seem surprising since, unlike $\mathrm{H}^1_0(D)$, the definition of the weighted space $\mathrm{H}^1(D;M)$ does not explicitly enforce a zero boundary condition on ∂D on members of the space; rather, this property is implicit in the presence of the weight. The resulting connection between $\mathrm{H}^1(D;M)$ and $\mathrm{H}^1_0(D)$ is helpful for the purpose of developing Galerkin methods for (1.7), since the construction of finite-dimensional subspaces of $\mathrm{H}^1_0(D)$ and the analysis of their approximation properties are, by now, well-developed and well-understood.

In Section 3 we shall revisit the weak formulation (1.7) of the initial boundary value problem. We shall formulate a backward Euler semidiscretization of the weak formulation and show that this has a unique solution. We shall then use a compactness argument to establish the existence of weak solutions to the initial-boundary-value problem in the case of a (-1)-convex U. We also show the uniqueness of the weak solution. In the process, we shall prove the unconditional stability of the temporal semidiscretization in the $\ell^\infty(0,T;\mathrm{L}^2(D))$ and $\ell^2(0,T;\mathrm{H}^1_0(D;M))$ norms. Elliptic and parabolic operators with unbounded drift coefficients, albeit in nonconservative form, have been considered recently by Cerrai, Da Prato, Lunardi, Metafune and others (see, for example, [11, 14, 15, 25, 26]); the technique herein, based on semidiscretization in time and passage to the limit using a weak compactness argument, is different from the semigroup theoretic approach used in those papers. Our arguments do not invoke compact embedding of (Maxwellian-)weighted Sobolev spaces, and therefore no growth/decay conditions (such as a Muckenhaupt condition) need to be imposed on the Maxwellian M. This is important from the point of view of the applications we have in mind: as was noted in Example 1.2 above, in FENE type models for dilute polymers the parameter b is typically much larger than 1, and therefore the Maxwellian, for such b, decays to 0 very rapidly at the boundary of the domain, – much more rapidly than could be accommodated by the Muckenhaupt condition or related growth conditions (see, for example, Theorem 3 in [18]).

In Section 4 we develop the fully-discrete method and, using the stability results from Section 3, we derive a bound on the global error in terms of the approximation error in a suitably defined spectral projection operator.

In Section 5 we give the precise definition of our projection operator: its nonstandard form stems from a *decomposition lemma*, Lemma 5.2, for elements of an anisotropic Sobolev space. The result can be seen as a variant, in Sobolev spaces, of the Malgrange Preparation Theorem [19].

We complete our convergence analysis in Section 6 by showing that the method exhibits an optimal convergence order with respect to the discretization parameters in the Maxwellian-weighted norm $\|\cdot\|_{\ell^2(0,T;\mathrm{H}^1_0(D;M))}$.

Section 7 is devoted to numerical experiments that illustrate the performance of the method. Since the case of two space dimensions ($d = 2$) is sufficiently representative, for ease of presentation in Sections 5, 6 and 7 we have confined ourselves to this case; all of our results in Sections 5 and 6 have obvious extensions to three space dimensions. The stability bounds and existence and uniqueness results presented in Sections 3 and 4 are valid in any number of space dimensions.

2. The Brascamp–Lieb inequality. Suppose that D is a convex open set, $D \subset \mathbb{R}^d$ (e.g. $D = B(\underset{\sim}{0}, \sqrt{b}\,)$, $b > 2$). Consider a probability measure μ supported on D with density $\exp(-V(\underset{\sim}{q}))$, $\underset{\sim}{q} \in D$, with respect to the Lebesgue measure $\mathrm{d}\underset{\sim}{q}$ on $\mathbb{R}^d$, where V is a convex function on D. In particular,

$$\mu(B) = \int_B \mathrm{d}\mu = \int_B \exp(-V(\underset{\sim}{q}))\,\mathrm{d}\underset{\sim}{q},$$

for any μ-measurable set $B \subset D$, with $\mu(D) = 1$. The following geometric functional inequality comes from the paper of Bobkov & Ledoux [8].

THEOREM 2.1 (Brascamp–Lieb inequality). *Assume that V is a twice continuously differentiable and strictly convex function on a convex open set $D \subset \mathbb{R}^d$, i.e., for each $\underset{\sim}{q} \in D$, the Hessian*

$$H(\underset{\sim}{q}) := \left(\frac{\partial^2 V(\underset{\sim}{q})}{\partial q_i \partial q_j} \right)$$

is a (strictly) positive definite matrix. Then, for any sufficiently smooth function f,

$$\mathrm{Var}_\mu(f) := \mathbb{E}_\mu[(f - \mathbb{E}_\mu[f])^2] \le \int_D \langle H^{-1}(\underset{\sim}{q}) \underset{\sim}{\nabla}_q f, \underset{\sim}{\nabla}_q f \rangle \, \mathrm{d}\mu, \qquad \textit{where} \quad \mathbb{E}_\mu[f] = \int_D f \, \mathrm{d}\mu.$$

In terms of simpler notation, the Brascamp–Lieb inequality can be restated as follows

$$\int_D \left[f(\underset{\sim}{q}) - \int_D f(\underset{\sim}{p}) \, \mathrm{e}^{-V(\underset{\sim}{p})} \, \mathrm{d}\underset{\sim}{p} \right]^2 \mathrm{e}^{-V(\underset{\sim}{q})} \, \mathrm{d}\underset{\sim}{q} \le \int_D \langle H^{-1}(\underset{\sim}{q}) \underset{\sim}{\nabla}_q f, \underset{\sim}{\nabla}_q f \rangle \, \mathrm{e}^{-V(\underset{\sim}{q})} \, \mathrm{d}\underset{\sim}{q},$$

for any sufficiently smooth function f.

COROLLARY 2.2. *Assume that V is a twice continuously differentiable and α-convex function on $D = B(\underset{\sim}{0}, \sqrt{b}\,)$, in the sense that there exists $c_0 > 0$ and $\alpha \in \mathbb{R}$ such that, for each $\underset{\sim}{q} \in D$ the Hessian $H(\underset{\sim}{q})$ of V satisfies $H(q) \ge c_0(1 - |\underset{\sim}{q}|^2/b)^\alpha \, \mathrm{Id}$, where Id is the $d \times d$ identity matrix. Then, for any sufficiently smooth function f,*

$$\int_D \left[f(\underset{\sim}{q}) - \int_D f(\underset{\sim}{p}) \, \mathrm{e}^{-V(\underset{\sim}{p})} \, \mathrm{d}\underset{\sim}{p} \right]^2 \mathrm{e}^{-V(\underset{\sim}{q})} \, \mathrm{d}\underset{\sim}{q} \le \frac{1}{c_0} \int_D \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right)^{-\alpha} \mathrm{e}^{-V(\underset{\sim}{q})} \, |\underset{\sim}{\nabla}_q f(\underset{\sim}{q})|^2 \, \mathrm{d}\underset{\sim}{q}.$$

Proof. Under the hypotheses of the corollary,

$$\underset{\sim}{\xi}^{\mathrm{T}} H(\underset{\sim}{q}) \underset{\sim}{\xi} \ge c_0 \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right)^\alpha |\underset{\sim}{\xi}|^2 \qquad \forall \underset{\sim}{\xi} \in \mathbb{R}^d, \quad |\underset{\sim}{q}| < \sqrt{b}.$$

Since $H(\underset{\sim}{q})$ is a symmetric matrix, we deduce that

$$\langle H(\underset{\sim}{q})^{-1} \underset{\sim}{\eta}, \underset{\sim}{\eta} \rangle = \underset{\sim}{\eta}^{\mathrm{T}} H(\underset{\sim}{q})^{-1} \underset{\sim}{\eta} \le \frac{1}{c_0} \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right)^{-\alpha} |\underset{\sim}{\eta}|^2 \qquad \forall \underset{\sim}{\eta} \in \mathbb{R}^d, \quad |\underset{\sim}{q}| < \sqrt{b}.$$

In particular, taking $\underset{\sim}{\eta} = \underset{\sim}{\nabla}_q f$, we obtain

$$\langle H(q)^{-1} \underset{\sim}{\nabla}_q f, \underset{\sim}{\nabla}_q f \rangle \le \frac{1}{c_0} \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right)^{-\alpha} |\underset{\sim}{\nabla}_q f(\underset{\sim}{q})|^2.$$

The Brascamp–Lieb inequality then implies the stated result. ☐

2.1. Application to the FENE potential. Let $D = B(\underset{\sim}{0}, \sqrt{b}\,)$ where $b > 2$, and define

$$U_\beta(s) := -\frac{\beta}{2} \ln \left(1 - \frac{2s}{b} \right),$$

where $0 \le s < \frac{b}{2}$, $\beta = b - 2\gamma$, $0 \le \gamma \le 1$. The FENE potential corresponds to $\beta = b$ (*i.e.*, to $\gamma = 0$). Further, let

$$C(\beta) := \int_D \mathrm{e}^{-U_\beta(\frac{1}{2}|\underset{\sim}{q}|^2)} \, \mathrm{d}\underset{\sim}{q}, \quad M_\beta(\underset{\sim}{q}) := \frac{1}{C(\beta)} \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right)^{\frac{b}{2}} = \frac{C(b)}{C(\beta)} M(\underset{\sim}{q}),$$

$$V(\underset{\sim}{q}) := U_\beta\left(\tfrac{1}{2} |\underset{\sim}{q}|^2 \right) + \ln C(\beta) = -\frac{\beta}{2} \ln \left(1 - \frac{|\underset{\sim}{q}|^2}{b} \right) + \ln C(\beta).$$

Note that the exponent in M_β is $b/2$, not $\beta/2$. Then,

$$\mu(D) = \int_D \mathrm{e}^{-V(\underset{\sim}{q})}\, \mathrm{d}\underset{\sim}{q} = 1, \quad \mathrm{e}^{-V(\underset{\sim}{q})} = \frac{1}{C(\beta)}\left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{\frac{\beta}{2}},$$

and therefore,

$$\int_D \left[f(\underset{\sim}{q}) - \int_D f(\underset{\sim}{p}) \frac{1}{C(\beta)}\left(1 - \frac{|\underset{\sim}{p}|^2}{b}\right)^{\frac{\beta}{2}} \mathrm{d}\underset{\sim}{p} \right]^2 \frac{1}{C(\beta)}\left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{\frac{\beta}{2}} \mathrm{d}\underset{\sim}{q}$$

$$\leq \int_D \langle H^{-1}(\underset{\sim}{q})\, \underset{\sim}{\nabla}_q f, \underset{\sim}{\nabla}_q f\rangle \frac{1}{C(\beta)}\left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{\frac{\beta}{2}} \mathrm{d}\underset{\sim}{q}.$$

In order to further bound the right-hand side above, note that, for all $\underset{\sim}{\xi} \in \mathbb{R}^d$ and all $\underset{\sim}{q} \in D$,

$$\sum_{i=1,\, j=1}^{d} \xi_i \xi_j \frac{\partial^2 V(\underset{\sim}{q})}{\partial q_i \partial q_j} = \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{-2} \left\{ \frac{\beta}{b}|\underset{\sim}{\xi}|^2 \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right) + \frac{2\beta}{b^2}\langle \underset{\sim}{\xi}, \underset{\sim}{q}\rangle^2 \right\} \geq \frac{\beta}{b}\left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{-1} |\underset{\sim}{\xi}|^2.$$

Thus, the assumptions of the above corollary are satisfied with $c_0 = \beta/b$ and $\alpha = -1$. Hence,

$$\int_D \left[f(\underset{\sim}{q}) - \int_D f(\underset{\sim}{p}) M_\beta(\underset{\sim}{p}) \left(1 - \frac{|\underset{\sim}{p}|^2}{b}\right)^{-\gamma} \mathrm{d}\underset{\sim}{p} \right]^2 M_\beta(\underset{\sim}{q}) \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{-\gamma} \mathrm{d}\underset{\sim}{q}$$

$$\leq \frac{b}{\beta} \int_D |\underset{\sim}{\nabla}_q f(\underset{\sim}{q})|^2 M_\beta(\underset{\sim}{q}) \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{1-\gamma} \mathrm{d}\underset{\sim}{q},$$

where $\gamma \in [0,1]$. We shall consider the two extreme cases: $\gamma = 0$ and $\gamma = 1$.

2.1.1. Case 1. Let $\gamma = 0$ (whereupon $\beta = b$). Then, by writing $M(\underset{\sim}{q}) := M_b(\underset{\sim}{q})$, taking $f = \hat{\psi}/\sqrt{M}$ and bounding, for $\underset{\sim}{q} \in D$, the factor $1 - |\underset{\sim}{q}|^2/b$ on the right-hand side by 1, we get

$$\int_D \left[\hat{\psi} - \sqrt{M(\underset{\sim}{q})} \int_D \hat{\psi}(\underset{\sim}{p}) \sqrt{M(\underset{\sim}{p})}\, \mathrm{d}\underset{\sim}{p} \right]^2 \mathrm{d}\underset{\sim}{q} \leq \int_D |\underset{\sim}{\nabla}_M \hat{\psi}|^2 \, \mathrm{d}\underset{\sim}{q}.$$

This implies the following Friedrichs inequality, by noting that $\mathrm{Ker}(\underset{\sim}{\nabla}_M) = \{\lambda\sqrt{M} \,:\, \lambda \in \mathbb{R}\}$:

$$\inf_{c \in \mathrm{Ker}(\underset{\sim}{\nabla}_M)} \int_D |\hat{\psi} - c\,|^2 \, \mathrm{d}\underset{\sim}{q} \leq \int_D |\underset{\sim}{\nabla}_M \hat{\psi}|^2 \, \mathrm{d}\underset{\sim}{q}. \tag{2.1}$$

2.1.2. Case 2. Let $\gamma = 1$, take $f = \hat{\psi}/\sqrt{M}$ and note that M_β and M only differ by the multiplicative factor $C(b)/C(\beta)$, where $\beta = b - 2$ with $b > 2$. Then,

$$\int_D \left[\hat{\psi}(\underset{\sim}{q}) - \frac{C(b)\sqrt{M(\underset{\sim}{q})}}{C(b-2)} \int_D \hat{\psi}(\underset{\sim}{p}) M_\beta(\underset{\sim}{p}) \left(1 - \frac{|\underset{\sim}{p}|^2}{b}\right)^{-1} \mathrm{d}\underset{\sim}{p} \right]^2 \left(1 - \frac{|\underset{\sim}{q}|^2}{b}\right)^{-1} \mathrm{d}\underset{\sim}{q} \leq \frac{b}{b-2} \int_D |\underset{\sim}{\nabla}_M \hat{\psi}|^2 \, \mathrm{d}\underset{\sim}{q}.$$

Hence, we obtain the following Hardy–Friedrichs inequality:

$$\inf_{c \in \mathrm{Ker}(\underset{\sim}{\nabla}_M)} \int_D \frac{|\hat{\psi} - c\,|^2}{1 - \frac{|\underset{\sim}{q}|^2}{b}} \, \mathrm{d}\underset{\sim}{q} \leq \frac{b}{b-2} \int_D |\underset{\sim}{\nabla}_M \hat{\psi}|^2 \, \mathrm{d}\underset{\sim}{q}. \tag{2.2}$$

This can be seen as a refinement of the Friedrichs inequality (2.1) in the sense that the left-hand side of (2.2) is an upper bound on the left-hand side of (2.1) (at the expense of increasing the multiplicative constant on the right-hand side of (2.1) from 1 to $b/(b-2)$, $b > 2$).

The inequalities (2.1) and (2.2) hold, in particular, for any $\hat{\psi} \in \sqrt{M}\,\mathrm{C}^\infty(\overline{D})$. Next, we shall show by a density argument that they are also valid for all $\hat{\psi} \in \mathrm{H}^1(D;M)$.

Recall from Example 1.2 that the FENE Maxwellian M is a weight function of type 3 on D. According to [29], Theorem 3.2.2a, the weighted Sobolev space $\mathrm{H}^1_M(D) = \{v \in \mathrm{L}^2_M(D) : \underset{\sim}{\nabla}_q v \in \mathrm{L}^2_M(D)^d\}$ is a Hilbert space with respect to the norm $\|\cdot\|_{\mathrm{H}^1_M(D)}$ defined by

$$\|v\|_{\mathrm{H}^1_M(D)} := \left(\|v\|^2_{\mathrm{L}^2_M(D)} + \|\underset{\sim}{\nabla}_q v\|^2_{\mathrm{L}^2_M(D)}\right)^{\frac{1}{2}},$$

and $\mathrm{L}^2_M(D) = (1/\sqrt{M})\,\mathrm{L}^2(D)$ is a Hilbert space with respect to the norm $\|\cdot\|_{\mathrm{L}^2_M(D)}$ defined by $\|v\|_{\mathrm{L}^2_M(D)} := \|\sqrt{M}v\|$, where $\|\cdot\|$ denotes the $\mathrm{L}^2(D)$ norm induced by the $\mathrm{L}^2(D)$ inner product $(\cdot,\cdot)$. By [29], Theorem 3.2.2c, $\mathrm{C}^\infty(\overline{D})$ is dense in both $\mathrm{H}^1_M(D)$ and $\mathrm{L}^2_M(D)$; see also Chapter I, §7, in Kufner [21]. Thus, $\sqrt{M}\,\mathrm{C}^\infty(\overline{D})$ is dense in the Hilbert spaces $\mathrm{H}^1(D;M)$ and $\mathrm{L}^2(D)$, whereby it is also dense in $\mathrm{H}^1_0(D;M)$; therefore $\mathrm{H}^1_0(D;M)$ is dense in $\mathrm{L}^2(D)$. In any case, it follows that (2.1) and (2.2) hold for all $\hat{\psi} \in \mathrm{H}^1(D;M)$. In particular, we see from (2.2) that each $\hat{\psi} \in \mathrm{H}^1(D;M) \cap \mathrm{C}(\overline{D})$ must vanish on ∂D, and hence $\mathrm{H}^1(D;M) \cap \mathrm{C}^1(\overline{D}) \subset \mathrm{H}^1_0(D) \cap \mathrm{C}^1(\overline{D})$.

Conversely, it follows from Hardy's inequality stated in Triebel [29] (see Section 3.2.6, Lemma 1, part (a), with $p = 2$, $\mu = 0$, $m = 1$) and Poincaré's inequality on $\mathrm{H}^1_0(D)$ that

$$\int_D \frac{|\hat{\psi}(\underset{\sim}{q})|^2}{\left|1 - \frac{|\underset{\sim}{q}|^2}{b}\right|^2}\,\mathrm{d}\underset{\sim}{q} \le C(b)\|\underset{\sim}{\nabla}_q \hat{\psi}\|^2_{\mathrm{L}^2(D)} \qquad \forall \hat{\psi} \in \mathrm{H}^1_0(D).$$

Since $\underset{\sim}{\nabla}_M \hat{\psi} = \underset{\sim}{\nabla}_q \hat{\psi} + \frac{1}{2}\underset{\sim}{q}U'\left(\frac{1}{2}|\underset{\sim}{q}|^2\right)\hat{\psi}$, we have, by the triangle inequality, that

$$\|\underset{\sim}{\nabla}_M \hat{\psi}\| \le \|\underset{\sim}{\nabla}_q \hat{\psi}\| + \frac{1}{2}\sqrt{b}\left(\int_D \frac{|\hat{\psi}(\underset{\sim}{q})|^2}{\left|1 - \frac{|\underset{\sim}{q}|^2}{b}\right|^2}\,\mathrm{d}\underset{\sim}{q}\right)^{\frac{1}{2}}.$$

The last two inequalities give that $\mathrm{H}^1_0(D) \subset \mathrm{H}^1(D;M)$; hence, $\mathrm{H}^1_0(D) \cap \mathrm{C}^1(\overline{D}) \subset \mathrm{H}^1(D;M) \cap \mathrm{C}^1(\overline{D})$. Thus, for the FENE potential, $\mathrm{H}^1(D;M) \cap \mathrm{C}^1(\overline{D}) = \mathrm{H}^1_0(D) \cap \mathrm{C}^1(\overline{D}) = \mathrm{H}^1_0(D;M) \cap \mathrm{C}^1(\overline{D})$, $\mathrm{H}^1_0(D) \subset \mathrm{H}^1_0(D;M)$, and $\mathrm{H}^1_0(D;M)$ is continuously and densely imbedded into $\mathrm{L}^2(D)$. The same statements apply for any Maxwellian M that is a weight function of type 3 on D and stems from a potential $U \in \mathrm{C}^\infty(D)$ that is α-convex on D with $\alpha = -1$. These observations will be relevant in Section 3, and in Section 5 for the choice of the Galerkin subspaces of $\mathrm{H}^1_0(D;M)$ from which approximations to $\hat{\psi} \in \mathrm{H}^1_0(D;M)$ are sought. Thus we assume in what follows that $U \in \mathrm{C}^\infty(D)$ is (-1)-convex.

3. Backward Euler semidiscretization: existence and uniqueness of weak solutions. As was noted in the Introduction, by setting $\hat{\psi}(\cdot,t) := \psi(\cdot,t)/\sqrt{M}$ for $t \in [0,T]$ and $\hat{\varphi} := \varphi/\sqrt{M}$ in (1.6) and writing $\hat{\psi}_0 := \psi_0/\sqrt{M}$, we arrive at the following weak formulation of the initial-boundary-value problem (1.3), (1.4), (1.5):

Given $\hat{\psi}_0 \in \mathrm{L}^2(D)$, find $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ such that (1.7) holds in the sense of distributions on $(0,T)$, and $\hat{\psi}(\cdot,0) = \hat{\psi}_0(\cdot)$.

The function ψ, representing a weak solution to the problem (1.6), is then recovered from $\hat{\psi}$ through the substitution $\psi := \sqrt{M}\,\hat{\psi}$. Thus, instead of constructing a Galerkin approximation to

ψ, our aim is to construct a Galerkin approximation to $\hat{\psi}$ from a finite-dimensional subspace of the function space $\mathrm{H}^1_0(D;M)$; we shall then produce an approximation to ψ by multiplying the approximation to $\hat{\psi}$ by $\sqrt{M}$. First, however, we shall construct a time-semidiscretization of (1.7) and use a compactness argument to show the existence of weak solutions; we shall then also show the uniqueness of weak solutions.

Let $N_T \geq 1$ be an integer, $\Delta t = T/N_T$, and $t^n = n\Delta t$, for $n = 0, 1, \ldots, N_T$. Discretizing (1.7) in time using the backward Euler method yields the following semi-discrete numerical scheme.

