

FINITE ELEMENT APPROXIMATION OF FINITELY EXTENSIBLE NONLINEAR ELASTIC DUMBBELL MODELS FOR DILUTE POLYMERS

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Abstract. We construct a Galerkin finite element method for the numerical approximation of weak solutions to a general class of coupled FENE-type finitely extensible nonlinear elastic dumbbell models that arise from the kinetic theory of dilute solutions of polymeric liquids with noninteracting polymer chains. The class of models involves the unsteady incompressible Navier–Stokes equations in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3 , for the velocity and the pressure of the fluid, with an elastic extra-stress tensor appearing on the right-hand side in the momentum equation. The extra-stress tensor stems from the random movement of the polymer chains and is defined through the associated probability density function that satisfies a Fokker–Planck type parabolic equation, a crucial feature of which is the presence of a centre-of-mass diffusion term. We require no structural assumptions on the drag term in the Fokker–Planck equation; in particular, the drag term need not be corotational. We perform a rigorous passage to the limit as first the spatial discretization parameter, and then the temporal discretization parameter tend to zero, and show that a (sub)sequence of these finite element approximations converges to a weak solution of this coupled Navier–Stokes–Fokker–Planck system. The passage to the limit is performed under minimal regularity assumptions on the data: a square-integrable and divergence-free initial velocity datum u_0 for the Navier–Stokes equation and a nonnegative initial probability density function ψ_0 for the Fokker–Planck equation, which has finite relative entropy with respect to the Maxwellian M .

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1. INTRODUCTION

This paper is concerned with the construction and convergence analysis of a finite element method for the numerical approximation of weak solutions to a system of nonlinear partial differential equations that arises from the kinetic theory of dilute polymer solutions. The mathematical model under consideration couples the incompressible Navier–Stokes equations, with the divergence of the elastic extra-stress tensor appearing on its right-hand side, to a high-dimensional Fokker–Planck equation with an unbounded drift term, whose transport coefficients depend on the fluid velocity and whose solution is a probability density function featuring in the

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definition of the elastic extra stress tensor. The existence and exponential equilibration of global weak solutions to the system was proved in two substantial recent papers, [7, 9], for both finitely extensible nonlinear bead-spring chain type polymer models and Hookean type bead-spring chain models, using a delicate combination of entropy estimates and weak compactness arguments applied to sequences of approximations that were generated by a temporal semidiscretization of the system. Weak solutions to the Navier–Stokes–Fokker–Planck system, whose existence was thus shown, were also shown to satisfy the natural energy inequality originating from the formal balance law for the system. In this paper, we construct a fully-discrete numerical approximation of the model and show that, as the spatial mesh size tends to zero, a subsequence of the sequence of numerical solutions converges to a weak solution of the temporally semidiscrete scheme, a subsequence of whose solutions is, in turn, known from [7] to converge to a weak solution of the coupled Navier–Stokes–Fokker–Planck system as the time step tends to zero. Hence we deduce that a subsequence of the sequence of numerical approximations converges to a weak solution of the problem. To the best of our knowledge, this is the first example of a general family of fully-discrete, convergent numerical methods for the coupled Navier–Stokes–Fokker–Planck system. The key contributions of the paper are the following: (1) the finite element method constructed here reproduces at the discrete level the energy inequality satisfied by weak solutions of the Navier–Stokes–Fokker–Planck system; and (2) convergence to weak solutions is established under minimal regularity assumptions on the data: a square-integrable and divergence-free initial velocity datum for the Navier–Stokes equation and a nonnegative initial probability density function for the Fokker–Planck equation, which has finite relative entropy with respect to the Maxwellian of the model.