Given $\hat{\psi}^0 := \hat{\psi}_0 = \psi_0/\sqrt{M} \in \mathrm{L}^2(D)$, find $\hat{\psi}^n \in \mathrm{H}^1_0(D;M)$, $n = 1, \ldots, N_T$, such that

$$\int_D \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\, \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}^{n+1}\, \underset{\sim}{q}\, \hat{\psi}^{n+1}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda} \int_D \underset{\sim}{\nabla}_M \hat{\psi}^{n+1} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} = 0$$
$$\forall \hat{\varphi} \in \mathrm{H}^1_0(D;M), \quad n = 0, \ldots, N_T - 1. \tag{3.1}$$

Let us first show that for any Δt, sufficiently small, this problem has a unique solution. To this end, we consider the bilinear form $B(\cdot,\cdot)$ defined on $\mathrm{H}^1_0(D;M) \times \mathrm{H}^1_0(D;M)$ by

$$B(\hat{\psi}, \hat{\varphi}) := \frac{1}{\Delta t} \int_D \hat{\psi}\, \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}^{n+1}\, \underset{\sim}{q}\, \hat{\psi}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda} \int_D \underset{\sim}{\nabla}_M \hat{\psi} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q},$$

and, for $\hat{\psi}^n \in \mathrm{L}^2(D)$ fixed, we define the linear functional $\ell(\hat{\psi}^n; \cdot)$ on $\mathrm{H}^1_0(D;M)$ by

$$\ell(\hat{\psi}^n; \hat{\varphi}) := \frac{1}{\Delta t} \int_D \hat{\psi}^n\, \hat{\varphi}\, \mathrm{d}\underset{\sim}{q}.$$

Clearly,

$$B(\hat{\psi}, \hat{\psi}) \geq \frac{1}{\Delta t} \left(1 - \Delta t \lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right) \int_D |\hat{\psi}|^2\, \mathrm{d}\underset{\sim}{q} + \frac{1}{4\lambda} \int_D |\underset{\sim}{\nabla}_M \hat{\psi}|^2\, \mathrm{d}\underset{\sim}{q},$$

and therefore, on assuming that $\Delta t \lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)} < 1$ and letting

$$c_{\Delta t} := \frac{1}{\Delta t} \left(1 - \Delta t \lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right) (> 0)\,,$$

we deduce that

$$B(\hat{\psi}, \hat{\psi}) \geq \min\left(c_{\Delta t}, \frac{1}{4\lambda}\right) \|\hat{\psi}\|^2_{\mathrm{H}^1_0(D;M)}. \tag{3.2}$$

Also, by a simple application of the Cauchy–Schwarz inequality, $B(\cdot,\cdot)$ is a bounded bilinear functional on $\mathrm{H}^1_0(D;M) \times \mathrm{H}^1_0(D;M)$ and, for any $\hat{\psi}^n \in \mathrm{L}^2(D)$, $\ell(\hat{\psi}^n; \cdot)$ is a bounded linear functional on $\mathrm{H}^1_0(D;M)$. Since $\mathrm{H}^1_0(D;M)$ is a Hilbert space with norm $\|\cdot\|_{\mathrm{H}^1_0(D;M)}$, the Lax–Milgram Theorem implies the existence of a unique solution $\hat{\psi}^{n+1} \in \mathrm{H}^1_0(D;M)$ such that

$$B(\hat{\psi}^{n+1}, \hat{\varphi}) = \ell(\hat{\psi}^n; \hat{\varphi}) \qquad \forall \hat{\varphi} \in \mathrm{H}^1_0(D;M), \qquad n = 0, 1, \ldots, N_T - 1. \tag{3.3}$$

As $\hat{\psi}^0 \in \mathrm{L}^2(D)$, we have thus shown that, for any $\Delta t = T/N_T$ such that $\Delta t \lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)} < 1$, the problem (3.1) has a unique solution $\{\hat{\psi}^n \in \mathrm{H}^1_0(D;M) : n = 1, \ldots, N_T\}$.

For the purposes of the convergence analysis which will be carried out below, we consider an extended version of the scheme (3.1) with a non-zero right-hand side:

$$\int_D \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\, \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}^{n+1}\, \underset{\sim}{q}\, \hat{\psi}^{n+1}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda} \int_D \underset{\sim}{\nabla}_M \hat{\psi}^{n+1} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q}$$
$$= \int_D \mu^{n+1} \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} + \int_D \underset{\sim}{\nu}^{n+1} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\, \mathrm{d}\underset{\sim}{q} \qquad \forall \hat{\varphi} \in \mathrm{H}^1_0(D;M), \quad n = 0, \ldots, N_T - 1, \tag{3.4}$$

where $\mu^{n+1} \in \mathrm{L}^2(D)$ and $\underset{\sim}{\nu}^{n+1} \in \mathrm{L}^2(D)^d$ for all $n \geq 0$. We have the following stability result for the extended scheme (3.4).

LEMMA 3.1 (*The first stability inequality*). *Let* $\Delta t = T/N_T$, $N_T \geq 1$, $\underset{\approx}{\kappa} \in \mathrm{C}[0,T]^{d\times d}$, $\hat{\psi}^0 \in \mathrm{L}^2(D)$, *and define* $c_0 := 1 + 4\lambda b\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}$. *If* Δt *is such that* $0 < c_0\Delta t \leq 1/2$, *then we have, for all* m *such that* $1 \leq m \leq N_T$,

$$\|\hat{\psi}^m\|^2 + \sum_{n=0}^{m-1} \Delta t \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}} \right\|^2 + \sum_{n=0}^{m-1} \frac{\Delta t}{2\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 \leq \mathrm{e}^{2c_0 m\Delta t} \left\{ \|\hat{\psi}^0\|^2 + \sum_{n=0}^{m-1} 2\Delta t \left(\|\mu^{n+1}\|^2 + 4\lambda \|\underset{\sim}{\nu}^{n+1}\|^2 \right) \right\}. \tag{3.5}$$

We shall denote the right-hand side of (3.5) *by* $\mathfrak{S}(\hat{\psi}^0, \mu, \underset{\sim}{\nu}, m\Delta t)$.

Proof. Let $0 \leq n \leq N_T - 1$. Setting $\hat{\varphi} = \hat{\psi}^{n+1}$, we write the first term in (3.4) as

$$\int_D \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\, \hat{\psi}^{n+1}\, \mathrm{d}\underset{\sim}{q} = \frac{1}{2\Delta t}\left(\|\hat{\psi}^{n+1}\|^2 - \|\hat{\psi}^n\|^2 \right) + \frac{1}{2\Delta t}\|\hat{\psi}^{n+1} - \hat{\psi}^n\|^2$$

using the identity $(a-b)a = \frac{1}{2}(a^2 - b^2) + \frac{1}{2}(a-b)^2$.

Applying the Cauchy–Schwarz inequality to the transport term in (3.4), we have

$$\int_D (\underset{\approx}{\kappa}^{n+1}\, \underset{\sim}{q}\, \hat{\psi}^{n+1}) \cdot \underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\, \mathrm{d}\underset{\sim}{q} \leq \|\underset{\approx}{\kappa}^{n+1} \underset{\sim}{q}\|_{\mathrm{L}^\infty(D)} \int_D |\hat{\psi}^{n+1}|\, |\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}|\, \mathrm{d}\underset{\sim}{q} \leq \sqrt{b}\, |\underset{\approx}{\kappa}^{n+1}|\, \|\hat{\psi}^{n+1}\|\, \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|.$$

Combining these results and applying the Cauchy-Schwarz inequality to the right-hand side terms in (3.4), we have

$$\begin{aligned} &\|\hat{\psi}^{n+1}\|^2 + \|\hat{\psi}^{n+1} - \hat{\psi}^n\|^2 + \frac{\Delta t}{\lambda}\|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 \\ &\quad\leq \|\hat{\psi}^n\|^2 + 2\Delta t\sqrt{b}\, |\underset{\approx}{\kappa}^{n+1}| \|\hat{\psi}^{n+1}\| \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\| \\ &\qquad + 2\Delta t \|\mu^{n+1}\| \|\hat{\psi}^{n+1}\| + 2\Delta t \|\underset{\sim}{\nu}^{n+1}\| \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\| \\ &\quad =: \|\hat{\psi}^n\|^2 + \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{T}_3. \end{aligned}$$

Using the inequality $2ab \leq \varepsilon a^2 + \frac{1}{\varepsilon} b^2$ on each of T_1 and T_3, we deduce that

$$\begin{aligned} \mathrm{T}_1 &\leq \varepsilon \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 + \frac{1}{\varepsilon}\Delta t^2 b |\underset{\approx}{\kappa}^{n+1}|^2 \|\hat{\psi}^{n+1}\|^2, \\ \mathrm{T}_3 &\leq \varepsilon \|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 + \frac{1}{\varepsilon}\Delta t^2 \|\underset{\sim}{\nu}^{n+1}\|^2. \end{aligned}$$

Choosing $\varepsilon = \Delta t/(4\lambda)$ then gives

$$\begin{aligned} &\|\hat{\psi}^{n+1}\|^2 + \|\hat{\psi}^{n+1} - \hat{\psi}^n\|^2 + \frac{\Delta t}{2\lambda}\|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 \\ &\quad\leq \|\hat{\psi}^n\|^2 + 4\Delta t \lambda b |\underset{\approx}{\kappa}^{n+1}|^2 \|\hat{\psi}^{n+1}\|^2 + 4\Delta t \lambda \|\underset{\sim}{\nu}^{n+1}\|^2 + \mathrm{T}_2. \end{aligned}$$

Similarly, we have

$$\mathrm{T}_2 \leq \Delta t \|\hat{\psi}^{n+1}\|^2 + \Delta t \|\mu^{n+1}\|^2,$$

and therefore, on defining $c_0 := 1 + 4\lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}$, we get that

$$\begin{aligned} &(1 - c_0\Delta t)\|\hat{\psi}^{n+1}\|^2 + \|\hat{\psi}^{n+1} - \hat{\psi}^n\|^2 + \frac{\Delta t}{2\lambda}\|\underset{\sim}{\nabla}_M \hat{\psi}^{n+1}\|^2 \\ &\quad\leq \|\hat{\psi}^n\|^2 + \Delta t \|\mu^{n+1}\|^2 + 4\Delta t \lambda \|\underset{\sim}{\nu}^{n+1}\|^2. \end{aligned}$$

As $c_0\Delta t \le \frac{1}{2}$, dividing through by $(1 - c_0\Delta t)$ and using the fact that $1 \le \frac{1}{1-c_0\Delta t} \le 2$, we have

$$
\begin{aligned}
&\|\hat\psi^{n+1}\|^2 + \|\hat\psi^{n+1} - \hat\psi^n\|^2 + \frac{\Delta t}{2\lambda}\|\underset{\sim}{\nabla}_M \hat\psi^{n+1}\|^2 \\
&\quad \le \frac{1}{1-c_0\Delta t}\left(\|\hat\psi^n\|^2 + \Delta t\|\mu^{n+1}\|^2 + 4\Delta t\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right) \\
&\qquad \le (1+2c_0\Delta t)\|\hat\psi^n\|^2 + 2\Delta t\left(\|\mu^{n+1}\|^2 + 4\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right).
\end{aligned}
\tag{3.6}
$$

Summing over $n = 0, \dots, m-1$ in (3.6) we obtain

$$
\begin{aligned}
&\|\hat\psi^m\|^2 + \sum_{n=0}^{m-1}\Delta t\left\|\frac{\hat\psi^{n+1} - \hat\psi^n}{\sqrt{\Delta t}}\right\|^2 + \sum_{n=0}^{m-1}\frac{\Delta t}{2\lambda}\|\underset{\sim}{\nabla}_M \hat\psi^{n+1}\|^2 \\
&\quad \le \left\{\|\hat\psi^0\|^2 + \sum_{n=0}^{m-1} 2\Delta t\left(\|\mu^{n+1}\|^2 + 4\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right)\right\} + 2c_0\sum_{n=0}^{m-1}\Delta t\|\hat\psi^n\|^2,
\end{aligned}
\tag{3.7}
$$

for all $m \in \{1, \dots, N_T\}$. Inequality (3.7) has the form

$$
\alpha_m + \sum_{n=0}^{m-1}\Delta t\,\beta_n \le (\alpha_0 + \gamma_m) + 2c_0\sum_{n=0}^{m-1}\Delta t\,\alpha_n, \qquad 1 \le m \le N_T,
$$

where $(\alpha_m)_{m\ge0}$, $(\beta_m)_{m\ge0}$ and $(\gamma_m)_{m\ge1}$ are three sequences of non-negative real numbers, and the sequence $(\gamma_m)_{m\ge1}$ is nondecreasing. Hence, by induction (or by a discrete Gronwall Lemma),

$$
\alpha_m + \sum_{n=0}^{m-1}\Delta t\,\beta_n \le (1+2c_0\Delta t)^m\alpha_0 + (1+2c_0\Delta t)^{m-1}\gamma_m, \qquad 1 \le m \le N_T.
$$

On taking

$$
\begin{aligned}
&\alpha_m := \|\hat\psi^m\|^2, \qquad \beta_m := \left\|\frac{\hat\psi^{m+1} - \hat\psi^m}{\sqrt{\Delta t}}\right\|^2 + \frac{1}{2\lambda}\|\underset{\sim}{\nabla}_M \hat\psi^{m+1}\|^2, \\
&\gamma_m := \sum_{n=0}^{m-1} 2\Delta t\left(\|\mu^{n+1}\|^2 + 4\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right)
\end{aligned}
$$

and using that

$$
(1+2c_0\Delta t)^{m-1} \le (1+2c_0\Delta t)^m \le \mathrm{e}^{2c_0 m\Delta t}, \qquad m \ge 1,
$$

we then deduce that

$$
\begin{aligned}
&\|\hat\psi^m\|^2 + \sum_{n=0}^{m-1}\Delta t\left\|\frac{\hat\psi^{n+1} - \hat\psi^n}{\sqrt{\Delta t}}\right\|^2 + \sum_{n=0}^{m-1}\frac{\Delta t}{2\lambda}\|\underset{\sim}{\nabla}_M \hat\psi^{n+1}\|^2 \\
&\quad \le \mathrm{e}^{2c_0 m\Delta t}\left\{\|\hat\psi^0\|^2 + \sum_{n=0}^{m-1} 2\Delta t\left(\|\mu^{n+1}\|^2 + 4\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right)\right\}, \qquad 1 \le m \le N_T.
\end{aligned}
$$

That completes the proof. □

We shall now use this stability result to show the existence of weak solutions via a weak compactness argument. We shall also show the uniqueness of the weak solution.

THEOREM 3.2. *Suppose that $\hat\psi_0 \in \mathrm{L}^2(D)$ and $\underset{\approx}{\kappa} \in \mathrm{C}[0,T]^{d\times d}$. Then, there exists a unique function $\hat\psi \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ such that $\hat\psi \in \mathrm{C}_{\text{weak}}([0,T];\mathrm{L}^2(D))$,*

$$
(\hat\psi(\cdot,0) - \hat\psi_0, \hat w) = 0 \qquad \forall \hat w \in \mathrm{L}^2(D),
$$

and

$$-(\hat{\psi}_0, \hat{\varphi}(\cdot,0)) - \int_0^T \int_D \hat{\psi}\frac{\partial \hat{\varphi}}{\partial t}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}\,\underset{\sim}{q}\,\hat{\psi})\cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t$$
$$+\frac{1}{2\lambda}\int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi}\cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M)), \quad \hat{\varphi}(\cdot,T)=0. \quad (3.8)$$

The function $\psi = \sqrt{M}\hat{\psi}$ *will be referred to as the weak solution of the initial-boundary-value problem* (1.3), (1.4), (1.5). $\mathrm{C}_{\mathrm{weak}}([0,T];\mathrm{L}^2(D))$ *denotes the set of all weakly continuous functions from* $[0,T]$ *into* $\mathrm{L}^2(D)$.

Proof. Step 1. Let us denote by $\hat{\psi}^{\Delta t} \in \mathrm{C}([0,T];\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ the continuous piecewise linear interpolant, with respect to $t \in [0,T]$, of the semidiscrete solution $\{\hat{\psi}^n : n = 0,\dots,N_T\}$ to (3.1), defined by

$$\hat{\psi}^{\Delta t}(\cdot,t)|_{[t^n,t^{n+1}]} := \frac{t-t^n}{\Delta t}\hat{\psi}^{n+1} + \frac{t^{n+1}-t}{\Delta t}\hat{\psi}^n, \qquad t \in [t^n,t^{n+1}], \quad n=0,\dots,N_T-1,$$

and let

$$\hat{\psi}^{\Delta t,+}(\cdot,t) := \hat{\psi}^{n+1}(\cdot), \qquad \hat{\psi}^{\Delta t,-}(\cdot,t) := \hat{\psi}^{n}(\cdot), \qquad t \in [t^n,t^{n+1}], \quad n=0,\dots,N_T-1.$$

We shall denote by $\hat{\psi}^{\Delta t,(\pm)}$ any one of the functions $\hat{\psi}^{\Delta t}$, $\hat{\psi}^{\Delta t,+}$, $\hat{\psi}^{\Delta t,-}$ defined above.

Using analogous notation for $\underset{\approx}{\kappa}$, equation (3.1), with $\hat{\varphi} \in \mathrm{H}^1_0(D;M)$ replaced by $\hat{\varphi}(t,\cdot) \in \mathrm{H}^1_0(D;M)$ for $t \in (0,T]$ where $\hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$, and summed over $n = 0,\dots,N_T-1$, yields

$$\int_0^T \int_D \frac{\partial \hat{\psi}^{\Delta t}}{\partial t}\,\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}^{\Delta t,+}\,\underset{\sim}{q}\,\hat{\psi}^{\Delta t,+})\cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t$$
$$+\frac{1}{2\lambda}\int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi}^{\Delta t,+}\cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)). \quad (3.9)$$

It follows from (3.5) with $\mu = 0$ and $\underset{\sim}{v} = \underset{\sim}{0}$ in (3.5) that

$$\begin{aligned} &(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t} \quad \text{is bounded in} \quad \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)),\\ &(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t} \quad \text{is bounded in} \quad \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)),\\ &\left\{\frac{\hat{\psi}^{\Delta t,+}-\hat{\psi}^{\Delta t,-}}{\sqrt{\Delta t}}\right\} \quad \text{is bounded} \quad \mathrm{L}^2(0,T;\mathrm{L}^2(D)). \end{aligned}$$

The first two of these imply that we can extract a subsequence from $(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t}$, which for the sake of notational simplicity we still denote by $(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t}$, such that, as $\Delta t \to 0_+$,

$$(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t} \quad \text{weak--}\ast \text{ converges in} \quad \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)), \quad (3.10)$$
$$(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t} \quad \text{weakly converges in} \quad \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)). \quad (3.11)$$

Now, (3.10) implies the existence of $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D))$ such that

$$\int_0^T (\hat{\psi}^{\Delta t}(t) - \hat{\psi}(t), \hat{\varphi}(t))\,\mathrm{d}t \to 0 \quad \text{as} \quad \Delta t \to 0_+ \qquad \forall \hat{\varphi} \in \mathrm{L}^1(0,T;\mathrm{L}^2(\Omega)). \quad (3.12)$$

On the other hand (3.11) implies the existence of $\hat{\psi}^*$ such that

$$\int_0^T \langle \hat{\psi}^{\Delta t}(t) - \hat{\psi}^*(t), \hat{\varphi}(t)\rangle\,\mathrm{d}t \to 0 \quad \text{as} \quad \Delta t \to 0_+ \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)'), \quad (3.13)$$

where $\langle \cdot, \cdot \rangle$ is the duality pairing between the Hilbert space $\mathrm{H}^1_0(D;M)$ and its dual space $\mathrm{H}^1_0(D;M)'$.

Now, the function space $\mathrm{H}^1_0(D;M)$ is continuously and densely imbedded into $\mathrm{L}^2(D)$; *i.e.*, the imbedding operator i from $\mathrm{H}^1_0(D;M)$ into $\mathrm{L}^2(D)$ is a continuous linear operator. The dual operator i' from $\mathrm{L}^2(D)'$ into $\mathrm{H}^1_0(D;M)'$ (cf. Definition 1, Ch. VII, §1 of Yoshida [31]) satisfies

$$\langle i(g), h' \rangle = \langle g, i'(h') \rangle \qquad \forall g \in \mathrm{H}^1_0(D;M), \quad \forall h' \in \mathrm{L}^2(D)'. \tag{3.14}$$

According to Theorem 2, Ch. VII, §1 of Yoshida [31], i' is a continuous linear operator from $\mathrm{L}^2(D)'$ into $\mathrm{H}^1_0(D;M)'$. Since $i(\mathrm{H}^1_0(D;M)) = \mathrm{H}^1_0(D;M)$ is dense in $\mathrm{L}^2(D)$, it follows from (3.14) that i' is bijective from $\mathrm{L}^2(D)'$ onto its range in $\mathrm{H}^1_0(D;M)'$. Further, since i is bijective, it follows from (3.14) (by *reductio ad absurdum*, for example,) that $i'(\mathrm{L}^2(D)')$ is dense in $\mathrm{H}^1_0(D;M)'$. Thus $\mathrm{L}^2(D)'$ can be identified with a dense subspace, $i'(\mathrm{L}^2(D)')$ of $\mathrm{H}^1_0(D;M)'$. Finally, identifying, by means of the Riesz representation theorem, $\mathrm{L}^2(D)$ with $\mathrm{L}^2(D)'$, we deduce that $\mathrm{H}^1_0(D;M) \subset \mathrm{L}^2(D) = \mathrm{L}^2(D)' \subset \mathrm{H}^1_0(D;M)'$, so that each space is dense in the next one in the chain, with continuous embedding. Hence, $\langle \hat{\psi}, \hat{\varphi} \rangle = (\hat{\psi}, \hat{\varphi})$ for all $\hat{\psi} \in \mathrm{H}^1_0(D;M)$ and all $\hat{\varphi} \in \mathrm{L}^2(D)$. Returning to (3.13), we then deduce that

$$\int_0^T (\hat{\psi}^{\Delta t}(t) - \hat{\psi}^*(t), \hat{\varphi}(t))\,\mathrm{d}t = \int_0^T \langle \hat{\psi}^{\Delta t}(t) - \hat{\psi}^*(t), \hat{\varphi}(t) \rangle\,\mathrm{d}t \to 0 \quad \text{as } \Delta t \to 0_+ \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{L}^2(D)).$$

Subtracting this from (3.12) yields

$$\int_0^T (\hat{\psi}(t) - \hat{\psi}^*(t), \hat{\varphi}(t))\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{L}^2(D)),$$

and therefore $\hat{\psi} = \hat{\psi}^* \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$.

It remains to show that the weak–$*$ limits $\hat{\psi}^\pm$ of the sequences $(\hat{\psi}^{\Delta t,(\pm)})_{\Delta t}$ in $\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))$ are also equal to $\hat{\psi}$. We shall show below that $\hat{\psi}^+ = \hat{\psi}^-$. Once we have done so, recalling from the definitions of $\hat{\psi}^{\Delta t}$ and $\hat{\psi}^{\Delta t,\pm}$ that

$$\hat{\psi}^{\Delta t}(\cdot,t) - \hat{\psi}^\pm(\cdot,t) = \frac{t-t^n}{\Delta t}(\hat{\psi}^{\Delta t,+}(\cdot,t) - \hat{\psi}^+(\cdot,t)) + \frac{t^{n+1}-t}{\Delta t}(\hat{\psi}^{\Delta t,-}(\cdot,t) - \hat{\psi}^-(\cdot,t))$$

for all $t \in [t^n, t^{n+1}]$ and $n = 0, \ldots, N_T - 1$, and passing to the weak–$*$ limit in $\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))$ as $\Delta t \to 0_+$, will imply that $\hat{\psi} = \hat{\psi}^\pm$.

To show that $\hat{\psi}^+ = \hat{\psi}^-$, we proceed as follows. Observe that

$$\begin{aligned}
\int_0^T (\hat{\psi}^{\Delta t,+} - \hat{\psi}^{\Delta t,-}, \hat{\varphi})\,\mathrm{d}t &= \sum_{n=0}^{N_T-1} \left(\hat{\psi}^{n+1} - \hat{\psi}^n, \int_{t^n}^{t^{n+1}} \hat{\varphi}(\cdot,t)\,\mathrm{d}t \right) \\
&= \sum_{n=0}^{N_T-1} \sqrt{\Delta t} \left(\frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}}, \int_{t^n}^{t^{n+1}} \hat{\varphi}(\cdot,t)\,\mathrm{d}t \right) \\
&\leq \sum_{n=0}^{N_T-1} \sqrt{\Delta t} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}} \right\| \left(\int_{t^n}^{t^{n+1}} \|\hat{\varphi}(\cdot,t)\|\,\mathrm{d}t \right) \\
&\leq \left(\sum_{n=0}^{N_T-1} \Delta t \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}} \right\|^2 \right)^{\frac{1}{2}} \left(\sum_{n=0}^{N_T-1} \left(\int_{t^n}^{t^{n+1}} \|\hat{\varphi}(\cdot,t)\|\,\mathrm{d}t \right)^2 \right)^{\frac{1}{2}} \\
&\leq \left(\sum_{n=0}^{N_T-1} \Delta t \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}} \right\|^2 \right)^{\frac{1}{2}} \left(\sum_{n=0}^{N_T-1} \Delta t \int_{t^n}^{t^{n+1}} \|\hat{\varphi}(\cdot,t)\|^2\,\mathrm{d}t \right)^{\frac{1}{2}} \\
&= \left\| \frac{\hat{\psi}^{\Delta t,+} - \hat{\psi}^{\Delta t,-}}{\sqrt{\Delta t}} \right\| \sqrt{\Delta t}\, \|\hat{\varphi}\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))},
\end{aligned}$$

for any $\hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{L}^2(D)) \subset \mathrm{L}^1(0,T;\mathrm{L}^2(D))$. Since the first factor on the right-hand side is bounded, independent of Δt, on passing to the limit $\Delta t \to 0_+$, it follows that

$$\lim_{\Delta t \to 0_+} \int_0^T (\hat{\psi}^{\Delta t,+} - \hat{\psi}^{\Delta t,-}, \hat{\varphi})\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{L}^2(D)).$$

Therefore,

$$\int_0^T (\hat{\psi}^{+} - \hat{\psi}^{-}, \hat{\varphi})\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{L}^2(D)).$$

This, in turn, implies that $\hat{\psi}^+ = \hat{\psi}^-$. Thereby, as has been argued above, $\hat{\psi} = \hat{\psi}^+ = \hat{\psi}^-$.

Step 2. Next we pass to the limit $\Delta t \to 0_+$ in (3.9). Integrating by parts in the first term appearing on the left-hand side of equation (3.9), with $\hat{\varphi} \in \mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M)) \hookrightarrow \mathrm{C}([0,T];\mathrm{H}^1_0(D;M))$, we deduce that

$$\begin{aligned}(\hat{\psi}^{\Delta t}(\cdot,T), \hat{\varphi}(\cdot,T)) &- (\hat{\psi}^{\Delta t}(\cdot,0), \hat{\varphi}(\cdot,0)) \\ &- \int_0^T \int_D \hat{\psi}^{\Delta t} \frac{\partial \hat{\varphi}}{\partial t}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}^{\Delta t,+}\,\underset{\sim}{q}\,\hat{\psi}^{\Delta t,+}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t \\ &\qquad + \frac{1}{2\lambda} \int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi}^{\Delta t,+} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M)). \qquad (3.15)\end{aligned}$$

As $\hat{\psi}^{\Delta t}(\cdot,0) := \hat{\psi}_0(\cdot)$ and the sequence $(\underset{\approx}{\kappa}^{\Delta t,+})_{\Delta t}$ converges (strongly) in $\mathrm{L}^\infty(0,T)$ to $\underset{\approx}{\kappa}$, passing to the limit $\Delta t \to 0_+$ in (3.15) we deduce that the associated limiting function $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ satisfies (3.8). In particular, on choosing $\hat{\varphi} = \hat{\zeta} \cdot \hat{w} \in \mathrm{C}^\infty_0(0,T) \otimes \mathrm{H}^1_0(D;M)$ in (3.8), where $\hat{\zeta} \in \mathrm{C}^\infty_0(0,T)$ and $\hat{w} \in \mathrm{H}^1_0(D;M)$ are arbitrary, it follows from (3.8) that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\hat{\psi}, \hat{w}) - ((\underset{\approx}{\kappa}\,\underset{\sim}{q})\hat{\psi}, \underset{\sim}{\nabla}_M \hat{w}) + \frac{1}{2\lambda}(\underset{\sim}{\nabla}_M \hat{\psi}, \underset{\sim}{\nabla}_M \hat{w}) = 0 \qquad \forall \hat{w} \in \mathrm{H}^1_0(D;M), \qquad (3.16)$$

in the sense of distributions on $(0,T)$, with $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$. Hence, the limiting function $\hat{\psi}$ satisfies (1.7), as required.

Step 3. It remains to show that $\hat{\psi}$ also satisfies the required initial condition. We proceed as follows. Since, for $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$, the second and third term on the left-hand side of (3.16) belong to $\mathrm{L}^2(0,T)$ for every $\hat{w} \in \mathrm{H}^1_0(D;M)$, the same is true of the first term on the left-hand side of (3.16). Therefore, $t \in [0,T] \mapsto (\hat{\psi}(\cdot,t), \hat{w})$ belongs to $\mathrm{H}^1(0,T)$ for all $\hat{w} \in \mathrm{H}^1_0(D;M)$. By the Sobolev embedding $\mathrm{H}^1(0,T) \hookrightarrow \mathrm{C}[0,T]$ we deduce that, for every $\hat{w} \in \mathrm{H}^1_0(D;M)$, $t \in [0,T] \mapsto (\hat{\psi}(\cdot,t), \hat{w})$ is a.e. equal to a function that is defined and continuous on $[0,T]$; *i.e.*, $\hat{\psi} \in \mathrm{C}_{\mathrm{weak}}([0,T];\mathrm{L}^2(D))$. Thus it makes sense to multiply (3.16) by $\hat{\zeta} \in \mathrm{H}^1(0,T)$, such that $\hat{\zeta}(T) = 0$, integrate over $[0,T]$ and integrate by parts with respect to t in the first term to deduce, on writing $\hat{\varphi} = \hat{\zeta} \cdot \hat{w}$, that

$$\begin{aligned}-(\hat{\psi}(\cdot,0), \hat{\varphi}(\cdot,0)) &- \int_0^T \int_D \hat{\psi} \frac{\partial \hat{\varphi}}{\partial t}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}\,\underset{\sim}{q}\,\hat{\psi}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t \\ &+ \frac{1}{2\lambda} \int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{H}^1(0,T) \otimes \mathrm{H}^1_0(D;M), \quad \hat{\varphi}(\cdot,T) = 0. \quad (3.17)\end{aligned}$$

Applying (3.8) with $\hat{\varphi} \in \mathrm{H}^1(0,T) \otimes \mathrm{H}^1_0(D;M) \subset \mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M))$ and comparing with (3.17) it follows that

$$(\hat{\psi}(\cdot,0) - \hat{\psi}_0, \hat{\varphi}(\cdot,0)) = 0 \qquad \forall \hat{\varphi} \in \mathrm{H}^1(0,T) \otimes \mathrm{H}^1_0(D;M), \quad \hat{\varphi}(\cdot,T) = 0,$$

and therefore, since $\mathrm{H}^1_0(D;M)$ is dense in $\mathrm{L}^2(D)$, it follows that $(\hat{\psi}(\cdot,0)-\hat{\psi}_0,\hat{w})=0$ for all $\hat{w}\in\mathrm{L}^2(D)$, which shows that the limiting function $\hat{\psi}$ satisfies the initial condition $\hat{\psi}(\cdot,0)=\hat{\psi}_0$ (and therefore $\psi=\sqrt{M}\hat{\psi}$ satisfies the corresponding initial condition $\psi(\cdot,0)=\psi_0$ $(=\sqrt{M}\hat{\psi}_0)$).

Step 4. Let us show that $\psi=\sqrt{M}\hat{\psi}$, with $\hat{\psi}\in\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))\cap\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ defined by (3.8), is the *unique* weak solution to the initial-boundary-value problem. We begin by observing that, for any $\hat{\psi}\in\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))\cap\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$,

$$\left|\int_0^T\left\{((\underset{\approx}{\kappa}\,\underset{\sim}{q})\hat{\psi},\underset{\sim}{\nabla}_M\hat{\varphi})-\frac{1}{2\lambda}(\underset{\sim}{\nabla}_M\hat{\psi},\underset{\sim}{\nabla}_M\hat{\varphi})\right\}\mathrm{d}t\right|\leq C\|\hat{\psi}\|_{\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))}|\hat{\varphi}|_{\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))}$$

for all $\hat{\varphi}\in\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$, where $C:=\left(b\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}+1/(4\lambda^2)\right)^{\frac{1}{2}}$. Thus, it follows from (3.8) that there is $G\in\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)')$ such that

$$-(\hat{\psi}_0,\hat{\varphi}(\cdot,0))-\int_0^T\int_D\hat{\psi}\frac{\partial\hat{\varphi}}{\partial t}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t=\int_0^T\langle G,\hat{\varphi}\rangle\,\mathrm{d}t\qquad\forall\hat{\varphi}\in\mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M)),\quad\hat{\varphi}(\cdot,T)=0.$$

Hence,

$$-\int_0^T\left\langle\hat{\psi},\frac{\partial\hat{\varphi}}{\partial t}\right\rangle\mathrm{d}t=\int_0^T\langle G,\hat{\varphi}\rangle\,\mathrm{d}t\qquad\forall\hat{\varphi}\in\mathrm{C}^\infty_0(0,T;\mathrm{H}^1_0(D;M)).$$

By virtue of Lemma 1.1, §1.1 in Ch. 3 of Temam [28] with $X=\mathrm{H}^1_0(D;M)'$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\psi},\hat{w}\rangle=\langle G,\hat{w}\rangle\qquad\forall\hat{w}\in\mathrm{H}^1_0(D;M),$$

in the sense of distributions on $(0,T)$, and $\hat{\psi}$ is almost everywhere equal to a continuous function from $[0,T]$ into $\mathrm{H}^1_0(D;M)'$. In fact, since $\hat{\psi}\in\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ and

$$\frac{\partial\hat{\psi}}{\partial t}=G\in\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)'),$$

it follows from Lemma 1.2, §1.2 in Ch. 3 of Temam [28] (with $V=\mathrm{H}^1_0(D;M)$, $H=\mathrm{L}^2(D)$ and $V'=\mathrm{H}^1_0(D;M)'$) that $\hat{\psi}$ is a.e. equal to a continuous function from $[0,T]$ into $\mathrm{L}^2(D)$ and the following identity holds in the sense of distributions of $(0,T)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\hat{\psi}\|^2=2\left\langle\frac{\partial\hat{\psi}}{\partial t},\hat{\psi}\right\rangle.$$

Now, suppose that $\hat{\psi}\in\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))\cap\mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ is a weak solution of the initial-boundary-value problem, defined by (3.8). Then, for any $s\in(0,T]$,

$$\begin{aligned}\int_0^s\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\hat{\psi}\|^2\,\mathrm{d}t&=\int_0^s\left\langle\frac{\partial\hat{\psi}}{\partial t},\hat{\psi}\right\rangle\mathrm{d}t=\int_0^s\langle G,\hat{\psi}\rangle\,\mathrm{d}t\\&=\int_0^s\left\{((\underset{\approx}{\kappa}\,\underset{\sim}{q})\hat{\psi},\underset{\sim}{\nabla}_M\hat{\psi})-\frac{1}{2\lambda}(\underset{\sim}{\nabla}_M\hat{\psi},\underset{\sim}{\nabla}_M\hat{\psi})\right\}\mathrm{d}t.\end{aligned}$$

Therefore,

$$\begin{aligned}\frac{1}{2}\left(\|\hat{\psi}(s)\|^2-\|\hat{\psi}_0\|^2\right)+\frac{1}{2\lambda}\|\underset{\sim}{\nabla}_M\hat{\psi}\|^2_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))}&=\int_0^s((\underset{\approx}{\kappa}\,\underset{\sim}{q})\hat{\psi},\underset{\sim}{\nabla}_M\hat{\psi})\mathrm{d}t\\&\leq\sqrt{b}\|\underset{\approx}{\kappa}\|_{\mathrm{L}^\infty(0,T)}\|\hat{\psi}\|_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))}\|\underset{\sim}{\nabla}_M\hat{\psi}\|_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))}\quad\text{for a.e. } s\in(0,T].\end{aligned}$$

This implies that

$$\|\hat\psi(s)\|^2 + \frac{1}{2\lambda}\|\nabla_M \hat\psi\|^2_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))} \leq \|\hat\psi_0\|^2 + 2\lambda\, b\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\|\hat\psi\|^2_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))} \quad \text{for a.e. } s \in (0,T].$$

Thus, by Gronwall's Lemma, any weak solution $\hat\psi$ to (3.8) satisfies the following energy inequality

$$\|\hat\psi(s)\|^2_{\mathrm{L}^\infty(0,s;\mathrm{L}^2(D))} + \frac{1}{2\lambda}\|\nabla_M \hat\psi\|^2_{\mathrm{L}^2(0,s;\mathrm{L}^2(D))} \leq \|\hat\psi_0\|^2 \exp\left(2s\lambda\, b\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right) \quad \text{for a.e. } s \in (0,T].$$

Note, in particular, that if $\hat\psi_0 = 0$, then $\hat\psi(\cdot,s) = 0$ in $\mathrm{L}^2(D)$ for a.e. $s \in (0,T]$, which in turn implies the uniqueness of a weak solution. ◻

We shall next show that $\psi = \sqrt{M}\hat\psi$ has the usual properties of a probability density function: if ψ_0 is non-negative and has unit integral over D, then the same is true of $\psi(\cdot,t)$ for all $t \in [0,T]$.

LEMMA 3.3. *Let $\psi_0 \in \mathfrak{H}$, and let $\psi = \sqrt{M}\hat\psi$ where $\hat\psi \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)) \cap \mathrm{C}_{\mathrm{weak}}([0,T];\mathrm{L}^2(D))$ is the weak solution to* (3.8) *subject to the initial condition $\hat\psi_0 = \psi_0/\sqrt{M}$* (i.e., *the function ψ is the weak solution of the initial-boundary-value problem* (1.3), (1.4), (1.5)). *Then,*

$$\int_D \psi(\underset{\sim}{q},t)\,\mathrm{d}\underset{\sim}{q} = \int_D \psi_0(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} \qquad \forall t \in [0,T).$$

Furthermore if $\psi_0 \geq 0$ a.e. on D, then $\psi(\cdot,t) \geq 0$ a.e. on D for all $t \in [0,T]$.

Proof. Fix any $t \in (0,T)$, and let $\varepsilon \in (0, T-t]$. Consider the function $\hat\varphi_\varepsilon$ defined by

$$\hat\varphi_\varepsilon(\underset{\sim}{q},s) := \begin{cases} \sqrt{M} & \text{for } s \in [0,t], \\ \sqrt{M}(t+\varepsilon-s)/\varepsilon & \text{for } s \in [t,t+\varepsilon), \\ 0 & \text{for } s \in [t+\varepsilon,T]. \end{cases}$$

Clearly, $\hat\varphi_\varepsilon \in \mathrm{H}^1(0,T;\mathrm{H}^1_0(D;M))$ and $\hat\varphi_\varepsilon(\cdot,T) = 0$. Taking $\hat\varphi_\varepsilon$ as test function in (3.8) we obtain

$$-(\hat\psi_0,\sqrt{M}\,) + \frac{1}{\varepsilon}\int_t^{t+\varepsilon} (\hat\psi(\cdot,s),\sqrt{M}\,)\,\mathrm{d}s = 0.$$

Passing to the limit $\varepsilon \to 0_+$ yields

$$-(\hat\psi_0,\sqrt{M}\,) + (\hat\psi(\cdot,t),\sqrt{M}\,) = 0,$$

whereby $(\psi(\cdot,t),1) = (\psi_0,1)$, as required, for all $t \in (0,T)$; for $t = 0$ the equality holds trivially.

Now, suppose that $\psi_0 \in \mathfrak{H}$ and $\psi_0 \geq 0$; then, $\hat\psi_0 \in \mathrm{L}^2(D)$ and $\hat\psi_0 \geq 0$. For Δt as in Lemma 3.5, consider the sequence of functions $(\hat\psi^n)_{n=0}^{N_T} \subset \mathrm{H}^1_0(D;M)$ defined by (3.3). By Lemma 3.5 below (with $L = 0$), we have that $([\hat\psi^n]_-)_{n=0}^{N_T} \subset \mathrm{H}^1_0(D;M)$. It follows from (3.3) that

$$B([\hat\psi^{n+1}]_-\,,\,[\hat\psi^{n+1}]_-) = B(\hat\psi^{n+1}\,,\,[\hat\psi^{n+1}]_-) = \ell(\hat\psi^n;[\hat\psi^{n+1}]_-).$$

Suppose, for induction, that $\hat\psi^n \geq 0$; this is certainly true for $n = 0$, since $\hat\psi^0 = \hat\psi_0 \geq 0$. Hence,

$$\ell(\hat\psi^n;[\hat\psi^{n+1}]_-) = \frac{1}{\Delta t}\int_D \hat\psi^n(\underset{\sim}{q})[\hat\psi^{n+1}(\underset{\sim}{q})]_-\,\mathrm{d}\underset{\sim}{q} \leq 0.$$

Therefore, $B([\hat\psi^{n+1}]_-\,,\,[\hat\psi^{n+1}]_-) \leq 0$; thus, (3.2) implies that $\|[\hat\psi^{n+1}]_-\|_{\mathrm{H}^1_0(D;M)} \leq 0$, whereby $[\hat\psi^{n+1}]_- = 0$ and hence $\hat\psi^{n+1} \geq 0$. By induction, $\hat\psi^n \geq 0$ for all $n = 0,1,\dots,N_T$. Therefore, each of the functions $\hat\psi^{\Delta t}$, $\hat\psi^+$ and $\hat\psi^-$, defined in the proof of Theorem 3.2, is non-negative on $D \times [0,T]$. Hence the limiting function $\hat\psi$ of the sequence(s), as $\Delta t \to 0_+$, is also non-negative on $D \times [0,T]$. ◻

Remark 3.4. *We note in passing that if* $\underset{\sim}{q}^T \underset{\approx}{\kappa}(t)\, \underset{\sim}{q} \leq 0$ *for a.e.* $t \in [0,T]$ *then, by considering the expression,* $B([\hat{\psi}^{n+1} - L\sqrt{M}\,]_+ \,,\, [\hat{\psi}^{n+1} - L\sqrt{M}\,]_+)$ *one can show by induction, as in the proof above, with*

$$L = \text{ess.sup}_{\underset{\sim}{q} \in D} \hat{\psi}_0(\underset{\sim}{q})/\sqrt{M(\underset{\sim}{q})},$$

that $B([\hat{\psi}^{n+1} - L\sqrt{M}\,]_+ \,,\, [\hat{\psi}^{n+1} - L\sqrt{M}\,]_+) = 0$ *for all* $n = 0, 1, \ldots, N_T - 1$*. Consequently, by* (3.2)*,* $[\hat{\psi}^{n+1} - L\sqrt{M}\,]_+ = 0$*;* i.e., $\hat{\psi}^{n+1} \leq L\sqrt{M}$*. This then implies, on passage to the limit* $\Delta t \to 0_+$*, that*

$$\text{ess.sup}_{(\underset{\sim}{q},t) \in D \times [0,T]} \hat{\psi}(\underset{\sim}{q}, t)/\sqrt{M(\underset{\sim}{q})} \leq \text{ess.sup}_{\underset{\sim}{q} \in D} \hat{\psi}_0(\underset{\sim}{q})/\sqrt{M(\underset{\sim}{q})}.$$

Hence,

$$\text{ess.sup}_{(\underset{\sim}{q},t) \in D \times [0,T]} \psi(\underset{\sim}{q}, t)/M(\underset{\sim}{q}) \leq \text{ess.sup}_{\underset{\sim}{q} \in D} \psi_0(\underset{\sim}{q})/M(\underset{\sim}{q}),$$

which can be thought of as a maximum principle for the initial-boundary value problem.