We shall now describe the Navier–Stokes–Fokker–Planck system under consideration, arising from the kinetic theory of dilute polymer solutions. The solvent is an incompressible, viscous, isothermal Newtonian fluid confined to a bounded open set $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3 , with a Lipschitz-continuous boundary $\partial\Omega$. For the sake of simplicity of presentation we shall suppose that Ω has ‘solid boundary’ $\partial\Omega$; the velocity field \underline{u} will then satisfy the no-slip boundary condition $\underline{u} = \underline{0}$ on $\partial\Omega$. The polymer chains, which are suspended in the solvent, are assumed not to interact with each other. The conservation of momentum and mass equations for the solvent then have the form of the incompressible Navier–Stokes equations in which the elastic *extra-stress* tensor $\underline{\tau}$ (*i.e.*, the polymeric part of the Cauchy stress tensor), appears as a source term:

Given $T \in \mathbb{R}_{>0}$, find $\underline{u} : (\underline{x}, t) \in \overline{\Omega} \times [0, T] \mapsto \underline{u}(\underline{x}, t) \in \mathbb{R}^d$ and $p : (\underline{x}, t) \in \Omega \times (0, T] \mapsto p(\underline{x}, t) \in \mathbb{R}$ such that

$$\frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla_{\underline{x}}) \underline{u} - \nu \Delta_{\underline{x}} \underline{u} + \nabla_{\underline{x}} p = \underline{f} + \nabla_{\underline{x}} \cdot \underline{\tau} \quad \text{in } \Omega \times (0, T], \tag{1.1a}$$

$$\nabla_{\underline{x}} \cdot \underline{u} = 0 \quad \text{in } \Omega \times (0, T], \tag{1.1b}$$

$$\underline{u} = \underline{0} \quad \text{on } \partial\Omega \times (0, T], \tag{1.1c}$$

$$\underline{u}(\underline{x}, 0) = \underline{u}_0(\underline{x}) \quad \forall \underline{x} \in \Omega. \tag{1.1d}$$

It is assumed that each of the equations above has been written in its nondimensional form; \underline{u} denotes a nondimensional velocity, defined as the velocity field scaled by the characteristic flow speed U_0 ; $\nu \in \mathbb{R}_{>0}$ is the reciprocal of the Reynolds number, *i.e.* the ratio of the kinematic viscosity coefficient of the solvent and $L_0 U_0$, where L_0 is a characteristic length-scale of the flow; p is the nondimensional pressure and \underline{f} is the nondimensional density of body forces.

In a *bead-spring chain model*, consisting of $K + 1$ beads coupled with K elastic springs to represent a polymer chain, the extra-stress tensor $\underline{\tau}$ is defined by the *Kramers expression* as a weighted average of ψ , the probability density function of the (random) conformation vector $\underline{q} := (q_1^T, \dots, q_K^T)^T \in \mathbb{R}^{Kd}$ of the chain (*cf.* (1.7) below, in the case of $K = 1$), with q_i representing the d -component conformation/orientation vector of the i th spring. The Kolmogorov equation satisfied by ψ is a second-order parabolic equation, the Fokker–Planck equation, whose transport coefficients depend on the velocity field \underline{u} . The domain D of admissible conformation vectors $D \subset \mathbb{R}^{Kd}$ is a K -fold Cartesian product $D_1 \times \dots \times D_K$ of balanced convex open sets $D_i \subset \mathbb{R}^d$, $i = 1, \dots, K$; the term *balanced* means that $q_i \in D_i$ if, and only if, $-q_i \in D_i$. Hence, in particular, $\underline{0} \in D_i$, $i = 1, \dots, K$.

Typically D_i is the whole of \mathbb{R}^d or a bounded open d -dimensional ball centred at the origin $\mathfrak{Q} \in \mathbb{R}^d$ for each $i = 1, \dots, K$. When $K = 1$, the model is referred to as the *dumbbell model*.

Henceforth we shall confine ourselves to the case of $K = 1$ – the dumbbell model; then, $D = D_1$, and we shall simply write D instead of D_1 . Concerning extensions to the case of $K \geq 1$, the reader is referred to the concluding remarks in Section 5.

Let $\mathcal{O} \subset [0, \infty)$ denote the image of D under the mapping $\underline{q} \in D \mapsto \frac{1}{2}|\underline{q}|^2$, and consider the *spring potential* $U \in C^2(\mathcal{O}; \mathbb{R}_{\geq 0})$. Clearly, $0 \in \mathcal{O}$. We shall suppose that $U(0) = 0$ and that U is monotonic increasing and unbounded on \mathcal{O} . The elastic spring-force $\underline{F} : D \subseteq \mathbb{R}^d \rightarrow \mathbb{R}^d$ of the spring is defined by

$$\underline{F}(\underline{q}) = U'(\tfrac{1}{2}|\underline{q}|^2) \underline{q}. \quad (1.2)$$

Remark 1.1. In the Hookean dumbbell model the spring force is defined by $\underline{F}(\underline{q}) = \underline{q}$, with $\underline{q} \in D = \mathbb{R}^d$, corresponding to $U(s) = s$, $s \in \mathcal{O} = [0, \infty)$. This model is physically unrealistic as it admits an arbitrarily large extension.

We shall therefore assume in what follows that D is a *bounded* open ball, centred at the origin $\mathfrak{Q} \in \mathbb{R}^d$, with boundary ∂D . We shall further suppose that there exist constants $c_j > 0$, $j = 1, 2, 3, 4$, and $\gamma > 1$ such that the (normalized) Maxwellian M , defined by

$$M(\underline{q}) = \frac{1}{\mathcal{Z}} e^{-U(\frac{1}{2}|\underline{q}|^2)}, \quad \mathcal{Z} := \int_D e^{-U(\frac{1}{2}|\underline{q}|^2)} d\underline{q}, \quad (1.3)$$

and the associated spring potential U satisfy

$$c_1 [\text{dist}(\underline{q}, \partial D)]^\gamma \leq M(\underline{q}) \leq c_2 [\text{dist}(\underline{q}, \partial D)]^\gamma \quad \forall \underline{q} \in D, \quad (1.4a)$$

$$c_3 \leq [\text{dist}(\underline{q}, \partial D)] U'(\tfrac{1}{2}|\underline{q}|^2) \leq c_4 \quad \forall \underline{q} \in D. \quad (1.4b)$$

Observe that

$$M(\underline{q}) \nabla_{\underline{q}} [M(\underline{q})]^{-1} = -[M(\underline{q})]^{-1} \nabla_{\underline{q}} M(\underline{q}) = \nabla_{\underline{q}} U(\tfrac{1}{2}|\underline{q}|^2) = U'(\tfrac{1}{2}|\underline{q}|^2) \underline{q}. \quad (1.5)$$

Since $[U(\frac{1}{2}|\underline{q}|^2)]^2 = (-\log M(\underline{q}) + \text{Const.})^2$, it follows from (1.4a), (1.4b) that (if $\gamma > 1$, as has been assumed here,)

$$\int_D \left[1 + [U(\tfrac{1}{2}|\underline{q}|^2)]^2 + [U'(\tfrac{1}{2}|\underline{q}|^2)]^2 \right] M(\underline{q}) d\underline{q} < \infty. \quad (1.6)$$

Remark 1.2. In the FENE (finitely extensible nonlinear elastic) dumbbell model the spring force is given by $\underline{F}(\underline{q}) = (1 - |\underline{q}|^2/b)^{-1} \underline{q}$, $\underline{q} \in D = B(\mathfrak{Q}, b^{\frac{1}{2}})$, corresponding to $U(s) = -\frac{b}{2} \log(1 - \frac{2s}{b})$, $s \in \mathcal{O} = [0, \frac{b}{2})$. Here $B(\mathfrak{Q}, b^{\frac{1}{2}})$ is a bounded open ball in \mathbb{R}^d centred at the origin $\mathfrak{Q} \in \mathbb{R}^d$ and of fixed radius $b^{\frac{1}{2}}$, with $b > 0$. Direct calculations show that the Maxwellian M and the elastic potential U of the FENE model satisfy the conditions (1.4a), (1.4b) with $\gamma := \frac{b}{2}$ provided that $b > 2$. Thus, (1.6) also holds for $b > 2$.