Lemma 3.5. *Suppose that* $\hat{\varphi} \in \mathrm{H}^1_0(D; M)$ *and* $L \geq 0$*. Then,*

$$\underset{\sim}{\nabla}_M [\,\hat{\varphi} - L\sqrt{M}\,]_+ = \begin{cases} \underset{\sim}{\nabla}_M (\,\hat{\varphi} - L\sqrt{M}\,) = \underset{\sim}{\nabla}_M \hat{\varphi} & \text{if } \varphi > L\sqrt{M}, \\ 0 & \text{if } \varphi \leq L\sqrt{M}; \end{cases} \tag{3.18}$$

and

$$\underset{\sim}{\nabla}_M [\,\hat{\varphi} + L\sqrt{M}\,]_- = \begin{cases} \underset{\sim}{\nabla}_M (\,\hat{\varphi} + L\sqrt{M}\,) = \underset{\sim}{\nabla}_M \hat{\varphi} & \text{if } \varphi < L\sqrt{M}, \\ 0 & \text{if } \varphi \geq L\sqrt{M}. \end{cases} \tag{3.19}$$

Furthermore, $[\,\hat{\varphi} - L\sqrt{M}\,]_+$ *and* $[\,\hat{\varphi} + L\sqrt{M}\,]_-$ *belong to* $\mathrm{H}^1_0(D; M)$*.*

Proof. We shall prove (3.18); the proof of (3.19) is analogous, *mutatis mutandis*. We begin by noting that since $L \geq 0$ and $\sqrt{M} > 0$ on D,

$$|[\,\hat{\varphi} - L\sqrt{M}\,]_+| \leq |\hat{\varphi}|. \tag{3.20}$$

Following [2], for any $\varepsilon > 0$, we define the following regularization of $[\,\cdot\,]_+$:

$$p_{+,\varepsilon}(s) := \begin{cases} (s^2 + \varepsilon^2)^{\frac{1}{2}} - \varepsilon & \text{if } s > 0, \\ 0 & \text{if } s \leq 0. \end{cases}$$

Clearly, $0 \leq p_{+,\varepsilon}(s) \leq [s]_+$ for all $s \in \mathbb{R}$. Observe that

$$\underset{\sim}{\nabla}_M [\,\hat{\varphi} - L\sqrt{M}\,]_+ = \underset{\sim}{\nabla}_q [\,\hat{\varphi} - L\sqrt{M}\,]_+ + \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)[\,\hat{\varphi} - L\sqrt{M}\,]_+$$

in the sense of d-component distributions on D. Let $\underset{\sim}{\eta} \in \mathrm{C}^\infty_0(D)^d$ be fixed. Then, on recalling the definition of the distributional derivative,

$$\begin{aligned} \langle \underset{\sim}{\nabla}_M [\,\hat{\varphi} - L\sqrt{M}\,]_+ \,,\, \underset{\sim}{\eta} \rangle &= \langle \underset{\sim}{\nabla}_q [\,\hat{\varphi} - L\sqrt{M}\,]_+ + \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)[\,\hat{\varphi} - L\sqrt{M}\,]_+ \,,\, \underset{\sim}{\eta} \rangle \\ &= -\langle [\,\hat{\varphi} - L\sqrt{M}\,]_+ \,,\, \underset{\sim}{\nabla}_q \cdot \underset{\sim}{\eta} \rangle + \langle \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)[\,\hat{\varphi} - L\sqrt{M}\,]_+ \,,\, \underset{\sim}{\eta} \rangle \\ &= -\int_D [\,\hat{\varphi} - L\sqrt{M}\,]_+ (\underset{\sim}{\nabla}_q \cdot \underset{\sim}{\eta}) \,\mathrm{d}\underset{\sim}{q} + \int_D \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)[\,\hat{\varphi} - L\sqrt{M}\,]_+ \cdot \underset{\sim}{\eta} \,\mathrm{d}\underset{\sim}{q}. \end{aligned}$$

Let χ_S denote the characteristic function of a set $S \subset D$. Since $\underset{\sim}{\eta}$ has compact support in D, by Lebesgue's Dominated Convergence Theorem we deduce that

$$\langle \underset{\sim}{\nabla}_M [\,\hat{\varphi} - L\sqrt{M}\,]_+\,,\, \underset{\sim}{\eta} \rangle = - \lim_{\varepsilon\to 0_+} \int_D p_{+,\varepsilon}(\hat{\varphi} - L\sqrt{M}\,)(\underset{\sim}{\nabla}_q \cdot \underset{\sim}{\eta})\,\mathrm{d}\underset{\sim}{q}$$
$$+ \lim_{\varepsilon\to 0_+} \int_D \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2) p_{+,\varepsilon}(\hat{\varphi} - L\sqrt{M}\,)\cdot \underset{\sim}{\eta}\,\mathrm{d}\underset{\sim}{q}$$
$$= \lim_{\varepsilon\to 0_+} \int_D p'_{+,\varepsilon}(\hat{\varphi} - L\sqrt{M}\,)\underset{\sim}{\nabla}_q(\hat{\varphi} - L\sqrt{M}\,)\cdot \eta\,\mathrm{d}\underset{\sim}{q} + \lim_{\varepsilon\to 0} \int_D \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2) p_{+,\varepsilon}(\hat{\varphi} - L\sqrt{M}\,)\cdot \underset{\sim}{\eta}\,\mathrm{d}\underset{\sim}{q}$$
$$= \int_D \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_q(\hat{\varphi} - L\sqrt{M}\,)\cdot \eta\,\mathrm{d}\underset{\sim}{q} + \int_D \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)(\hat{\varphi} - L\sqrt{M}\,)\cdot \underset{\sim}{\eta}\,\mathrm{d}\underset{\sim}{q}$$
$$= \int_D \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q}) \left\{ \underset{\sim}{\nabla}_q(\hat{\varphi} - L\sqrt{M}\,) + \tfrac{1}{2}\underset{\sim}{q} U'(\tfrac{1}{2}|\underset{\sim}{q}|^2)(\hat{\varphi} - L\sqrt{M}\,)\right\}\cdot \underset{\sim}{\eta}\,\mathrm{d}\underset{\sim}{q}$$
$$= \int_D \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M(\hat{\varphi} - L\sqrt{M}\,)\cdot \underset{\sim}{\eta}\,\mathrm{d}\underset{\sim}{q} = \langle \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M(\hat{\varphi} - L\sqrt{M}\,)\,,\, \underset{\sim}{\eta}\rangle.$$

Since the above chain of equalities holds for all $\underset{\sim}{\eta} \in \mathrm{C}_0^\infty(D)^d$, it follows that $\underset{\sim}{\nabla}_M[\,\hat{\varphi} - L\sqrt{M}\,]_+ = \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M(\hat{\varphi} - L\sqrt{M}\,)$. As $\sqrt{M} \in \mathrm{Ker}(\underset{\sim}{\nabla}_M)$, we deduce that $\chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M(\hat{\varphi} - L\sqrt{M}\,) = \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M\hat{\varphi}$, and that proves (3.18). Now, since $\underset{\sim}{\nabla}_M[\,\hat{\varphi} - L\sqrt{M}\,]_+ = \chi_{\hat{\varphi} > L\sqrt{M}}(\underset{\sim}{q})\,\underset{\sim}{\nabla}_M\hat{\varphi}$, and the right-hand side in this equality belongs to $\mathrm{L}^2(D)$ (recall that $\hat{\varphi} \in \mathrm{H}^1_0(D;M)$ by hypothesis), it follows that $\underset{\sim}{\nabla}_M[\,\hat{\varphi} - L\sqrt{M}\,]_+ \in \mathrm{L}^2(D)$. Hence, and by (3.20), $[\,\hat{\varphi} - L\sqrt{M}\,]_+ \in \mathrm{H}^1_0(D;M)$, as required. ◻

Next we shall show that if $\underset{\approx}{\kappa} \in \mathrm{H}^1(0,T)^{d\times d}$ and $\hat{\psi}_0 \in \mathrm{H}^1_0(D;M)$, then we have stability in stronger norms, and that the weak solution $\hat{\psi} \in \mathrm{L}^\infty(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M))$ whose existence and uniqueness has just been established, is in fact more regular: it belongs to the function space $\mathrm{H}^1(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^\infty(0,T;\mathrm{H}^1_0(D;M))$.

LEMMA 3.6 (The second stability inequality). *Let $\Delta t = T/N_T$, $N_T \geq 1$, $\underset{\approx}{\kappa} \in \mathrm{H}^1(0,T)^{d\times d}$ and $\hat{\psi}^0 \in \mathrm{H}^1_0(D;M)$, and define $c_0 := 1 + 4\lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}$. If Δt is such that $0 < c_0\Delta t \leq 1/2$, then, for all m such that $1 \leq m \leq N_T$, we have*

$$\Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\right\|^2 + \frac{1}{4\lambda}\|\underset{\sim}{\nabla}_M \hat{\psi}^m\|^2 + \frac{1}{2\lambda}\sum_{n=0}^{m-1}\Delta t \left\| \underset{\sim}{\nabla}_M \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\sqrt{\Delta t}}\right\|^2$$
$$\leq \mathrm{e}^{2c_1 m\Delta t}\Bigg\{ 2\Delta t \sum_{n=0}^{m-1}\|\mu^{n+1}\|^2 + 12\lambda \max_{1\leq n\leq m}\|\underset{\sim}{\nu}^n\|^2 + \Delta t\sum_{n=1}^{m-1}\left\|\frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t}\right\|^2$$
$$+ \frac{1}{\lambda}\|\underset{\sim}{\nabla}_M\hat{\psi}^0\|^2 + \left(b\,\|\underset{\approx}{\kappa}_t\|^2_{\mathrm{L}^2(0,T)} + 12\lambda b\,\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right)\mathfrak{S}(\hat{\psi}^0,\mu,\underset{\sim}{\nu},m\Delta t)\Bigg\}, \qquad (3.21)$$

where $\mathfrak{S}(\hat{\psi}^0,\mu,\underset{\sim}{\nu},m\Delta t)$ is the expression on the right-hand side of the first stability inequality and $c_1 = 4\lambda(1 + b\,\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)})$.

Proof. The proof is similar to that of the previous lemma, except we now select as our test function $\hat{\varphi} = (\hat{\psi}^{n+1} - \hat{\psi}^n)/\Delta t$, multiply the resulting identity by Δt and sum over $n = 0,\dots,m-1$, where $m \geq 1$. Thus,

$$\Delta t \sum_{n=0}^{m-1}\left\|\frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\right\|^2 + \frac{1}{4\lambda}\left(\|\underset{\sim}{\nabla}_M\hat{\psi}^m\|^2 - \|\underset{\sim}{\nabla}_M\hat{\psi}^0\|^2\right) + \frac{1}{4\lambda}\sum_{n=0}^{m-1}\left\|\underset{\sim}{\nabla}_M\hat{\psi}^{n+1} - \underset{\sim}{\nabla}_M\hat{\psi}^n\right\|^2$$
$$= \Delta t\sum_{n=0}^{m-1}\left(\mu^{n+1}, \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\right) + \Delta t \sum_{n=0}^{m-1}\left(\underset{\sim}{\nu}^{n+1} + (\underset{\approx}{\kappa}^{n+1}\underset{\sim}{q})\hat{\psi}^{n+1}, \underset{\sim}{\nabla}_M\frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}\right)$$
$$=: \mathrm{T}_1 + \mathrm{T}_2.$$

Let us consider the term T_2, and define the functions

$$\underset{\sim}{A}^{n+1} = \underset{\sim}{\nu}^{n+1} + (\underset{\approx}{\kappa}^{n+1}\underset{\sim}{q})\hat{\psi}^{n+1}, \qquad n = 0, \ldots, m-1.$$

After summation by parts, we have that

$$\begin{aligned}
\mathrm{T}_2 &= -(\underset{\sim}{A}^1, \underset{\sim}{\nabla}_M \hat{\psi}^0) + (\underset{\sim}{A}^m, \underset{\sim}{\nabla}_M \hat{\psi}^m) - \Delta t \sum_{n=1}^{m-1} \left(\frac{\underset{\sim}{A}^{n+1} - \underset{\sim}{A}^n}{\Delta t}, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) \\
&= -(\underset{\sim}{A}^1, \underset{\sim}{\nabla}_M \hat{\psi}^0) + (\underset{\sim}{A}^m, \underset{\sim}{\nabla}_M \hat{\psi}^m) - \Delta t \sum_{n=1}^{m-1} \left(\frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t}, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) \\
&\quad -\Delta t \sum_{n=1}^{m-1} \left(\frac{\underset{\approx}{\kappa}^{n+1} - \underset{\approx}{\kappa}^n}{\Delta t}\, \underset{\sim}{q}\, \hat{\psi}^n, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) - \Delta t \sum_{n=1}^{m-1} \left((\underset{\approx}{\kappa}^{n+1}\underset{\sim}{q}) \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}, \underset{\sim}{\nabla}_M \hat{\psi}^n \right).
\end{aligned}$$

Hence,

$$\begin{aligned}
&\Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 + \frac{1}{4\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^m\|^2 + \frac{1}{4\lambda} \sum_{n=0}^{m-1} \left\| \underset{\sim}{\nabla}_M \hat{\psi}^{n+1} - \underset{\sim}{\nabla}_M \hat{\psi}^n \right\|^2 \\
&\quad = \frac{1}{4\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^0\|^2 - (\underset{\sim}{A}^1, \underset{\sim}{\nabla}_M \hat{\psi}^0) + (\underset{\sim}{A}^m, \underset{\sim}{\nabla}_M \hat{\psi}^m) + \Delta t \sum_{n=0}^{m-1} \left(\mu^{n+1}, \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right) \\
&\qquad -\Delta t \sum_{n=1}^{m-1} \left(\frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t}, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) - \Delta t \sum_{n=1}^{m-1} \left(\frac{\underset{\approx}{\kappa}^{n+1} - \underset{\approx}{\kappa}^n}{\Delta t}\, \underset{\sim}{q}\, \hat{\psi}^n, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) \\
&\qquad -\Delta t \sum_{n=1}^{m-1} \left((\underset{\approx}{\kappa}^{n+1}\underset{\sim}{q}) \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t}, \underset{\sim}{\nabla}_M \hat{\psi}^n \right) \\
&\qquad =: \mathrm{S}_1 + \cdots + \mathrm{S}_7.
\end{aligned}$$

Clearly,

$$\begin{aligned}
\mathrm{S}_2 &\le \|\underset{\sim}{A}^1\| \|\underset{\sim}{\nabla}_M \hat{\psi}^0\| \\
&\le \left(\|\underset{\sim}{\nu}^1\| + \sqrt{b}\, |\underset{\approx}{\kappa}^1|\, \|\hat{\psi}^1\| \right) \|\underset{\sim}{\nabla}_M \hat{\psi}^0\| \\
&\le \frac{1}{4\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^0\|^2 + \lambda \left(\|\underset{\sim}{\nu}^1\| + \sqrt{b}\, |\underset{\approx}{\kappa}^1|\, \|\hat{\psi}^1\| \right)^2.
\end{aligned}$$

Similarly,

$$\begin{aligned}
\mathrm{S}_3 &\le \|\underset{\sim}{A}^m\| \|\underset{\sim}{\nabla}_M \hat{\psi}^m\| \\
&\le \left(\|\underset{\sim}{\nu}^m\| + \sqrt{b}\, |\underset{\approx}{\kappa}^m|\, \|\hat{\psi}^m\| \right) \|\underset{\sim}{\nabla}_M \hat{\psi}^m\| \\
&\le \frac{1}{8\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^m\|^2 + 2\lambda \left(\|\underset{\sim}{\nu}^m\| + \sqrt{b}\, |\underset{\approx}{\kappa}^m|\, \|\hat{\psi}^m\| \right)^2.
\end{aligned}$$

Next, we have

$$\begin{aligned}
\mathrm{S}_4 &\le \left(\Delta t \sum_{n=0}^{m-1} \|\mu^{n+1}\|^2 \right)^{\frac{1}{2}} \left(\Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 \right)^{\frac{1}{2}} \\
&\le \frac{1}{4} \Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 + \Delta t \sum_{n=0}^{m-1} \|\mu^{n+1}\|^2.
\end{aligned}$$

Similarly,

$$\mathrm{S}_5 \leq \left(\Delta t \sum_{n=1}^{m-1} \left\| \frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t} \right\|^2 \right)^{\frac{1}{2}} \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right)^{\frac{1}{2}}$$

and

$$\begin{aligned}
\mathrm{S}_6 &\leq \sqrt{b} \left(\Delta t \sum_{n=1}^{m-1} \left| \frac{\underset{\approx}{\kappa}^{n+1} - \underset{\approx}{\kappa}^n}{\Delta t} \right|^2 \|\hat{\psi}^n\|^2 \right)^{\frac{1}{2}} \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right)^{\frac{1}{2}} \\
&\leq \sqrt{b}\, \|\underset{\approx}{\kappa}_t\|_{\mathrm{L}^2(t^1,t^m)} \max_{1\leq n\leq m-1} \|\hat{\psi}^n\| \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

Finally,

$$\begin{aligned}
\mathrm{S}_7 &\leq \sqrt{b} \left(\Delta t \sum_{n=1}^{m-1} |\underset{\approx}{\kappa}^{n+1}|^2 \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 \right)^{\frac{1}{2}} \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right)^{\frac{1}{2}} \\
&\leq \sqrt{b}\, \|\underset{\approx}{\kappa}\|_{\mathrm{L}^\infty(t^2,t^m)} \left(\Delta t \sum_{n=1}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 \right)^{\frac{1}{2}} \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right)^{\frac{1}{2}} \\
&\leq \frac{1}{4} \Delta t \sum_{n=1}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 + b\, \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(t^2,t^m)} \left(\Delta t \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right).
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 + \frac{1}{4\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^m\|^2 + \frac{1}{2\lambda} \sum_{n=0}^{m-1} \left\| \underset{\sim}{\nabla}_M \hat{\psi}^{n+1} - \underset{\sim}{\nabla}_M \hat{\psi}^n \right\|^2 \\
&\quad \leq 2\Delta t \sum_{n=0}^{m-1} \|\mu^{n+1}\|^2 + 12\lambda \max_{1\leq n\leq m} \|\underset{\sim}{\nu}^n\|^2 + \Delta t \sum_{n=1}^{m-1} \left\| \frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t} \right\|^2 \\
&\qquad + \left(b\, \|\underset{\approx}{\kappa}_t\|^2_{\mathrm{L}^2(t^1,t^m)} + 12\lambda b\, \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(t_1,t_m)}\right) \max_{1\leq n\leq m} \|\hat{\psi}^n\|^2 \\
&\qquad\quad + \frac{1}{\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^0\|^2 + 8\lambda(1 + b\, \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(t^2,t^m)}) \left(\frac{\Delta t}{4\lambda} \sum_{n=1}^{m-1} \|\underset{\sim}{\nabla}_M \hat{\psi}^n\|^2 \right).
\end{aligned}$$

By an analogous argument, based on the discrete Gronwall Lemma, as in the proof of the first stability inequality, we then deduce that

$$\begin{aligned}
&\Delta t \sum_{n=0}^{m-1} \left\| \frac{\hat{\psi}^{n+1} - \hat{\psi}^n}{\Delta t} \right\|^2 + \frac{1}{4\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^m\|^2 + \frac{1}{2\lambda} \sum_{n=0}^{m-1} \left\| \underset{\sim}{\nabla}_M \hat{\psi}^{n+1} - \underset{\sim}{\nabla}_M \hat{\psi}^n \right\|^2 \\
&\quad \leq \mathrm{e}^{2c_1 m\Delta t} \Bigg\{ 2\Delta t \sum_{n=0}^{m-1} \|\mu^{n+1}\|^2 + 12\lambda \max_{1\leq n\leq m} \|\underset{\sim}{\nu}^n\|^2 + \Delta t \sum_{n=1}^{m-1} \left\| \frac{\underset{\sim}{\nu}^{n+1} - \underset{\sim}{\nu}^n}{\Delta t} \right\|^2 \\
&\qquad + \frac{1}{\lambda} \|\underset{\sim}{\nabla}_M \hat{\psi}^0\|^2 + \left(b\, \|\underset{\approx}{\kappa}_t\|^2_{\mathrm{L}^2(0,T)} + 12\lambda b\, \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right) \max_{1\leq n\leq m} \|\hat{\psi}^n\|^2 \Bigg\},
\end{aligned}$$

where $c_1 = 4\lambda(1 + b\,\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)})$. Now, using the first stability inequality, the last term in the curly bracket is bounded by $(b\,\|\underset{\approx}{\kappa}_t\|^2_{\mathrm{L}^2(0,T)} + 12\lambda b\,\|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)})\,\mathfrak{S}(\hat{\psi}^0, \mu, \underset{\sim}{\nu}, m\Delta t)$, and hence the required bound. □

Once again, we denote by $\hat{\psi}^{\Delta t} \in \mathrm{H}^1(0,T;\mathrm{L}^2(D)) \cap \mathrm{C}([0,T];\mathrm{H}^1_0(D;M))$ the continuous piecewise linear interpolant, with respect to $t \in [0,T]$, of the solution $\{\hat{\psi}^n \,:\, n = 0, \dots, N_T\}$ to (3.1) defined by

$$\hat{\psi}^{\Delta t}(\cdot,t)|_{[t^n,t^{n+1}]} := \frac{t - t^n}{\Delta t}\hat{\psi}^{n+1} + \frac{t^{n+1} - t}{\Delta t}\hat{\psi}^n, \qquad t \in [t^n, t^{n+1}], \quad n = 0, \dots, N_T - 1,$$

and let

$$\hat{\psi}^{\Delta t,+}(\cdot,t) := \hat{\psi}^{n+1}(\cdot), \qquad \hat{\psi}^{\Delta t,-}(\cdot,t) := \hat{\psi}^n(\cdot), \qquad t \in [t^n, t^{n+1}], \quad n = 0, \dots, N_T - 1.$$

Using analogous notation for $\underset{\approx}{\kappa}$, (3.1) summed for $n = 0, \dots, N_T - 1$ can be restated as:

$$\int_0^T \int_D \frac{\partial \hat{\psi}^{\Delta t}}{\partial t}\,\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}^{\Delta t,+}\,\underset{\sim}{q}\,\hat{\psi}^{\Delta t,+}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t \\ + \frac{1}{2\lambda}\int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi}^{\Delta t,+} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)). \quad (3.22)$$

It follows from (3.21) with $\mu = 0$ and $\underset{\sim}{\nu} = \underset{\sim}{0}$ in (3.5) that

$$\begin{aligned} &(\hat{\psi}^{\Delta t})_{\Delta t} \quad \text{is bounded in} \quad \mathrm{L}^\infty(0,T;\mathrm{H}^1_0(D;M)), \\ &(\hat{\psi}^{\Delta t})_{\Delta t} \quad \text{is bounded in} \quad \mathrm{H}^1(0,T;\mathrm{L}^2(D)) \hookrightarrow \mathrm{C}([0,T];\mathrm{L}^2(D)), \\ &\left\{\frac{\hat{\psi}^{\Delta t,+} - \hat{\psi}^{\Delta t,-}}{\sqrt{\Delta t}}\right\} \quad \text{is bounded} \quad \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)). \end{aligned}$$

Passing to the limit $\Delta t \to 0_+$ and denoting by $\hat{\psi}$ the (common) weak(−(∗)) limit of $(\hat{\psi}^{\Delta t})_{\Delta t}$ in the function space $\mathrm{L}^\infty(0,T;\mathrm{H}^1_0(D;M)) \cap \mathrm{H}^1(0,T;\mathrm{L}^2(D))$, we deduce from (3.22) (in the same way as before) that

$$\int_0^T \int_D \frac{\partial \hat{\psi}}{\partial t}\,\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t - \int_0^T \int_D (\underset{\approx}{\kappa}\,\underset{\sim}{q}\,\hat{\psi}) \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t \\ + \frac{1}{2\lambda}\int_0^T \int_D \underset{\sim}{\nabla}_M \hat{\psi} \cdot \underset{\sim}{\nabla}_M \hat{\varphi}\,\mathrm{d}\underset{\sim}{q}\,\mathrm{d}t = 0 \qquad \forall \hat{\varphi} \in \mathrm{L}^2(0,T;\mathrm{H}^1_0(D;M)), \quad (3.23)$$

$\hat{\psi}(\cdot,0) = \hat{\psi}_0(\cdot)$, and $\hat{\psi}$ satisfies the energy inequality

$$\|\hat{\psi}\|^2_{\mathrm{H}^1(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M \hat{\psi}\|^2_{\mathrm{L}^\infty(0,T;\mathrm{L}^2(D))} \le C(b, \lambda, \underset{\approx}{\kappa}, T)\|\hat{\psi}_0\|^2_{\mathrm{H}^1_0(D;M)}.$$

By uniqueness of the weak solution, it follows that the function $\hat{\psi}$ thus constructed coincides with the weak solution of (3.8); in other words, the weak solution $\hat{\psi}$ of (3.8) belongs to $\mathrm{H}^1(0,T;\mathrm{L}^2(D)) \cap \mathrm{L}^\infty(0,T;\mathrm{H}^1_0(D;M))$ provided that $\underset{\approx}{\kappa} \in \mathrm{H}^1(0,T)^{d\times d}$ and $\hat{\psi}_0 \in \mathrm{H}^1_0(D;M)$.

The stability results (3.5) and (3.21) will be useful in Section 4, but for now we note that setting $\mu = 0$ and $\underset{\sim}{\nu} = \underset{\sim}{0}$ in (3.5) and (3.21) demonstrates the unconditional stability of the time semidiscretization in various norms. We also note that, evidently, any fully-discrete method based on the semidiscrete scheme (3.1) and conforming Galerkin discretization in $\underset{\sim}{q}$ using a finite-dimensional subspace $\mathcal{P}_N$ of $\mathrm{H}^1_0(D;M)$ will be unconditionally stable in the norms appearing on the left-hand sides of (3.5) and (3.21).

4. The fully-discrete method. Let $\mathcal{P}_N(D)$ be a finite-dimensional subspace of $\mathrm{H}^1_0(D;M)$ that will be chosen below and let $\hat\psi^n_N \in \mathcal{P}_N(D)$ be the solution at time level n of our fully-discrete Galerkin method:

$$\int_D \frac{\hat\psi^{n+1}_N - \hat\psi^n_N}{\Delta t}\,\hat\varphi \,\mathrm{d}\underset{\sim}{q} - \int_D (\underset{\approx}{\kappa}^{n+1}\,\underset{\sim}{q}\,\hat\psi^{n+1}_N)\cdot \underset{\sim}{\nabla}_M\hat\varphi\,\mathrm{d}\underset{\sim}{q} + \frac{1}{2\lambda}\int_D \underset{\sim}{\nabla}_M\hat\psi^{n+1}_N\cdot\underset{\sim}{\nabla}_M\hat\varphi\,\mathrm{d}\underset{\sim}{q} = 0,$$
$$\forall\hat\varphi\in\mathcal{P}_N(D),\quad n=0,\dots,N_T-1, \tag{4.1}$$
$$\hat\psi^0_N(\cdot) := \text{the } \mathrm{L}^2(D) \text{ orthogonal projection of } \hat\psi_0(\cdot)=\hat\psi(\cdot,0) \text{ onto } \mathcal{P}_N(D). \tag{4.2}$$

REMARK 4.1. *If the linear space $\mathcal{P}_N(D)$ is selected so that $\sqrt{M}\in\mathcal{P}_N(D)$, then, since $\sqrt{M}\in$* Ker$(\underset{\sim}{\nabla}_M)$, *it follows on taking $\hat\varphi=\sqrt{M}$ in* (4.1) *that*

$$\int_D \sqrt{M(\underset{\sim}{q})}\,\hat\psi^n_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} = \int_D \sqrt{M(\underset{\sim}{q})}\,\hat\psi^0_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q},\qquad n=1,\dots,N_T,$$

whereby, on letting $\psi^n_N := \sqrt{M}\hat\psi^n_N$, we have that

$$\int_D \psi^n_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} = \int_D \psi^0_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q},\qquad n=1,\dots,N_T.$$

The function ψ^n_N represents an approximation to the probability density function $\psi=\sqrt{M}\hat\psi$ at $t=t^n$. Since, by Lemma 3.3, $\int_D\psi(\underset{\sim}{q},t)\,\mathrm{d}\underset{\sim}{q}=\int_D\psi_0(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q}=1$ for all $t\geq 0$, we deduce, by choosing $\mathcal{P}_N(D)$ so that $\sqrt{M}\in\mathcal{P}_N(D)$, this integral identity is preserved under discretization.

Our objective is to derive a bound on the global error

$$\begin{aligned} e^n_N &= \hat\psi(\cdot,t^n)-\hat\psi^n_N\\ &= \Big(\hat\psi(\cdot,t^n)-\hat\Pi_N\hat\psi(\cdot,t^n)\Big)+\Big(\hat\Pi_N\hat\psi(\cdot,t^n)-\hat\psi^n_N\Big) =: \eta^n+\xi^n,\end{aligned}$$

where $\hat\Pi_N\hat\psi(\cdot,t^n)\in\mathcal{P}_N(D)$ is a certain projection of $\hat\psi(\cdot,t^n)$ onto $\mathcal{P}_N(D)$ that will be defined below. For the moment, the specific choices of $\mathcal{P}_N\subset\mathrm{H}^1_0(D;M)$ and $\hat\Pi_N$ are irrelevant.

We begin by bounding norms of ξ in terms of suitable norms of η. Substituting ξ into (4.1), setting $\hat\varphi=\xi^{n+1}$, and noting that $\xi^n=\hat\psi(\cdot,t^n)-\hat\psi^n_N-\eta^n$, we have

$$\begin{aligned}\int_D \frac{\xi^{n+1}-\xi^n}{\Delta t}\,\xi^{n+1}\,\mathrm{d}\underset{\sim}{q} - \int_D(\underset{\approx}{\kappa}^{n+1}\,\underset{\sim}{q}\,\xi^{n+1})\cdot\underset{\sim}{\nabla}_M\xi^{n+1}\,\mathrm{d}\underset{\sim}{q}+\frac{1}{2\lambda}\int_D\underset{\sim}{\nabla}_M\xi^{n+1}\cdot\underset{\sim}{\nabla}_M\xi^{n+1}\,\mathrm{d}\underset{\sim}{q}\\ =\int_D\mu^{n+1}\,\xi^{n+1}\,\mathrm{d}\underset{\sim}{q}+\int_D\underset{\sim}{\nu}^{n+1}\cdot\underset{\sim}{\nabla}_M\xi^{n+1}\,\mathrm{d}\underset{\sim}{q}-\frac{1}{2\lambda}\int_D\underset{\sim}{\nabla}_M\eta^{n+1}\cdot\underset{\sim}{\nabla}_M\xi^{n+1}\,\mathrm{d}\underset{\sim}{q},\end{aligned} \tag{4.3}$$

for $n=0,\dots,N_T-1$, where

$$\mu^{n+1} := \left(\frac{\hat\psi(\cdot,t^{n+1})-\hat\psi(\cdot,t^n)}{\Delta t}-\frac{\partial\hat\psi}{\partial t}(\cdot,t^{n+1})\right)-\frac{\eta^{n+1}-\eta^n}{\Delta t}, \tag{4.4}$$

$$\underset{\sim}{\nu}^{n+1} := \underset{\approx}{\kappa}^{n+1}\underset{\sim}{q}\eta^{n+1}-\frac{1}{2\lambda}\underset{\sim}{\nabla}_M\eta^{n+1}. \tag{4.5}$$

Since $\mathcal{P}_N(D)\subset\mathrm{H}^1_0(D;M)$, (4.3) is in the form of (3.4); hence, applying Lemma 3.1, we obtain

$$\begin{aligned}&\|\xi^m\|^2+\frac{1}{2\lambda}\sum_{n=0}^{m-1}\Delta t\|\underset{\sim}{\nabla}_M\xi^{n+1}\|^2\\ &\quad\leq \mathrm{e}^{2c_0m\Delta t}\left\{\|\xi^0\|^2+\sum_{n=0}^{m-1}2\Delta t\left(\|\mu^{n+1}\|^2+4\lambda\|\underset{\sim}{\nu}^{n+1}\|^2\right)\right\},\quad m=1,\dots,N_T.\end{aligned} \tag{4.6}$$

Let us first consider the term $\|\xi^0\|$ on the right-hand side of (4.6). Since $\hat{\psi}_N^0$ is the $\mathrm{L}^2(D)$ orthogonal projection of $\hat{\psi}(\cdot,0) = \hat{\psi}_0$ onto $\mathcal{P}_N(D)$, we have

$$(\xi^0, \hat{\varphi}_N) = (e_N^0, \hat{\varphi}_N) - (\eta^0, \hat{\varphi}_N) = -(\eta^0, \hat{\varphi}_N) \qquad \forall \hat{\varphi}_N \in \mathcal{P}_N(D).$$

Setting $\hat{\varphi}_N = \xi^0$ here and applying the Cauchy–Schwarz inequality on the right-hand side yields

$$\|\xi^0\| \leq \|\eta^0\|. \tag{4.7}$$

By the triangle inequality we have the following bound on $\|\underset{\sim}{\nu}^{n+1}\|$:

$$\|\underset{\sim}{\nu}^{n+1}\| \leq \sqrt{b}|\underset{\approx}{\kappa}^{n+1}|\,\|\eta^{n+1}\| + \frac{1}{2\lambda}\|\underset{\sim}{\nabla}_M \eta^{n+1}\|, \quad n = 0, \dots, N_T - 1.$$

Hence for the third term on the right-hand-side of (4.6), we have

$$\begin{aligned}
\sum_{n=0}^{m-1} 8\lambda \Delta t \|\underset{\sim}{\nu}^{n+1}\|^2 &\leq \sum_{n=0}^{m-1} \Delta t \left(16\lambda b |\underset{\approx}{\kappa}^{n+1}|^2 \|\eta^{n+1}\|^2 + \frac{4}{\lambda}\|\underset{\sim}{\nabla}_M \eta^{n+1}\|^2\right) \\
&\leq 4c_2 \sum_{n=0}^{m-1} \Delta t \|\eta^{n+1}\|^2_{\mathrm{H}^1_0(D;M)} \\
&= 4c_2 \|\eta\|^2_{\ell^2(0,t^m;\mathrm{H}^1_0(D;M))}, \qquad m = 1, \dots, N_T,
\end{aligned}$$

where $c_2 := \max\left(1/\lambda\,,\, 4\lambda b \|\underset{\approx}{\kappa}\|^2_{\mathrm{L}^\infty(0,T)}\right)$.

It remains to bound $\|\mu^{m+1}\|$. We begin by observing that

$$\begin{aligned}
\|\mu^{m+1}\| &\leq \left\| \frac{\hat{\psi}(\cdot, t^{n+1}) - \hat{\psi}(\cdot, t^n)}{\Delta t} - \frac{\partial \hat{\psi}}{\partial t}(\cdot, t^{n+1}) \right\| + \left\| \frac{\eta^{n+1} - \eta^n}{\Delta t} \right\| \\
&:= I + II.
\end{aligned}$$

For term I, applying Taylor's Theorem with integral remainder yields

$$\frac{\hat{\psi}(\cdot, t^{n+1}) - \hat{\psi}(\cdot, t^n)}{\Delta t} - \frac{\partial \hat{\psi}}{\partial t}(\cdot, t^{n+1}) = -\frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} (t^{n+1} - t)\frac{\partial^2 \hat{\psi}}{\partial t^2}(\cdot, t)\,\mathrm{d}t,$$

and it follows that

$$I \leq \sqrt{\Delta t} \left(\int_{t^n}^{t^{n+1}} \left\| \frac{\partial^2 \hat{\psi}}{\partial t^2}(\cdot, t) \right\|^2 \mathrm{d}t \right)^{\frac{1}{2}}.$$

For term II we have the following bound:

$$\begin{aligned}
II = \left\| \frac{\eta^{n+1} - \eta^n}{\Delta t} \right\| &= \left\{ \int_D \left(\frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \frac{\partial \eta}{\partial t}(\underset{\sim}{q}, t)\,\mathrm{d}t \right)^2 \mathrm{d}\underset{\sim}{q} \right\}^{\frac{1}{2}} \\
&\leq \left\{ \int_D \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \left| \frac{\partial \eta}{\partial t}(\underset{\sim}{q}, t) \right|^2 \mathrm{d}t\,\mathrm{d}\underset{\sim}{q} \right\}^{\frac{1}{2}} \\
&= \frac{1}{\sqrt{\Delta t}} \left\{ \int_{t^n}^{t^{n+1}} \left\| \frac{\partial \eta}{\partial t}(\cdot, t) \right\|^2 \mathrm{d}t \right\}^{\frac{1}{2}}.
\end{aligned}$$

With the bounds derived on I and II we now have that

$$\sum_{n=0}^{m-1} 2\Delta t\|\mu^{n+1}\|^2 \leq 4\sum_{n=0}^{m-1}\Delta t^2\int_{t^n}^{t^{n+1}}\left\|\frac{\partial^2\hat{\psi}}{\partial t^2}(\cdot,t)\right\|^2 \mathrm{d}t + 4\sum_{n=0}^{m-1}\int_{t^n}^{t^{n+1}}\left\|\frac{\partial \eta}{\partial t}(\cdot,t)\right\|^2 \mathrm{d}t$$
$$= 4\Delta t^2\left\|\frac{\partial^2\hat{\psi}}{\partial t^2}\right\|^2_{\mathrm{L}^2(0,t^m;\mathrm{L}^2(D))} + 4\left\|\frac{\partial\eta}{\partial t}\right\|^2_{\mathrm{L}^2(0,t^m;\mathrm{L}^2(D))}.$$

Combining the bounds on the three terms on the right-hand side of (4.6) we deduce that

$$\|\xi^m\|^2 + \frac{1}{2\lambda}\sum_{n=0}^{m-1}\Delta t\|\underset{\sim}{\nabla}_M\xi^{n+1}\|^2$$
$$\leq \mathrm{e}^{2c_0 m\Delta t}\left(\|\eta^0\|^2 + 4c_2\|\eta\|^2_{\ell^2(0,t^m;\mathrm{H}^1_0(D;M))} + 4\left\|\frac{\partial\eta}{\partial t}\right\|^2_{\mathrm{L}^2(0,t^m;\mathrm{L}^2(D))}\right.$$
$$\left. + 4\Delta t^2\left\|\frac{\partial^2\hat{\psi}}{\partial t^2}\right\|^2_{\mathrm{L}^2(0,t^m;\mathrm{L}^2(D))}\right). \tag{4.8}$$

It remains to bound the first three terms in the bracket on the right-hand side of (4.8). To do so we need to make a specific choice of the finite-dimensional space $\mathcal{P}_N(D)$ from which approximations to $\hat{\psi} \in \mathrm{H}^1_0(D;M)$ are sought, and we also need to specify the projector $\hat{\Pi}_N$. These questions will be discussed in the next section. We shall then return, in Section 6, to the bound (4.8) and complete the convergence analysis of the numerical method.

5. Approximation results. Motivated by the behaviour of the FENE potential considered in Section 2, we have assumed at the end of Section 2 that U is (-1)-convex. Then, $\mathrm{H}^1_0(D) \subset \mathrm{H}^1_0(D;M)$. Therefore, any finite-dimensional space $\mathcal{P}_N(D) \subset \mathrm{H}^1_0(D)$ is, trivially, also contained in $\mathrm{H}^1_0(D;M)$. Further, $\mathrm{H}^1(D;M) \cap \mathrm{C}^1(\overline{D}) = \mathrm{H}^1_0(D) \cap \mathrm{C}^1(\overline{D})$; thus, from the viewpoint of $\mathrm{C}^1(\overline{D})$ functions, the function spaces $\mathrm{H}^1(D;M)$ and $\mathrm{H}^1_0(D)$ are indistinguishable.

Remark 5.1. *We noted in Remark 4.1 that if, in addition, $\sqrt{M} \in \mathcal{P}_N(D)$ then*

$$\int_D \psi^n_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q} = \int_D \psi^0_N(\underset{\sim}{q})\,\mathrm{d}\underset{\sim}{q}.$$

Since $\sqrt{M} \in \mathrm{H}^1_0(D)$, one can ensure that this integral identity holds by choosing $\mathcal{P}_N(D) = \sqrt{M}\mathcal{S}_N(D)$, where $\mathcal{S}_N(D)$ is a finite-dimensional subspace of $\mathrm{C}^1(\overline{D})$ such that $1 \in \mathcal{S}_N(D)$.

Our definition of $\mathcal{P}_N(D)$ and the choice of the projector $\hat{\Pi}_N : \mathrm{H}^1_0(D;M) \to \mathcal{P}_N(D)$ depend on the number d of space dimensions. Since the case of $d = 2$ is sufficiently representative, for the sake of brevity and ease of presentation we shall confine ourselves to two space dimensions, that is, when D is a disc of radius $\sqrt{b}$ in $\mathbb{R}^2$.

Let D_0 denote the slit disc

$$D_0 := D \setminus \{(q_1, 0) \,:\, 0 \leq q_1 < \sqrt{b}\}.$$

It is natural to transform D_0 into the rectangle $(r,\theta) \in R := (0,1)\times(0,2\pi)$ in a polar co-ordinate system, using the (bijective) change of variables

$$\underset{\sim}{q} = (q_1,q_2) = (\sqrt{b}\,r\cos\theta, \sqrt{b}\,r\sin\theta) \in D_0 \tag{5.1}$$

where $(r,\theta) \in R$. Given $f \in \mathrm{H}^1(D)$, we define $\tilde{f}$ on R by

$$\tilde{f}(r,\theta) = f(q_1,q_2), \qquad \underset{\sim}{q} = (q_1,q_2) \in D_0, \quad (r,\theta) \in R, \qquad q_1 = \sqrt{b}\,r\cos\theta, \quad q_2 = \sqrt{b}\,r\sin\theta.$$

Thus,

$$\|f\|^2_{\mathrm{H}^1(D)} = \|f\|^2_{\mathrm{H}^1(D_0)} = \int_0^1 r \int_0^{2\pi} \left(b|\tilde{f}|^2 + |D_r \tilde{f}|^2 + \left| \frac{D_\theta \tilde{f}}{r} \right|^2 \right) \mathrm{d}\theta \, \mathrm{d}r.$$

Motivated by this identity and writing, here and henceforth, $\tilde{w}(r) := r$ for our weight-function on the interval $(0,1)$, we define the space

$$\tilde{\mathrm{H}}^1_{\tilde{w}}(R) := \{\tilde{f} \in \mathrm{L}^2_{\tilde{w}}(R) \,:\, D_r \tilde{f} \in \mathrm{L}^2_{\tilde{w}}(R) \quad \text{and} \quad \frac{1}{r} D_\theta \tilde{f} \in \mathrm{L}^2_{\tilde{w}}(R)\}, \tag{5.2}$$

equipped with the norm $\|\cdot\|_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)}$ defined by

$$\|\tilde{f}\|^2_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)} := \int_0^1 \tilde{w}(r) \int_0^{2\pi} \left(|\tilde{f}|^2 + |D_r \tilde{f}|^2 + \left| \frac{D_\theta \tilde{f}}{r} \right|^2 \right) \mathrm{d}\theta \, \mathrm{d}r, \tag{5.3}$$

where $\mathrm{L}^2_{\tilde{w}}(R)$ is the $\tilde{w}$-weighted space of square-integrable functions on R, with the norm $\|\cdot\|_{\mathrm{L}^2_{\tilde{w}}(R)}$ defined by

$$\|\tilde{f}\|^2_{\mathrm{L}^2_{\tilde{w}}(R)} := \int_0^1 \tilde{w}(r) \int_0^{2\pi} |\tilde{f}(r,\theta)|^2 \, \mathrm{d}\theta \, \mathrm{d}r = \int_R |\tilde{f}(r,\theta)|^2 \, r \, \mathrm{d}r \, \mathrm{d}\theta.$$

We denote by $\tilde{\mathrm{H}}^1_{\tilde{w},0}(R)$ the subspace of $\tilde{\mathrm{H}}^1_{\tilde{w}}(R)$ consisting of all functions $\tilde{f}$ such that the trace $\tilde{f}(1,\cdot) = 0$. For $s,t \geq 0$ the space $\mathrm{H}^{s,t}(R)$ is defined as

$$\mathrm{H}^{s,t}(R) := \mathrm{H}^s(0,1;\mathrm{H}^t_p(0,2\pi)), \tag{5.4}$$

where the periodic Sobolev space $\mathrm{H}^t_p(0,2\pi)$ is given by

$$\mathrm{H}^t_p(0,2\pi) := \{\tilde{f} \in \mathrm{H}^t_{\mathrm{loc}}(\mathbb{R}) : \tilde{f}(\theta + 2\pi) = \tilde{f}(\theta) \quad \forall \theta \in \mathbb{R}\}.$$

Clearly, $\tilde{f} \in \tilde{\mathrm{H}}^1_{\tilde{w}}(R)$ implies that $f \in \mathrm{H}^1(D_0)$, and *vice versa*. We will also need weighted Sobolev spaces of the following form:

$$\mathrm{H}^{s,t}_{\tilde{w}}(R) := \mathrm{H}^s_{\tilde{w}}(0,1;\mathrm{H}^t_p(0,2\pi)), \tag{5.5}$$

equipped (for non-negative integers s and t) with the norm $\|\cdot\|_{\mathrm{H}^{s,t}_{\tilde{w}}(R)}$ defined by

$$\|\tilde{f}\|^2_{\mathrm{H}^{s,t}_{\tilde{w}}(R)} := \sum_{0 \leq i \leq s,\, 0 \leq j \leq t} \int_0^1 \tilde{w}(r) \int_0^{2\pi} |D^i_r D^j_\theta \, \tilde{f}(r,\theta)|^2 \, \mathrm{d}\theta \, \mathrm{d}r.$$

Similarly, for $s > \frac{1}{2}$, we define

$$\mathrm{H}^{s,t}_{\tilde{w},0}(R) := \mathrm{H}^s_{\tilde{w},0}(0,1;\mathrm{H}^t_p(0,2\pi)),$$

where $\mathrm{H}^s_{\tilde{w},0}(0,1)$ is the subspace of $\mathrm{H}^s_{\tilde{w}}(0,1)$ consisting of all functions that vanish (in the sense of the Trace Theorem) at $r = 1$. In particular, for $s = 1$, $\mathrm{H}^1_{\tilde{w},0}(0,1)$ denotes the set of all $\tilde{u} \in \mathrm{H}^1_{\tilde{w}}(0,1)$ such that $\tilde{u}(1) = 0$, endowed with the following inner product and norm:

$$(\tilde{u},\tilde{v})_{\mathrm{H}^1_{\tilde{w},0}(0,1)} := \int_0^1 \tilde{w}(r) \, D_r \tilde{u} \, D_r \tilde{v} \, \mathrm{d}r \qquad \text{and} \qquad \|\tilde{u}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} := \{(\tilde{u},\tilde{v})_{\mathrm{H}^1_{\tilde{w},0}(0,1)}\}^{\frac{1}{2}}.$$

Note that $\tilde{w}$ is a Jacobi weight function (*i.e.*, of the form $(1-s)^\alpha(1+s)^\beta$, $s \in (-1,1)$ with $\alpha, \beta > -1$) when transformed to $(-1,1)$.

We now introduce the projection operators that we will use. Due to the cartesian product structure of the set R it is natural to define distinct projection operators in the r and θ co-ordinate directions. In the θ-direction we use the orthogonal projection in the $\mathrm{L}^2(0,2\pi)$ inner product (*i.e.*, truncation of the Fourier series) denoted, for $N \geq 1$, by

$$P_N^F : \mathrm{L}^2(0,2\pi) \to \mathbb{S}_N(0,2\pi),$$

where $\mathbb{S}_N(0,2\pi)$ is the space of all trigonometric polynomials in $\theta \in [0,2\pi]$ of degree N or less.

The appropriate choice of projector in the r-direction is less immediate. We define, for $N \geq 1$,

$$P_N^J g : \mathrm{H}^1_{\tilde{w},0}(0,1) \to \mathbb{P}_{N,0}(0,1) \tag{5.6}$$

as the orthogonal projection in the $\mathrm{H}^1_{\tilde{w},0}(0,1)$ inner product, where $\mathbb{P}_{N,0}(0,1)$ is the space of all algebraic polynomials in $r \in [0,1]$, of degree N or less, that vanish at $r=1$.

It is tempting to define a two-dimensional projector onto $\mathbb{S}_N(0,2\pi) \otimes \mathbb{P}_{N,0}(0,1)$ as the tensor product of the projectors P_N^F and P_N^J. Unfortunately, this choice is inadequate due to the presence of the singular factor $1/r$ in the weighted Sobolev norm $\|\cdot\|_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)}$, and a different definition is required. In order to motivate our choice of the two-dimensional projector below, we state the following result that can be seen as a variant of the Malgrange Preparation Theorem [19].

Lemma 5.2. **(Decomposition Lemma)** *Suppose that (a,b) and (c,d) are nonempty bounded open intervals of $\mathbb{R}$, with $x \in (a,b)$ and $y \in (c,d)$, and $u \in \mathrm{W}^{1,q}((c,d);\mathrm{W}^{s,p}(a,b))$ where $1 \leq q \leq \infty$, $1 < p \leq \infty$, and $1/p < s \leq 1$. Then,*

(a) $u_y \in \mathrm{L}^q((c,d);\mathrm{C}^{s-1/p}[a,b])$;

(b) If there exists $x_0 \in [a,b]$ such that $u_y(x_0,y)=0$ for a.e. $y \in (c,d)$, then

$$u(x,y) = A(x) + (x-x_0)B(x,y),$$

where $A \in \mathrm{W}^{s,p}(a,b)$, $B \in \mathrm{W}^{1,q}((c,d);\mathrm{L}^t(a,b))$, with $1 \leq t < p$ and $1 + (1/p) < s + (1/t)$, and $(x-x_0)B \in \mathrm{W}^{1,q}((c,d);\mathrm{W}^{s,p}(a,b))$.

(c) If, in addition to $x_0 \in [a,b]$ as in part (b), there exists $x_1 \in [a,b]$ (which may, but need not, differ from x_0) such that $u(x_1,y)=0$ for a.e. $y \in (c,d)$, then $A(x_1)=0$ and $B(x_1,y)=0$ for all $y \in (c,d)$.

Proof. (a) Since $u \in \mathrm{W}^{1,q}((c,d);\mathrm{W}^{s,p}(a,b))$, we have $u_y \in \mathrm{L}^q((c,d);\mathrm{W}^{s,p}(a,b))$, and therefore, by the Sobolev Embedding Theorem, also $u_y \in \mathrm{L}^q((c,d);\mathrm{C}^{s-1/p}[a,b])$.

(b) It follows from (a) that

$$|u_y(x_1,y) - u_y(x_2,y)| \leq C(y)|x_1-x_2|^{s-1/p} \qquad \forall x_1,x_2 \in [a,b] \quad \text{and for a.e. } y \in (c,d),$$

where $C \in \mathrm{L}^q(c,d)$. Now, suppose that there exists $x_0 \in [a,b]$ such that $u_y(x_0,y)=0$ for a.e. $y \in (c,d)$. Let

$$v(x,y) := \begin{cases} u_y(x,y)/(x-x_0) & \text{when } x \in [a,b]\setminus\{x_0\}, \quad y \in (c,d), \\ 0 & \text{when } x = x_0, \quad y \in (c,d). \end{cases}$$

Clearly, $u_y(x,y) = (x-x_0)\,v(x,y)$. If $q \in [1,\infty)$, then

$$\begin{aligned} \left(\int_c^d \left(\int_a^b |v(x,y)|^t\,\mathrm{d}x\right)^{\frac{q}{t}} \mathrm{d}y\right)^{\frac{1}{q}} &= \left(\int_c^d \left(\int_a^b \frac{|u_y(x,y)-u_y(x_0,y)|^t}{|x-x_0|^t}\,\mathrm{d}x\right)^{\frac{q}{t}} \mathrm{d}y\right)^{\frac{1}{q}} \\ &\leq \left(\int_a^b \frac{\mathrm{d}x}{|x-x_0|^{t(1-(s-1/p))}}\right)^{\frac{1}{t}} \left(\int_c^d |C(y)|^q\,\mathrm{d}y\right)^{\frac{1}{q}} < \infty, \end{aligned}$$

since $0 < t(1-(s-1/p)) < 1$. If, on the other hand, $q = \infty$, then

$$\text{ess.sup}_{y\in(c,d)} \left(\int_a^b |v(x,y)|^t\,\mathrm{d}x\right)^{\frac{1}{t}} \leq \left(\int_a^b \frac{\mathrm{d}x}{|x-x_0|^{t(1-(s-1/p))}}\right)^{\frac{1}{t}} \cdot \text{ess.sup}_{y\in(c,d)}|C(y)| < \infty.$$

Either way $v \in \mathrm{L}^q((c,d);\mathrm{L}^t(a,b))$, which then implies that the function $y \mapsto \int_c^y v(x,\eta)\,\mathrm{d}\eta$ is absolutely continuous on $[c,d]$ for a.e. $x \in [a,b]$; moreover, it belongs to $\mathrm{W}^{1,q}(c,d)$ for a.e. $x \in [a,b]$. Further, the function $B : (x,y) \mapsto B(x,y) := \int_c^y v(x,\eta)\,\mathrm{d}\eta$, defined on $(a,b)\times(c,d)$, belongs to $\mathrm{W}^{1,q}((c,d);\mathrm{L}^t(a,b))$. Now,

$$u(x,y) = u(x,c) + (x-x_0)\int_c^y v(x,\eta)\,\mathrm{d}\eta =: A(x) + (x-x_0)B(x,y),$$

with $A \in \mathrm{W}^{s,p}(a,b)$, $B \in \mathrm{W}^{1,q}((c,d);\mathrm{L}^t(a,b))$, and $(x-x_0)B \in \mathrm{W}^{1,q}((c,d);\mathrm{W}^{s,p}(a,b))$.

(c) Now, let $x_1 \in [a,b]$ and $u(x_1,y) = 0$ for a.e. $y \in (c,d)$. Since then $u_y(x_1,y) = 0$ for a.e. $y \in (c,d)$, it follows from the definition of the function v in part (b) that $v(x_1,y) = 0$ for a.e. $y \in (c,d)$, irrespective of whether or not $x_1 \neq x_0$. Hence, recalling the definition of B, we also have that $B(x_1,y) = 0$ for all $y \in (c,d)$. Thus, $A(x_1) = u(x_1,y) - (x_1-x_0)B(x_1,y) = 0$. ☐

Suppose that $\tilde g \in \tilde{\mathrm{H}}^1_{\tilde w,0}(R)\cap \mathrm{H}^{1,1}(R)$. Then, necessarily, $D_\theta \tilde g(0,\theta) = 0$ for a.e. $\theta \in (0,2\pi)$, as otherwise $\|\tilde g\|_{\tilde{\mathrm{H}}^1_{\tilde w}(R)}$ would not be finite.[1] Furthermore, applying Lemma 5.2 with $x = r$, $y = \theta$, $(a,b) = (0,1)$, $(c,d) = (0,2\pi)$, $s = 1$, $p = q = 2$, $x_0 = 0$ and $x_1 = 1$, we deduce that $\tilde g$ has the decomposition

$$\tilde g(r,\theta) = \tilde g_1(r) + r\tilde g_2(r,\theta), \tag{5.7}$$

where $\tilde g_1 \in \mathrm{H}^1(0,1)$, $\tilde g_2 \in \mathrm{H}^1_p((0,2\pi);\mathrm{L}^t(0,1))$ with $1 \le t < 2$, and $r\tilde g_2 \in \mathrm{H}^1_p((0,2\pi);\mathrm{H}^1(0,1))$, $\tilde g_1(1) = 0$ (and therefore $\tilde g_1 \in \mathrm{H}^1_{\tilde w,0}(0,1)$), and $\tilde g_2(1,\theta) = 0$ for all $\theta \in (0,2\pi)$.

Assuming that $\tilde g \in \tilde{\mathrm{H}}^1_{\tilde w,0}(R)\cap\mathrm{H}^{1,1}(R)$, and $\tilde g_2(\cdot,\theta) \in \mathrm{H}^1_{\tilde w,0}(0,1)$ for all $\theta \in (0,2\pi)$, we now define

$$\tilde P^J_N \tilde g(\cdot,\theta) := P^J_N \tilde g_1(\cdot) + rP^J_{N-1}\tilde g_2(\cdot,\theta), \quad \theta \in (0,2\pi),$$

where $P^J_N : \mathrm{H}^1_{\tilde w,0}(0,1) \to \mathbb{P}_{N,0}(0,1)$ is the orthogonal projector defined in (5.6).

There are a number of approximation results available in the literature related to projectors in Jacobi-weighted inner products (see for example [5] or [10]). Since the setting here is specific, we need to establish the required approximation properties of the univariate projector P^J_N from first principles. The approximation properties of $\tilde P^J_N$ and of our two-dimensional projector $P^F_N \tilde P^J_N$ will then follow. The relevant results are stated in the next two lemmas.

Lemma 5.3. *Suppose that $\tilde g \in \mathrm{H}^k_{\tilde w,0}(0,1)$ with $k \ge 1$; then,*

$$\|\tilde g - P^J_N \tilde g\|_{\mathrm{H}^1_{\tilde w}(0,1)} \le cN^{1-k}\|\tilde g\|_{\mathrm{H}^k_{\tilde w}(0,1)}. \tag{5.8}$$

If, in addition, there exists $\alpha \in (0,1)$ such that $r \mapsto r^\alpha \tilde g(r) \in \mathrm{C}[0,1]$, then also

$$\|\tilde g - P^J_N \tilde g\|_{\mathrm{L}^2_{\tilde w}(0,1)} \le cN^{-k}\|\tilde g\|_{\mathrm{H}^k_{\tilde w}(0,1)}. \tag{5.9}$$

Proof. Let us first prove (5.8). Note that by Pythagoras' Theorem,

$$\|\tilde g - P^J_N\tilde g\|_{\mathrm{H}^1_{\tilde w,0}(0,1)} = \left(\|\tilde g\|^2_{\mathrm{H}^1_{\tilde w,0}(0,1)} - \|P^J_N\tilde g\|^2_{\mathrm{H}^1_{\tilde w,0}(0,1)}\right)^{\frac12} \le \|\tilde g\|_{\mathrm{H}^1_{\tilde w,0}(0,1)} \le \|\tilde g\|_{\mathrm{H}^k_{\tilde w}(0,1)}.$$

If $k = 1$, the right-most term in this chain is equal to $1\cdot N^{1-k}\|\tilde g\|_{\mathrm{H}^k_{\tilde w}(0,1)}$, while if $k \ge 2$ and $1 \le N < k-1$, then it is bounded by $(k-1)^{k-1}N^{1-k}\|\tilde g\|_{\mathrm{H}^k_{\tilde w}(0,1)}$.

[1] Note that by part (a) of the Decomposition Lemma, if $\tilde g \in \mathrm{H}^{1,1}(R)$, then $D_\theta\tilde g \in \mathrm{L}^2((0,2\pi);\mathrm{C}^{\frac12}[0,1])$. If $D_\theta \tilde g(0,\theta)$ were nonzero for $\theta \in S_0$ where S_0 is a subset of $(0,2\pi)$ of Lebesgue measure $\mathcal{L}_1(S_0) > 0$, then for each $\theta \in S_0$ there would exist a nonempty interval $[0,r_\theta] \subset [0,1]$ over which $|D_\theta\tilde g(\cdot,\theta)|$ is continuous and strictly positive and has, therefore, a positive lower bound (which may vary with θ). Now, $\int_0^1 |D_\theta\tilde g(r,\theta)|^2/r\,\mathrm{d}r \ge \int_0^{r_\theta}|D_\theta\tilde g(r,\theta)|^2/r\,\mathrm{d}r$ and the latter integral is divergent for each $\theta \in S_0$. As S_0 has positive measure, also $\int_0^{2\pi}\int_0^1 |D_\theta\tilde g(r,\theta)|^2/r\,\mathrm{d}r\,\mathrm{d}\theta = \infty$, which in turn contradicts $\tilde g \in \tilde{\mathrm{H}}^1_{\tilde w,0}(R)$. Thus $\mathcal{L}_1(S_0) = 0$, or S_0 is empty; in any case, $D_\theta\tilde g(0,\theta) = 0$ for a.e. $\theta \in (0,2\pi)$.

Finally, if $k \geq 2$ and $N \geq \max(2, k-1)$, then we recall that, by the definition of P_N^J,

$$\|\tilde{g} - P_N^J \tilde{g}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \leq \|\tilde{g} - \tilde{v}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \qquad \forall \tilde{v} \in \mathbb{P}_{N,0}(0,1).$$

Select, in particular,

$$\tilde{v}(r) = -\int_r^1 Q_{N-1}^J D_s \tilde{g}(s)\,\mathrm{d}s, \qquad r \in [0,1],$$

where Q_{N-1}^J is the orthogonal projector in $\mathrm{L}^2_{\tilde{w}}(0,1)$ onto $\mathbb{P}_{N-1}(0,1)$, the set of all algebraic polynomials of degree $N-1$ or less on the interval $[0,1]$. Thus,

$$\|\tilde{g} - P_N^J \tilde{g}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \leq \|D_r \tilde{g} - D_r \tilde{v}\|_{\mathrm{L}^2_{\tilde{w}}(0,1)} = \|D_r \tilde{g} - Q_{N-1}^J (D_r \tilde{g})\|_{\mathrm{L}^2_{\tilde{w}}(0,1)} \leq c\,(N-1)^{1-k} \|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)},$$

where the last bound (scaled from the standard interval $(-1,1)$ to $(0,1)$) comes from §5.7.1 of Canuto *et al.* [10], and is valid for $N \geq \max(2, k-1)$, $k \geq 2$. Hence, after bounding $(N-1)^{1-k}$ by $2^{k-1}N^{1-k}$ (recall that $N \geq 2$ by hypothesis), we deduce that

$$\|\tilde{g} - P_N^J \tilde{g}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \leq c\,2^{k-1} N^{1-k} \|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)}.$$

Now choosing $\hat{c} = \max\{(k-1)^{k-1}, c\,2^{k-1}\}$, with the convention that $0^0 := 1$, we have that

$$\|\tilde{g} - P_N^J \tilde{v}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \leq \hat{c} N^{1-k} \|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)}$$

for all $N \geq 1$ (regardless of whether or not $N \geq k-1$). Since by the Poincaré inequality

$$\|\tilde{v}\|_{\mathrm{L}^2_{\tilde{w}}(0,1)} \leq \frac{1}{\sqrt{2}} \|D_r \tilde{v}\|_{\mathrm{L}^2_{\tilde{w}}(0,1)} \qquad \forall \tilde{v} \in \mathrm{H}^1_{\tilde{w},0}(0,1) \tag{5.10}$$

$\|\cdot\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)}$ and $\|\cdot\|_{\mathrm{H}^1_{\tilde{w}}(0,1)}$ are equivalent norms on $\mathrm{H}^1_{\tilde{w},0}(0,1)$, we deduce (5.8) for any $N \geq 1$.

The proof of (5.9) is based on a duality argument. Let $e := \tilde{g} - P_N^J \tilde{g}$. It follows from the hypotheses on $\tilde{g}$ that $e \in \mathrm{L}^2_{\tilde{w}}(0,1)$, and $r \mapsto r^\alpha e(r) \in \mathrm{C}[0,1]$ with $\alpha \in (0,1)$.

Given any $e \in \mathrm{L}^2_{\tilde{w}}(0,1)$, consider the mixed Neumann–Dirichlet boundary-value problem:

$$-D_r(r D_r\, z_e(r)) = r\, e(r), \quad r \in (0,1), \qquad \lim_{r \to 0_+} r D_r z_e(r) = 0, \quad z_e(1) = 0. \tag{5.11}$$

By (5.10) and the Lax–Milgram Theorem, this has a unique weak solution $z_e \in \mathrm{H}^1_{\tilde{w},0}(0,1)$,

$$(z_e, v)_{\mathrm{H}^1_{\tilde{w},0}(0,1)} = (e, v)_{\mathrm{L}^2_{\tilde{w}}(0,1)} \qquad \forall v \in \mathrm{H}^1_{\tilde{w},0}(0,1), \qquad \text{and} \qquad \|z_e\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)} \leq \frac{3}{4} \|e\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)}. \tag{5.12}$$

We shall show that, in fact, $z_e \in \mathrm{H}^2_{\tilde{w},0}(0,1)$. To this end, note that

$$D_r z_e(r) = -\frac{1}{r} \int_0^r s\, e(s)\,\mathrm{d}s, \qquad r \in (0,1]. \tag{5.13}$$

Hence, $D_r z_e \in \mathrm{C}(0,1]$; and since $r \mapsto r^\alpha e(r) \in \mathrm{C}[0,1]$ with $\alpha \in (0,1)$, we have $\lim_{r \to 0_+} r\, e(r) = 0$, and therefore $\lim_{r \to 0_+} D_r z_e(r) = 0$. Now,

$$\begin{aligned}\int_0^1 \frac{1}{r} |D_r z_e(r)|^2\,\mathrm{d}r &\leq \frac{1}{2} \int_0^1 r\, |\ln r|^2\, |e(r)|^2\,\mathrm{d}r = \frac{1}{2} \int_0^1 |r^\alpha e(r)|^2 \cdot \frac{|\ln r|}{r^{2\alpha-1}}\,\mathrm{d}r \\ &\leq \max_{x \in [0,1]} |r^\alpha\, e(r)|^2 \int_0^1 \frac{|\ln r|}{r^{2\alpha-1}}\,\mathrm{d}r < \infty,\end{aligned}$$

by using in the left-most integral in the chain the identity (5.13) with $s = \sqrt{s}\,\sqrt{s}$, applying the Cauchy–Schwarz inequality in the inner integral, and exchanging the order of integration in the resulting double integral. Thus, it follows from (5.11) that $D_r^2 z_e = -(e + r^{-1} D_r z_e) \in \mathrm{L}^2_{\tilde{w}}(0,1) \cap \mathrm{C}(0,1]$ and, for any $\varepsilon \in (0,1)$,

$$\int_\varepsilon^1 r\,|D_r^2 z_e(r)|^2\,\mathrm{d}r + \int_\varepsilon^1 D_r z_e(r)\, D_r^2 z_e(r)\,\mathrm{d}r = -\int_\varepsilon^1 r\, e(r)\, D_r^2 z_e(r)\,\mathrm{d}r.$$

Hence, by computing explicitly the second integral on the left-hand side and applying Cauchy's inequality $|ab| \le \frac{1}{2}(a^2+b^2)$ on the right-hand side, we obtain

$$\int_\varepsilon^1 r\,|D_r^2 z_e(r)|^2\,\mathrm{d}r + |D_r z_e(1)|^2 \le \int_\varepsilon^1 r\,|e(r)|^2\,\mathrm{d}r + |D_r z_e(\varepsilon)|^2.$$

Passing to the limit $\varepsilon \to 0_+$, and omitting the second term on the left-hand side, we deduce that

$$\int_0^1 r\,|D_r^2 z_e(r)|^2\,\mathrm{d}r \le \int_0^1 r\,|e(r)|^2\,\mathrm{d}r.$$

Combining this with our earlier bound from (5.12), we have that

$$\|z_e\|^2_{\mathrm{H}^2_{\tilde{w}}(0,1)} \le \frac{7}{4}\|e\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)}. \tag{5.14}$$

We are now ready to embark on the analysis of the projection error in the $\mathrm{L}^2_{\tilde{w}}(0,1)$ norm. Recalling that $e = \tilde{g} - P_N^J \tilde{g} \in \mathrm{H}^1_{\tilde{w},0}(0,1)$, we deduce from the weak formulation (5.12), the definition of the orthogonal projector P_N^J, the Cauchy–Schwarz inequality, (5.8) and (5.14) that

$$\begin{aligned}
\|\tilde{g} - P_N^J\tilde{g}\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)} = (e, \tilde{g} - P_N^J\tilde{g})_{\mathrm{L}^2_{\tilde{w}}(0,1)} &= (z_e, \tilde{g} - P_N^J\tilde{g})_{\mathrm{H}^1_{\tilde{w},0}(0,1)} = (\tilde{g} - P_N^J\tilde{g}, z_e)_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \\
&= (\tilde{g} - P_N^J\tilde{g}, z_e - P_N^J z_e)_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \\
&\le \|\tilde{g} - P_N^J\tilde{g}\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \|z_e - P_N^J z_e\|_{\mathrm{H}^1_{\tilde{w},0}(0,1)} \\
&\le cN^{1-k}\|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)} \cdot N^{-1}\|z_e\|_{\mathrm{H}^2_{\tilde{w}}(0,1)} \\
&\le cN^{-k}\|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)}\|e\|_{\mathrm{L}^2_{\tilde{w}}(0,1)} \\
&= cN^{-k}\|\tilde{g}\|_{\mathrm{H}^k_{\tilde{w}}(0,1)}\|\tilde{g} - P_N^J\tilde{g}\|_{\mathrm{L}^2_{\tilde{w}}(0,1)}, \qquad k \ge 1.
\end{aligned}$$

Dividing the left-most and the right-most term in this chain by $\|\tilde{g} - P_N^J\tilde{g}\|_{\mathrm{L}^2_{\tilde{w}}(0,1)}$ gives (5.9). ☐

REMARK 5.4. *A sufficient condition for the existence of $\alpha \in (0,1)$ such that the function $r \mapsto r^\alpha \tilde{g}(r) \in \mathrm{C}[0,1]$ is that (by adopting the notation from Chapter 3 of Triebel [29])*

$$\tilde{g} \in \mathrm{W}^1_2((0,1); r^{\alpha+1}; r^{\alpha-1}) := \{\tilde{f} \in \mathrm{L}^2_{\mathrm{loc}}(0,1) \,:\, \int_0^1 r^{\alpha+1}|D_r\tilde{f}(r)|^2 + r^{\alpha-1}|\tilde{f}(r)|^2\,\mathrm{d}r < \infty\}.$$

As a matter of fact, if $\tilde{g} \in \mathrm{W}^1_2((0,1); r^{\alpha+1}; r^{\alpha-1})$ for some $\alpha \in (0,1)$, then $r \mapsto r^\alpha \tilde{g}(r) \in \mathrm{C}^{\frac{\alpha}{2}}[0,1]$. This follows from the following inequality: let $G(r) = r^\alpha \tilde{g}(r)$; then,

$$|G(r_1) - G(r_2)| \le |r_1 - r_2|^{\frac{\alpha}{2}} \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} \left(\int_0^1 r^{1+\alpha}|D_r\tilde{g}(r)|^2 + r^{\alpha-1}|\tilde{g}(r)|^2\,\mathrm{d}r\right)^{\frac{1}{2}}.$$

LEMMA 5.5. *Let $\tilde{g} \in \tilde{\mathrm{H}}^1_{\tilde{w},0}(R) \cap \mathrm{H}^{1,1}(R)$, with decomposition $\tilde{g}(r,\theta) = \tilde{g}_1(r) + r\tilde{g}_2(r,\theta)$, where $\tilde{g}_1 \in \mathrm{H}^1_{\tilde{w},0}(0,1)$ and $\tilde{g}_2(\cdot,\theta) \in \mathrm{H}^1_{\tilde{w},0}(0,1)$ for all $\theta \in (0,2\pi)$, and denote by $\tilde{\Pi}_N$ the two-dimensional projector onto $\mathbb{P}_{N_r}(0,1) \otimes \mathbb{S}_{N_\theta}(0,2\pi)$ defined, for positive integers N_θ and N_r, by*

$$(\tilde{\Pi}_N\tilde{g})(r,\theta) := (P^F_{N_\theta}\tilde{P}^J_{N_r}\tilde{g})(r,\theta) = (\tilde{P}^J_{N_r}P^F_{N_\theta}\tilde{g})(r,\theta).$$

If $\tilde{g}_1 \in \mathrm{H}^{k+1}_{\tilde{w}}(0,1)$ and $\tilde{g}_2 \in \mathrm{H}^{k+1,0}_{\tilde{w}}(R) \cap \mathrm{H}^{k,1}_{\tilde{w}}(R) \cap \mathrm{H}^{0,l+1}_{\tilde{w}}(R) \cap \mathrm{H}^{1,l}_{\tilde{w}}(R)$ for some $k, l \geq 1$, and there exists an $\alpha \in (0,1)$ such that, for each $\theta \in (0, 2\pi)$, $r \mapsto r^\alpha g_2(r,\theta) \in \mathrm{C}[0,1]$, then

$$\|\tilde{g} - \tilde{\Pi}_N \tilde{g}\|_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)} \leq C_1 N_r^{-k} \left(\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k+1,0}_{\tilde{w}}(R)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k,1}_{\tilde{w}}(R)} \right)^{\frac{1}{2}} + C_2 N_\theta^{-l} \left(\|\tilde{g}_2\|^2_{\mathrm{H}^{0,l+1}_{\tilde{w}}(R)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{1,l}_{\tilde{w}}(R)} \right)^{\frac{1}{2}}. \tag{5.15}$$

If $\tilde{g}_1 \in \mathrm{H}^{k}_{\tilde{w}}(0,1)$ and $\tilde{g}_2 \in \mathrm{H}^{k,0}_{\tilde{w}}(R) \cap \mathrm{H}^{0,l}_{\tilde{w}}(R)$ for some $k, l \geq 1$, and there exists an $\alpha \in (0,1)$ such that, for each $\theta \in (0, 2\pi)$, $r \mapsto r^\alpha g_2(r,\theta) \in \mathrm{C}[0,1]$, then

$$\|\tilde{g} - \tilde{\Pi}_N \tilde{g}\|_{\mathrm{L}^2_{\tilde{w}}(R)} \leq C_1 N_r^{-k} \left(\|\tilde{g}_1\|^2_{\mathrm{H}^{k}_{\tilde{w}}(0,1)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k,0}_{\tilde{w}}(R)} \right)^{\frac{1}{2}} + C_2 N_\theta^{-l} \|\tilde{g}_2\|_{\mathrm{H}^{0,l}_{\tilde{w}}(R)}. \tag{5.16}$$

Proof. The left-hand side in (5.15) is given by:

$$\begin{aligned}\|\tilde{g} - \tilde{\Pi}_N \tilde{g}\|^2_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)} &= \int_0^1 \tilde{w}(r) \int_0^{2\pi} \left\{ (\tilde{g} - \tilde{\Pi}_N \tilde{g})^2 + (D_r \tilde{g} - D_r(\tilde{\Pi}_N \tilde{g}))^2 \right\} \mathrm{d}\theta \, \mathrm{d}r \\ &\quad + \int_0^1 r^{-1} \int_0^{2\pi} (D_\theta \tilde{g} - D_\theta(\tilde{\Pi}_N \tilde{g}))^2 \, \mathrm{d}\theta \, \mathrm{d}r \\ &=: I + II.\end{aligned}$$

Let us first consider term I; we treat the two terms in the, inner, θ-integral in I separately. First, using the L^2-error bound for Fourier projection, as well as the fact that $\|P^F_{N_\theta}\|_{\mathcal{L}(\mathrm{L}^2_p(0,2\pi), \mathrm{L}^2_p(0,2\pi))} \leq 1$, we obtain

$$\begin{aligned}\|\tilde{g}(r,\cdot) - \tilde{\Pi}_N \tilde{g}(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} &\leq \left(\|\tilde{g}(r,\cdot) - P^F_{N_\theta} \tilde{g}(r,\cdot)\|_{\mathrm{L}^2(0,2\pi)} + \|P^F_{N_\theta}(\tilde{g}(r,\cdot) - \tilde{P}^J_{N_r} \tilde{g}(r,\cdot))\|_{\mathrm{L}^2(0,2\pi)} \right)^2 \\ &\leq \left(C_3 N_\theta^{-l} \|D^l_\theta \tilde{g}(r,\cdot)\|_{\mathrm{L}^2(0,2\pi)} + \|\tilde{g}(r,\cdot) - \tilde{P}^J_{N_r} \tilde{g}(r,\cdot)\|_{\mathrm{L}^2(0,2\pi)} \right)^2 \\ &\leq 2C_3^2 N_\theta^{-2l} \|D^l_\theta \tilde{g}(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} + 2\|\tilde{g}(r,\cdot) - \tilde{P}^J_{N_r} \tilde{g}(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} \\ &\leq 2C_3^2 N_\theta^{-2l} \|D^l_\theta \tilde{g}_2(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} + 2\|\tilde{g}(r,\cdot) - \tilde{P}^J_{N_r} \tilde{g}(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)},\end{aligned}$$

where $D^l_\theta \tilde{g} = r D^l_\theta \tilde{g}_2$ and $0 \leq r \leq 1$ have been used in the last line. Similarly,

$$\begin{aligned}&\|D_r \tilde{g}(r,\cdot) - D_r(\tilde{\Pi}_N \tilde{g}(r,\cdot))\|^2_{\mathrm{L}^2(0,2\pi)} \\ &\quad \leq 2C_3^2 N_\theta^{-2l} \|D_r D^l_\theta \tilde{g}(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} + 2\|D_r \tilde{g}(r,\cdot) - D_r(\tilde{P}^J_{N_r} \tilde{g}(r,\cdot))\|^2_{\mathrm{L}^2(0,2\pi)} \\ &\qquad \leq 4C_3^2 N_\theta^{-2l} (\|D^l_\theta \tilde{g}_2(r,\cdot)\|^2_{\mathrm{L}^2(0,2\pi)} + \|D_r D^l_\theta \tilde{g}_2(r,\cdot)\|^2_{L^2(0,2\pi)}) \\ &\qquad\quad + 2\|D_r \tilde{g}(r,\cdot) - D_r(\tilde{P}^J_{N_r} \tilde{g}(r,\cdot))\|^2_{\mathrm{L}^2(0,2\pi)}.\end{aligned}$$

Therefore,

$$I \leq 6C_3^2 N_\theta^{-2l} \int_0^{2\pi} \left(\|D^l_\theta \tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)} + \|D_r D^l_\theta \tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)} \right) \mathrm{d}\theta + 2 \int_0^{2\pi} \|\tilde{g}(\cdot,\theta) - \tilde{P}^J_{N_r} \tilde{g}(\cdot,\theta)\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)} \mathrm{d}\theta.$$

Now we bound the final term on the right-hand side of the last inequality:

$$
\begin{aligned}
&\|\tilde{g}(\cdot,\theta) - \tilde{P}^J_{N_r}\tilde{g}(\cdot,\theta)\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)} \le 2\|\tilde{g}_1 - P^J_{N_r}\tilde{g}_1\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)} + 2\|r(\tilde{g}_2(\cdot,\theta) - P^J_{N_r-1}\tilde{g}_2(\cdot,\theta))\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)}\\
&\quad \le C^2 N_r^{-2k}\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)}\\
&\qquad + 2\int_0^1 \tilde{w}(r)\left\{[r(\tilde{g}_2(r,\theta) - P^J_{N_r-1}\tilde{g}_2(r,\theta))]^2 + [D_r(r(\tilde{g}_2(r,\theta) - P^J_{N_r-1}\tilde{g}_2(r,\theta)))]^2\right\}\mathrm{d}r\\
&\quad = C^2 N_r^{-2k}\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)}\\
&\qquad + 2\int_0^1 \tilde{w}(r)\left\{(1+r^2)(\tilde{g}_2(r,\theta) - P^J_{N_r-1}\tilde{g}_2(r,\theta))^2 + r^2(D_r(\tilde{g}_2(r,\theta) - P^J_{N_r-1}\tilde{g}_2(r,\theta)))^2\right\}\mathrm{d}r\\
&\quad \le C^2 N_r^{-2k}\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + 4\|\tilde{g}_2(\cdot,\theta) - P^J_{N_r-1}\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)}\\
&\quad \le C_4^2 N_r^{-2k}\left(\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + \|\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)}\right),
\end{aligned}
$$

using the univariate $\|\cdot\|_{\mathrm{H}^1_{\tilde{w}}}$ error bound (5.8). Therefore,

$$
\begin{aligned}
I \le 6\,C_3^2 N_\theta^{-2l}\int_0^{2\pi}&\left(\|D^l_\theta\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)} + \|D_r D^l_\theta\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)}\right)\mathrm{d}\theta\\
&+ 2\,C_4^2 N_r^{-2k}\int_0^{2\pi}\left(\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + \|\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)}\right)\mathrm{d}\theta,
\end{aligned}
\tag{5.17}
$$

which is an optimal-order bound on I.

Next we consider II. Using the fact that θ-differentiation commutes with the projectors $P^J_{N_r}$ and $P^F_{N_\theta}$, we have

$$
\begin{aligned}
II &= \int_0^1 r^{-1}\int_0^{2\pi}|D_\theta(\tilde{g}(r,\theta) - \tilde{P}^J_{N_r}P^F_{N_\theta}\tilde{g}(r,\theta))|^2\mathrm{d}\theta\,\mathrm{d}r\\
&\le 2\int_0^1 r^{-1}\int_0^{2\pi}|D_\theta\tilde{g}(r,\theta) - P^F_{N_\theta}D_\theta\tilde{g}(r,\theta)|^2\mathrm{d}\theta\,\mathrm{d}r\\
&\quad + 2\int_0^1 r^{-1}\int_0^{2\pi}|P^F_{N_\theta}D_\theta\tilde{g}(r,\theta) - \tilde{P}^J_{N_r}(P^F_{N_\theta}D_\theta\tilde{g}(r,\theta))|^2\mathrm{d}\theta\,\mathrm{d}r.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
II &\le 2\int_0^1 r^{-1}\int_0^{2\pi}\left|rD_\theta\tilde{g}_2(r,\theta) - rP^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta)\right|^2\mathrm{d}\theta\,\mathrm{d}r\\
&\quad + 2\int_0^{2\pi}\int_0^1 r^{-1}|rP^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta) - \tilde{P}^J_{N_r}(rP^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta))|^2\,\mathrm{d}r\,\mathrm{d}\theta\\
&\le C_5^2 N_\theta^{-2l}\int_0^1\tilde{w}(r)\int_0^{2\pi}|D^{l+1}_\theta\tilde{g}_2(r,\theta)|^2\,\mathrm{d}\theta\,\mathrm{d}r\\
&\quad + 2\int_0^{2\pi}\int_0^1\tilde{w}(r)|P^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta) - P^J_{N_r-1}(P^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta))|^2\,\mathrm{d}r\,\mathrm{d}\theta\\
&\le C_5^2 N_\theta^{-2l}\int_0^{2\pi}\|D^{l+1}_\theta\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)}\,\mathrm{d}\theta + \; C_6^2 N_r^{-2k}\int_0^{2\pi}\|P^F_{N_\theta}D_\theta\tilde{g}_2(r,\theta)\|^2_{\mathrm{H}^k_{\tilde{w}}(0,1)}\,\mathrm{d}\theta.
\end{aligned}
$$

We have used the fact that $\tilde{P}^J_{N_r}(r\tilde{f}) = rP^J_{N_r-1}(\tilde{f})$ and the $\mathrm{L}^2_w(0,1)$ norm error bound for $P^J_{N_r}$ stated in (5.9). For the integral in the last line in the bound on II we have

$$\sum_{j=0}^{k}\int_0^1 \tilde{w}(r)\|P^F_{N_\theta} D_r^j D_\theta \tilde{g}_2(\cdot,r)\|^2_{\mathrm{L}^2(0,2\pi)}\mathrm{d}r \le \sum_{j=0}^{k}\int_0^1 \tilde{w}(r)\|D_r^j D_\theta \tilde{g}_2(\cdot,r)\|^2_{\mathrm{L}^2(0,2\pi)}\mathrm{d}r = \int_0^{2\pi} \|D_\theta \tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{H}^k_{\tilde{w}}(0,1)}\mathrm{d}\theta.$$

Therefore,

$$II \le C_5^2 N_\theta^{-2l}\int_0^{2\pi} \|D_\theta^{l+1}\tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)}\,\mathrm{d}\theta + C_6^2 N_r^{-2k}\int_0^{2\pi}\|D_\theta \tilde{g}_2(\cdot,\theta)\|^2_{\mathrm{H}^k_{\tilde{w}}(0,1)}\mathrm{d}\theta.$$

Combining the bounds for I and II obtain, with suitable constants C_1 and C_2,

$$\|\tilde{g} - P^F_{N_\theta}\tilde{P}^J_{N_r}\tilde{g}\|_{\tilde{\mathrm{H}}^1_{\tilde{w}}(R)} \le C_1 N_r^{-k}\left\{\int_0^{2\pi}(\|\tilde{g}_1\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k+1}_{\tilde{w}}(0,1)} + \|D_\theta\tilde{g}_2\|^2_{\mathrm{H}^k_{\tilde{w}}(0,1)})\,\mathrm{d}\theta\right\}^{\frac{1}{2}} + C_2 N_\theta^{-l}\left\{\int_0^{2\pi}(\|D_\theta^{l+1}\tilde{g}_2\|^2_{\mathrm{L}^2_{\tilde{w}}(0,1)} + \|D_\theta^l\tilde{g}_2\|^2_{\mathrm{H}^1_{\tilde{w}}(0,1)})\,\mathrm{d}\theta\right\}^{\frac{1}{2}}, \tag{5.18}$$

which is (5.15). The proof of the $\mathrm{L}^2_{\tilde{w}}(R)$ norm bound (5.16) is very similar: its main ingredients are, in fact, contained in the argument above. For the sake of brevity we omit the details. □

The bounds (5.15) and (5.16) can now be straightforwardly mapped from R to D_0 using (5.1). We define $\mathcal{P}_N(D)$ as $\mathbb{P}_{N_r,0}(0,1)\otimes\mathbb{S}_{N_\theta}(0,2\pi)$ mapped from R to D_0 using (5.1), and we suppose that $\hat{\psi}\in\mathcal{H}^{k+1,l+1}(D)$, with $k,l\ge 1$, where

$$\begin{aligned}\mathcal{H}^{k,l}(D) := \{g \in \mathrm{H}^1_0(D) \,:\, &\tilde{g}\in\tilde{\mathrm{H}}^1_{\tilde{w},0}(R)\cap\mathrm{H}^{1,1}(R), \text{with decomposition } \tilde{g}(r,\theta)=\tilde{g}_1(r)+r\tilde{g}_2(r,\theta),\\ &\tilde{g}_1\in\tilde{\mathrm{H}}^k_{\tilde{w},0}(0,1) \text{ and } \tilde{g}_2\in\mathrm{H}^{k,0}_{\tilde{w},0}(R)\cap\mathrm{H}^{k-1,1}_{\tilde{w}}(R)\cap\mathrm{H}^{0,l}_{\tilde{w}}(R)\cap\mathrm{H}^{1,l-1}_{\tilde{w}}(R),\\ &\text{and there exists } \alpha\in(0,1) \text{ such that, for each } \theta\in(0,2\pi),\ r\mapsto r^\alpha g_2(r,\theta)\in\mathrm{C}[0,1]\},\end{aligned}$$

equipped with the norm

$$\|g\|_{\mathcal{H}^{k,l}(D)} := \left(\|g\|^2_{\mathcal{H}^k_r(D)} + \|g\|^2_{\mathcal{H}^l_\theta(D)}\right)^{\frac{1}{2}},$$

where

$$\begin{aligned}\|g\|_{\mathcal{H}^k_r(D)} &:= \left(\|\tilde{g}_1\|^2_{\mathrm{H}^k_{\tilde{w}}(0,1)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k,0}_{\tilde{w}}(R)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{k-1,1}_{\tilde{w}}(R)}\right)^{\frac{1}{2}},\\ \|g\|_{\mathcal{H}^l_\theta(D)} &:= \left(\|\tilde{g}_2\|^2_{\mathrm{H}^{0,l}_{\tilde{w}}(R)} + \|\tilde{g}_2\|^2_{\mathrm{H}^{1,l-1}_{\tilde{w}}(R)}\right)^{\frac{1}{2}}.\end{aligned}$$

We define

$$\hat{\Pi}_N : \mathcal{H}^{1,1}(D)\to\mathcal{P}_N(D) \quad \text{by} \quad (\hat{\Pi}_N g)(q_1,q_2) = (\tilde{\Pi}_N\tilde{g})(r,\theta), \qquad g\in\mathcal{H}^{1,1}(D).$$

Thus, recalling that $\mathrm{H}^1_0(D;M)=\mathrm{H}^1_0(D)$, we deduce from (5.15) that

$$\|\hat{\psi}-\hat{\Pi}_N\hat{\psi}\|_{\mathrm{H}^1_0(D;M)} \le C_1 N_r^{-k}\|\hat{\psi}\|_{\mathcal{H}^{k+1}_r(D)} \ +\ C_2 N_\theta^{-l}\|\hat{\psi}\|_{\mathcal{H}^{l+1}_\theta(D)} \tag{5.19}$$

for all $\hat{\psi}\in\mathcal{H}^{k+1,l+1}(D)$, with $k,l\ge 1$. Similarly, we obtain from (5.16) that

$$\|\hat{\psi}-\hat{\Pi}_N\hat{\psi}\|_{\mathrm{L}^2(D)} \le C_1 N_r^{-k}\|\hat{\psi}\|_{\mathcal{H}^k_r(D)} \ +\ C_2 N_\theta^{-l}\|\hat{\psi}\|_{\mathcal{H}^l_\theta(D)} \tag{5.20}$$

for all $\hat{\psi}\in\mathcal{H}^{k,l}(D)$, with $k,l\ge 1$.

6. Convergence analysis of the numerical method. We see from (4.8) that in order to obtain bounds on the norms of ξ appearing on the left-hand side of (4.8) we need to bound the following terms:

$$\|\eta^0\| = \|\eta^0\|_{\mathrm{L}^2(D)}, \quad \|\eta\|_{\ell^2(0,T;\mathrm{H}^1_0(D;M))} \quad \text{and} \quad \left\|\frac{\partial \eta}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))}.$$

It follows from (5.19), (5.20) and the definition of $\eta := \hat{\psi} - \hat{\Pi}_N \hat{\psi}$ that

$$\|\eta^0\| \le \|\hat{\psi}_0 - \hat{\Pi}_N \hat{\psi}_0\| \le C_1 N_r^{-k} \|\hat{\psi}_0\|_{\mathcal{H}^k_r(D)} \; + \; C_2 N_\theta^{-l} \|\hat{\psi}_0\|_{\mathcal{H}^l_\theta(D)},$$

$$\|\eta\|_{\ell^2(0,T;\mathrm{H}^1_0(D;M))} \le C_1 N_r^{-k} \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{k+1}_r(D))} \; + \; C_2 N_\theta^{-l} \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{l+1}_\theta(D))},$$

$$\left\|\frac{\partial \eta}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))} \le C_1 N_r^{-k} \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^k_r(D))} \; + \; C_2 N_\theta^{-l} \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^l_\theta(D))},$$

with $k, l \ge 1$, provided that $\hat{\psi}$ is such that the norms on the right-hand sides of these inequalities are finite. Substituting these three bounds into the right-hand side of (4.8) we deduce that

$$\begin{aligned}
&\|\xi\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M \xi\|_{\ell^2(0,T;\mathrm{L}^2(D))} \\
&\quad \le C_1 N_r^{-k} \left(\|\hat{\psi}_0\|_{\mathcal{H}^k_r(D)} + \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{k+1}_r(D))} + \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^k_r(D))} \right) \qquad (6.1)\\
&\quad\quad + C_2 N_\theta^{-l} \left(\|\hat{\psi}_0\|_{\mathcal{H}^l_\theta(D)} + \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{l+1}_\theta(D))} + \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^l_\theta(D))} \right) + C_3 \Delta t \left\|\frac{\partial^2 \hat{\psi}}{\partial t^2}\right\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))}.
\end{aligned}$$

Note, also, that

$$\|\eta\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} \le C_1 N_r^{-k} \|\hat{\psi}\|_{\ell^\infty(0,T;\mathcal{H}^k_r(D))} + \; C_2 N_\theta^{-l} \|\hat{\psi}\|_{\ell^\infty(0,T;\mathcal{H}^l_\theta(D))}, \qquad (6.2)$$

$$\|\underset{\sim}{\nabla}_M \eta\|_{\ell^2(0,T;\mathrm{L}^2(D))} \le C_1 N_r^{-k} \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{k+1}_r(D))} + \; C_2 N_\theta^{-l} \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{l+1}_\theta(D))}. \qquad (6.3)$$

Thus, by the triangle inequality,

$$\begin{aligned}
&\|\hat{\psi} - \hat{\psi}_N\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M (\hat{\psi} - \hat{\psi}_N)\|_{\ell^2(0,T;\mathrm{L}^2(D))} \\
&\quad \le \|\xi\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M \xi\|_{\ell^2(0,T;\mathrm{L}^2(D))} + \|\eta\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M \eta\|_{\ell^2(0,T;\mathrm{L}^2(D))},
\end{aligned}$$

whereby (6.1), (6.2) and (6.3) give

$$\begin{aligned}
&\|\hat{\psi} - \hat{\psi}_N\|_{\ell^\infty(0,T;\mathrm{L}^2(D))} + \|\underset{\sim}{\nabla}_M (\hat{\psi} - \hat{\psi}_N)\|_{\ell^2(0,T;\mathrm{L}^2(D))} \\
&\quad \le C_1 N_r^{-k} \left(\|\hat{\psi}\|_{\ell^\infty(0,T;\mathcal{H}^k_r(D))} + \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{k+1}_r(D))} + \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^k_r(D))} \right) \\
&\quad\quad + C_2 N_\theta^{-l} \left(\|\hat{\psi}\|_{\ell^\infty(0,T;\mathcal{H}^l_\theta(D))} + \|\hat{\psi}\|_{\ell^2(0,T;\mathcal{H}^{l+1}_\theta(D))} + \left\|\frac{\partial \hat{\psi}}{\partial t}\right\|_{\mathrm{L}^2(0,T;\mathcal{H}^l_\theta(D))} \right) \\
&\quad\quad + C_3 \Delta t \left\|\frac{\partial^2 \hat{\psi}}{\partial t^2}\right\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))}.
\end{aligned}$$

We recall that $\psi = \sqrt{M}\hat{\psi}$, and we define $\psi_N^n := \sqrt{M}\hat{\psi}_N^n$. Consequently,

$$\begin{aligned}
&\|\psi - \psi_N\|_{\ell^\infty(0,T;\mathfrak{H})} + \|\psi - \psi_N\|_{\ell^2(0,T;\mathfrak{K})} \\
&\quad \leq C_1 N_r^{-k} \left(\left\| \frac{\psi}{\sqrt{M}} \right\|_{\ell^\infty(0,T;\mathcal{H}_r^k(D))} + \left\| \frac{\psi}{\sqrt{M}} \right\|_{\ell^2(0,T;\mathcal{H}_r^{k+1}(D))} + \left\| \frac{1}{\sqrt{M}} \frac{\partial \psi}{\partial t} \right\|_{\mathrm{L}^2(0,T;\mathcal{H}_r^k(D))} \right) \\
&\qquad + C_2 N_\theta^{-l} \left(\left\| \frac{\psi}{\sqrt{M}} \right\|_{\ell^\infty(0,T;\mathcal{H}_\theta^l(D))} + \left\| \frac{\psi}{\sqrt{M}} \right\|_{\ell^2(0,T;\mathcal{H}_\theta^{l+1}(D))} + \left\| \frac{1}{\sqrt{M}} \frac{\partial \psi}{\partial t} \right\|_{\mathrm{L}^2(0,T;\mathcal{H}_\theta^l(D))} \right) \\
&\qquad\quad + C_3 \Delta t \left\| \frac{1}{\sqrt{M}} \frac{\partial^2 \psi}{\partial t^2} \right\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(D))},
\end{aligned}$$

with $k, l \geq 1$, provided that ψ is such that the norms on the right-hand side are finite.

That completes the convergence analysis of the method in the case of $d = 2$. For $d = 3$ the argument is identical, and rests on a three-dimensional analogue of Lemma 5.2. We omit the details.

Starting from the second stability inequality stated in Lemma 3.6 and proceeding in an identical manner as above, one can derive analogous error bounds in the $h^1(0,T;\mathfrak{H})$ and $\ell^\infty(0,T;\mathfrak{K})$ norms.

REMARK 6.1. *In the case of the FENE Maxwellian, $\sqrt{M} \in \mathcal{P}_N$ if, and only if, there exists a positive integer m such that $b = 4m$ and $N_r \geq 2m$. In order to ensure that, more generally, $\sqrt{M} \in \mathcal{P}_N(D)$ regardless of the choice of M and the value of N_r, one could have instead defined the finite-dimensional space $\mathcal{P}_N(D)$ as $\sqrt{M}\mathcal{S}_N(D)$, where $\mathcal{S}_N(D)$ is $\mathbb{P}_{N_r}(0,1) \otimes \mathbb{S}_{N_\theta}(0,2\pi)$ mapped to D_0 using* (5.1)*. With only minor changes, the convergence analysis then still proceeds as above.*

7. Implementation of the numerical method. Numerical methods for solving the Fokker–Planck equation arising from the FENE dumbbell model for dilute polymeric fluids have been the focus of some attention recently; Du *et. al.* [16] developed a finite difference scheme which preserved unity and positivity of ψ, and Lozinski *et. al.* developed a spectral method for this problem. We briefly discuss the work of Lozinski *et. al.* here because the spectral method they developed is similar in spirit to the method we propose (see Lozinski's Ph.D. thesis [23] for a detailed discussion of their work, [13, 24] for the numerical method for 2D dumbbells and [12] for the 3D case). Their spectral method is based on the 'original' version of the Fokker–Planck equation:

$$\frac{\partial \psi}{\partial t} + \underset{\sim}{\nabla}_q \cdot \left(\underset{\approx}{\kappa} \underset{\sim}{q}\, \psi \right) = \frac{1}{2\,\lambda} \underset{\sim}{\nabla}_q \cdot \left(\underset{\sim}{\nabla}_q \psi + \underset{\sim}{F}(\underset{\sim}{q})\, \psi \right),$$

and does not involve any symmetrizing transformations using the Maxwellian. The method appears to work well in practice: its accuracy is identical that of the numerical method we present below. On the other hand, unlike the numerical method defined by (4.1) and (4.2) herein, the papers by Lozinski et al. cited above provide no theoretical underpinning of their method from the point of view of stability and accuracy. In this section we discuss the implementation of our spectral Galerkin method and present some computational results to demonstrate its accuracy and efficacy.

As in Section 5 we restrict our attention to the case $d = 2$ and suppose that $\hat{\psi} \in \mathcal{H}^{1,1}(D)$. It is natural to map $\underset{\sim}{q} = (q_1, q_2) \in D_0 \subset \mathbb{R}^2$ to $(r, \theta) \in R = (0,1) \times (0, 2\pi)$, and exploit the cartesian product structure of R to seek an approximate solution

$$\hat{\psi}_N(q_1, q_2) = \hat{\Psi}_N(r, \theta) \in \mathcal{P}_N(R) := \mathbb{P}_{N_r,0}(0,1) \otimes \mathbb{S}_{N_\theta}(0, 2\pi) = \mathrm{span}(B),$$

where B is a basis that will be defined below. As in Section 5, $\mathcal{P}_N(D)$ is $\mathcal{P}_N(R)$ mapped to D_0.

A number of different bases in polar coordinates have been proposed in the literature to ensure an efficient and robust implementation of spectral methods on the disc in $\mathbb{R}^2$. In particular, the complication introduced by the change of variables $(q_1, q_2) \mapsto (r, \theta)$ is the coordinate singularity at $r = 0$. This singularity was the genesis of the decomposition (5.7) for functions in $\tilde{\mathrm{H}}^1_{\tilde{w}}(R) \cap \mathrm{H}^{1,1}(R)$. On the other hand, we prefer to use a set of C^∞ basis functions for $\mathcal{P}_N(D)$. The constraints on tensor-product basis functions in (r, θ)-coordinates to ensure that they are in fact also $\mathrm{C}^\infty(D)$ (often referred to as the *pole condition*) were characterized by Eisen *et. al.* (see Theorems 1 and 2 in [17]). We can interpret the splitting (5.7) as a Sobolev space analogue of the pole condition. A number of bases have been proposed which satisfy the pole condition; see, for example, Chapter 18 of Boyd [9] for a discussion of many of the alternatives. Before introducing the basis we use in this work, we make the following observation.

REMARK 7.1. *Let $\hat{\psi}$ be the weak solution of* (1.7)*, and define $\hat{\psi}^*(\underset{\sim}{q},t) := \hat{\psi}(-\underset{\sim}{q},t)$. Supposing that $\hat{\psi}_0$ is invariant under the change of variable $\underset{\sim}{q} \mapsto -\underset{\sim}{q}$,* i.e.*, $\hat{\psi}_0(\underset{\sim}{q}) \equiv \hat{\psi}_0(-\underset{\sim}{q})$, on noting that the weak formulation* (1.7) *is also invariant under this change of variables, it follows that $\hat{\psi}$ and $\hat{\psi}^*$ are weak solutions to the same initial boundary-value problem. It follows by the uniqueness established in Section 3 that $\hat{\psi}(\underset{\sim}{q},t) \equiv \hat{\psi}^*(\underset{\sim}{q},t)$,* i.e.*, $\hat{\psi}(\underset{\sim}{q},t) = \hat{\psi}(-\underset{\sim}{q},t)$ for all $\underset{\sim}{q} \in D$ and all $t \in [0,T]$.*

The above remark demonstrates that (1.7) captures an important symmetry property of the dumbbell model of polymeric fluids: the configuration probability density function, ψ, is required to be symmetric about the origin in D because the beads of a dumbbell are indistinguishable. With this in mind, then, the basis we use is essentially the one proposed by Matsushima and Marcus [27] and Verkley [30], except that we ensure that the basis functions are zero at $r = 1$ so as to be in $\mathrm{H}^1_0(D)$, and that they are π-periodic in θ:

$$B = \{X_k^{il} \in \mathrm{C}^\infty(R) : X_k^{il}(r,\theta) = W_{lk}(r)\Phi_{il}(\theta), \quad k = 0,\dots,N_r; \quad i = 0,1; \quad l = 1,\dots,N_\theta\}, \tag{7.1}$$

where $W_{lk}(r) = r^{2l}(1-r^2)P_k^{(0,2l)}(2r^2-1)$, $P_k^{(\alpha,\beta)}(x)$ is the Jacobi polynomial of degree k with respect to the weight $(1-x)^\alpha(1+x)^\beta$, and $\Phi_{il}(\theta) = (1-i)\cos(2l\theta) + i\sin(2l\theta)$. $\mathcal{P}_N(R)$ is then a $N := (2N_\theta+1)(N_r+1)$-dimensional space. Each element of B satisfies the pole condition. The degree-of-freedom indexing scheme we use is given by $u := (2l-i)(N_r+1)+k+1$ for $1 \le u \le N$. This indexing scheme yields advantageous sparsity and band-matrix structure (cf. below).

It is now straightforward to determine the discretization matrices, which we label $\mathbf{M}$, $\mathbf{S}$ and $\mathbf{C}$ for mass, stiffness and convection respectively. We obtain the discretization matrices from the integrals in (4.1),

$$\mathbf{M} = \int_D \hat{\psi}_N^{n+1}\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}, \tag{7.2}$$

$$\mathbf{S} = \int_D \underset{\sim}{\nabla}_M\hat{\psi}_N^{n+1}\cdot\underset{\sim}{\nabla}_M\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}, \tag{7.3}$$

$$\mathbf{C}^{n+1} = \int_D (\underset{\approx}{\kappa}^{n+1}\,\underset{\sim}{q}\,\hat{\psi}_N^{n+1})\cdot\underset{\sim}{\nabla}_M\hat{\varphi}\,\mathrm{d}\underset{\sim}{q}, \tag{7.4}$$

for test functions $\hat{\varphi} \in \mathcal{P}_N(D)$. We transform these integrals to R, employ the ansatz $\hat{\Psi}_N^{n+1}(r,\theta) = \sum_{v=0}^N \hat{\Psi}_v^{n+1}X_v(r,\theta) \in \mathcal{P}_N(R)$ and set test functions to $X_u \in B$ for $1 \le u \le N$, yielding the following discretized forms of (7.2), (7.3) and (7.4) in polar coordinates,

$$\mathbf{M}_{uv} = \int_0^1 b\,r\,W_{lk}(r)W_{nm}(r)\,\mathrm{d}r\int_0^\pi \Phi_{jn}(\theta)\Phi_{il}(\theta)\,\mathrm{d}\theta, \tag{7.5}$$

$$\begin{aligned}\mathbf{S}_{uv} = &\int_0^1 r\,W'_{lk}(r)W'_{nm}(r)\,\mathrm{d}r\int_0^\pi \Phi_{jn}(\theta)\Phi_{il}(\theta)\,\mathrm{d}\theta\\ &+\int_0^1 \frac{1}{r}W_{lk}(r)W_{nm}(r)\,\mathrm{d}r\int \Phi'_{jn}(\theta)\Phi'_{il}(\theta)\,\mathrm{d}\theta\\ &+\int_0^1 \frac{b}{2}\frac{r^2}{1-r^2}\left(W_{lk}(r)W'_{nm}(r) + W'_{lk}(r)W_{nm}(r)\right)\,\mathrm{d}r\int_0^\pi \Phi_{jn}(\theta)\Phi_{il}(\theta)\,\mathrm{d}\theta\\ &+\int_0^1 \frac{b^2}{4}\frac{r^3}{(1-r^2)^2}W_{lk}(r)W_{nm}(r)\,\mathrm{d}r\int_0^\pi \Phi_{jn}(\theta)\Phi_{il}(\theta)\,\mathrm{d}\theta,\end{aligned} \tag{7.6}$$

$$\mathbf{C}_{uv}^{n+1} = \int_0^1 b\, r\, W_{lk}(r) W_{nm}(r)\, \mathrm{d}r \times \int_0^\pi \phi'_{il}(\theta)\phi_{jn}(\theta)(-\kappa_{11}^{n+1}\sin 2\theta - \kappa_{12}^{n+1}\sin^2\theta + \kappa_{21}\cos^2\theta)\, \mathrm{d}\theta$$
$$+ \int_0^1 \left(b\, r^2\, W'_{lk}(r) W_{nm}(r) + \frac{b^2}{2}\frac{r^3}{1-r^2} W_{lk}(r) W_{nm}(r) \right) \mathrm{d}r$$
$$\times \int_0^\pi \phi_{il}(\theta)\phi_{jn}(\theta)(\kappa_{11}^{n+1}\cos 2\theta + \frac{1}{2}(\kappa_{12}^{n+1} + \kappa_{21}^{n+1})\sin 2\theta)\, \mathrm{d}\theta. \tag{7.7}$$

With these definitions in hand, the numerical method is equivalent to solving the following linear system for the coefficient vector $\hat{\mathbf{\Psi}}_N^{n+1} \in \mathbb{R}^N$, $n = 0, 1, \ldots, N_T - 1$:

$$\left(\mathbf{M} + \Delta t \left(\frac{1}{2\lambda}\mathbf{S} - \mathbf{C}^{n+1} \right) \right) \hat{\mathbf{\Psi}}_N^{n+1} = \mathbf{M}\hat{\mathbf{\Psi}}_N^n, \tag{7.8}$$

and then the numerical approximation to the probability density function itself is obtained as $\psi_N^{n+1}(\underset{\sim}{q}) = \Psi_N^{n+1}(r,\theta) = \sqrt{M(r)}\, \hat{\Psi}_N^{n+1}(r,\theta)$.

We note that the matrices defined by (7.5), (7.6) and (7.7) have convenient sparsity and bandedness properties. Due to the orthogonality of the sinusoidal basis functions in the θ-direction, it is easy to show that for the degree-of-freedom indexing scheme given above **M** and **S** are block-diagonal matrices and **C** has non-zero blocks only for $l = n \pm \alpha$, $\alpha = 1, 2, 3$ (where α depends on $\underset{\approx}{\kappa}$). In addition, we can exploit some of the many recurrence relations satisfied by Jacobi polynomials in the integrals with respect to r. For example, by twice applying 22.7.18 in [1] to (7.5), we see that **M** is a pentadiagonal matrix. **S** and **C** share similar bandedness properties within their non-zero blocks. We evaluate the θ-integrals exactly using trigonometric identities, and, noting that the r-integrands are all polynomials, we use Gauss quadrature to evaluate the r-integrals to machine precision. **M** and **S** are constant matrices which can be pre-computed and reused, but if $\underset{\approx}{\kappa}$ is time-varying, we must reassemble **C** at every time step. However, it is easy to factor out the dependence of **C** on $\underset{\approx}{\kappa}$ so that the integrals that determine **C** need not be evaluated more than once.

We now present some numerical results. For simplicity we always use the Maxwellian (which satisfies the symmetry property required in Remark 7.1) as our initial condition, so that $\hat{\psi}_0 = \sqrt{M}$. One case that has attracted much interest in the literature is that of an *extensional flow*, for which

$$\underset{\approx}{\kappa} = \begin{bmatrix} \delta & 0 \\ 0 & -\delta \end{bmatrix}. \tag{7.9}$$

The plots in Figure 7.1 show the computed steady-state solution for $\delta = 1$ in (a), (b) and $\delta = 5$ in (c), (d). Similar plots for extensional flows are presented in [13]. From the figure, it is clear that $\hat{\Psi}$ can have an extremely sharp profile as $r \to 1$ and the sharpness depends strongly on δ. However, on multiplying by $\sqrt{M}$ to obtain ψ, we ameliorate this sharpness considerably.

(N_r, N_θ)	$\Vert\hat{\psi} - \hat{\psi}_{\mathrm{exact}}\Vert / \Vert\hat{\psi}_{\mathrm{exact}}\Vert$	$\Vert\hat{\psi} - \hat{\psi}_{\mathrm{exact}}\Vert_{\mathrm{H}_0^1(D;M)} / \Vert\hat{\psi}_{\mathrm{exact}}\Vert_{\mathrm{H}_0^1(D;M)}$
(10,10)	1.9887×10^{-3}	3.2475×10^{-3}
(15,15)	4.3479×10^{-6}	9.3672×10^{-6}
(20,20)	4.1911×10^{-9}	1.1289×10^{-8}
(25,25)	1.7870×10^{-12}	5.6226×10^{-12}

TABLE 7.1

Relative errors in the $\mathrm{L}^2(D)$ *and* $\mathrm{H}_0^1(D;M)$ *norms for an extensional flow (with* $b = 12$, $\lambda = 1$ *and* $\delta = 1$*) at steady-state.* $\hat{\psi}$ *is the computed steady-state solution obtained by taking 2000 time steps with* $\Delta t = 0.05$*, and* $\hat{\psi}_{\mathrm{exact}}$ *is given in* (7.10).

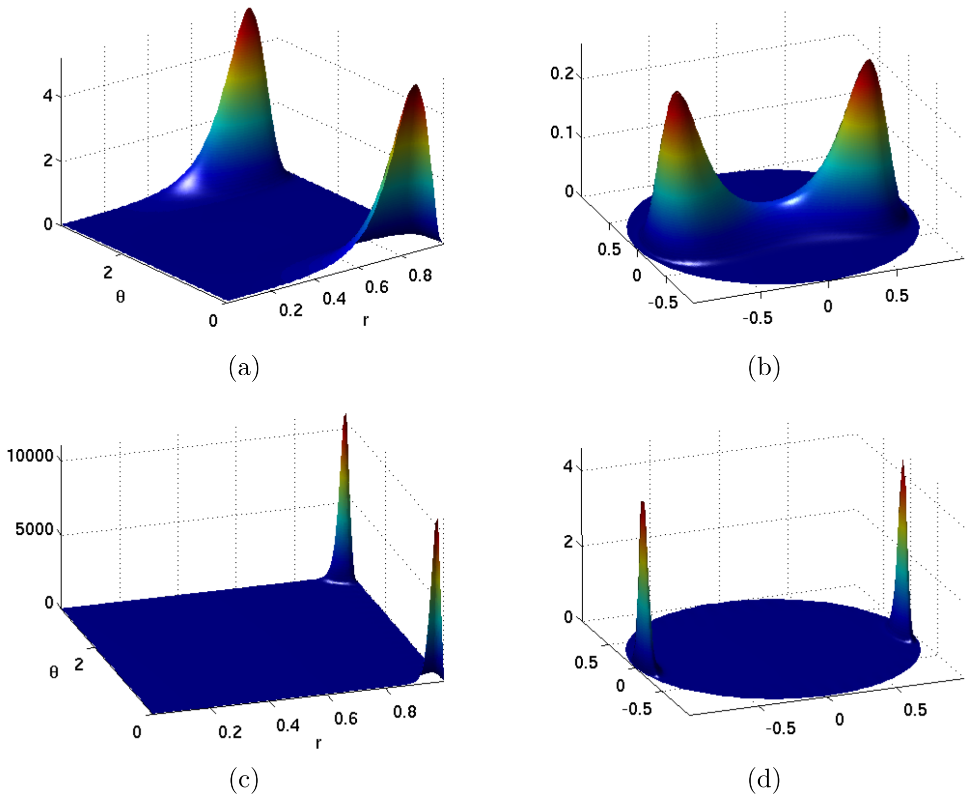

FIG. 7.1. *Steady state solution of the problem: (a) $\hat{\Psi}_N$ on $(0,1)\times(0,\pi)$ with $b=12$, $\lambda=1$, $\delta=1$ (extensional flow) and $(N_r,N_\theta)=(15,8)$, and (b) the corresponding probability density function ψ_N, scaled to the unit circle in the plane; (c) and (d) are analogous, except we have chosen $\delta=5$ and we now require $(N_r,N_\theta)=(40,20)$ to resolve the much sharper solution. Note that in both cases we have $\hat{\Psi}_N(1,\theta)=0$.*

(N_r,N_θ)	$\Vert\hat{\psi}-\hat{\psi}_{\text{exact}}\Vert/\Vert\hat{\psi}_{\text{exact}}\Vert$	$\Vert\hat{\psi}-\hat{\psi}_{\text{exact}}\Vert_{\mathrm{H}^1_0(D;M)}/\Vert\hat{\psi}_{\text{exact}}\Vert_{\mathrm{H}^1_0(D;M)}$
(10,10)	5.1683×10^{-2}	5.3525×10^{-2}
(20,20)	2.6450×10^{-5}	3.8198×10^{-5}
(30,30)	9.7029×10^{-10}	1.7190×10^{-9}
(40,40)	2.5862×10^{-11}	2.1422×10^{-11}

TABLE 7.2

Relative errors in the $\mathrm{L}^2(D)$ and $\mathrm{H}^1_0(D;M)$ norms for an extensional flow at steady-state. We have the same values of b and λ as in Table 7.1, but this time we took $\delta=2$. The time-stepping strategy to compute the steady-state solution was also the same as in Table 7.1.

To experimentally assess the spatial accuracy of our method we use the fact when $\underset{\approx}{\kappa}$ is a symmetric tensor the exact steady-state solution of the Fokker–Planck equation is given by (cf. [7])

$$\psi_{\text{exact}}(\underset{\sim}{q}) := CM(\underset{\sim}{q})\exp(\lambda\underset{\sim}{q}^T\underset{\approx}{\kappa}\underset{\sim}{q}), \tag{7.10}$$

where C is a normalization constant chosen so that $\int_D \psi_{\text{exact}}(\underset{\sim}{q})\mathrm{d}\underset{\sim}{q}=1$. Tables 7.1 and 7.2 show the relative error (in the $\mathrm{L}^2(D)$ and $\mathrm{H}^1_0(D;M)$ norms) between the exact and the computed steady-state solution for two different extensional flows. We can see from the data in the tables that the method converges rapidly in both cases. The case $\delta=2$ corresponds to a stronger extensional flow (and concomitantly a sharper solution profile) than when $\delta=1$, so it is to be expected that more modes are required in Table 7.2 to capture the solution to a given accuracy.

8. Conclusions. The Fokker–Planck equation (1.1) has been the subject of active research recently, as a component of the Navier–Stokes–Fokker–Planck model for dilute polymeric fluids. We focused our attention on Fokker–Planck equations with unbounded drift that arise from modelling polymer molecules as FENE dumbbells, which introduces the complication of a singularity in the potential $\underset{\sim}{q} \mapsto U(\underset{\sim}{q})$ as $\mathfrak{d}(\underset{\sim}{q}) \to 0$. The purpose of this paper was to develop a rigorous foundation for the numerical approximation of such Fokker–Planck equations.

We symmetrized the principal part of the differential operator by introducing the Maxwellian, M, and applied the transformation $\hat{\psi} = \psi/\sqrt{M}$. The resulting weak formulation (1.7) facilitated the development of a number of analytical results in Sections 3 and 4, including existence and uniqueness of weak solutions of the semi-discretized equation (3.1) and, on passing to the limit $\Delta t \to 0_+$, of (1.7) also. Using approximation results derived in Section 5, an optimal convergence rate for the fully discrete Galerkin spectral method (4.1), (4.2) was established for the case $d = 2$; an analogous procedure could be carried out for $d = 3$. Finally, Section 7 addressed issues directly related to the implementation of the numerical method, and computational results were presented to demonstrate the spectral rate of convergence of the method with respect to the spatial variables.

The goal of future work is to apply the results developed here to the coupled Navier–Stokes–Fokker–Planck model, building on the recent paper [4] where convergence to weak solutions of coupled Navier–Stokes–Fokker–Planck systems has been shown for a general class of Galerkin schemes (without convergence rates) in the special case when the velocity field $\underset{\sim}{u}$ is corotational (*i.e.*, $\underset{\sim}{q}^T \underset{\approx}{\kappa} \underset{\sim}{q} = 0$, with $\underset{\approx}{\kappa} = \underset{\approx}{\nabla}_x \underset{\sim}{u}$).

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