The governing equations of the general FENE-type dumbbell model with centre-of-mass diffusion are (1.1a)–(1.1d), where the extra-stress tensor $\underline{\tau}$, depending on the probability density function ψ , is defined by the *Kramers expression*:

$$\underline{\tau}(\psi) = k (\underline{\mathcal{C}}(\psi)) - k \rho(\psi) \underline{I}. \quad (1.7)$$

Here the dimensionless constant $k > 0$ is a constant multiple of the product of the Boltzmann constant k_B and the absolute temperature \mathbb{T} , \underline{I} is the unit $d \times d$ tensor, and

$$\underline{\mathcal{C}}(\psi)(\underline{x}, t) = \int_D \psi(\underline{x}, \underline{q}, t) \underline{q} \underline{q}^T U' \left(\tfrac{1}{2}|\underline{q}|^2 \right) d\underline{q}, \quad \text{and} \quad \rho(\psi)(\underline{x}, t) = \int_D \psi(\underline{x}, \underline{q}, t) d\underline{q}, \quad (1.8)$$

where $\rho(\psi)(\underline{x}, t)$ is the density of polymer chains located at \underline{x} at time t . The probability density function ψ is a solution of the Fokker–Planck equation

$$\frac{\partial \psi}{\partial t} + (\underline{u} \cdot \nabla_x) \psi + \nabla_q \cdot \left(\underline{\sigma}(\underline{u}) \underline{q} \psi \right) = \varepsilon \Delta_x \psi + \frac{1}{2\lambda} \nabla_q \cdot \left(M \nabla_q \left(\frac{\psi}{M} \right) \right) \quad \text{in } \Omega \times D \times (0, T], \quad (1.9)$$

with $\underline{\sigma}(\underline{u}) \equiv \nabla_x \underline{u}$, where $(\nabla_x \underline{u})(\underline{x}, t) \in \mathbb{R}^{d \times d}$ and $\{\nabla_x \underline{u}\}_{ij} = \frac{\partial u_i}{\partial x_j}$. In (1.9), $\varepsilon > 0$ is the centre-of-mass diffusion coefficient defined as $\varepsilon := (\ell_0/L_0)^2/(8\lambda)$ with $\ell_0 := \sqrt{k_B T/H}$ signifying the characteristic microscopic length-scale and $\lambda := (\zeta/4H)(U_0/L_0)$, where $\zeta > 0$ is a friction coefficient and $H > 0$ is a spring-constant. The dimensionless parameter $\lambda \in \mathbb{R}_{>0}$, called the Weissenberg number (and usually denoted by Wi), characterizes the elastic relaxation property of the fluid.

We impose the following boundary and initial conditions on ψ :

$$M \left[\frac{1}{2\lambda} \nabla_q \left(\frac{\psi}{M} \right) - \underline{\sigma}(\underline{u}) \underline{q} \left(\frac{\psi}{M} \right) \right] \cdot \frac{\underline{q}}{|\underline{q}|} = 0 \quad \text{on } \Omega \times \partial D \times (0, T], \quad (1.10a)$$

$$\varepsilon \nabla_x \psi \cdot \underline{n} = 0 \quad \text{on } \partial \Omega \times D \times (0, T], \quad (1.10b)$$

$$\psi(\cdot, \cdot, 0) = \psi_0(\cdot, \cdot) \geq 0 \quad \text{on } \Omega \times D, \quad (1.10c)$$

where \underline{q} is normal to ∂D , as D is a bounded ball centred at the origin in \mathbb{R}^d , and \underline{n} is normal to $\partial \Omega$. The initial condition ψ_0 is nonnegative, defined on $\Omega \times D$, with $\int_D \psi_0(\underline{x}, \underline{q}) \, d\underline{q} = 1$ for a.e. $\underline{x} \in \Omega$, and assumed to have finite relative entropy with respect to the Maxwellian M ; *i.e.* $\int_{\Omega \times D} \psi_0(\underline{x}, \underline{q}) \log(\psi_0(\underline{x}, \underline{q})/M(\underline{q})) \, d\underline{q} \, d\underline{x} < \infty$. The boundary and initial conditions for ψ have been chosen so as to ensure that

$$\int_D \psi(\underline{x}, \underline{q}, t) \, d\underline{q} = \int_D \psi(\underline{x}, \underline{q}, 0) \, d\underline{q} = 1 \quad \forall (\underline{x}, t) \in \Omega \times (0, T]. \quad (1.11)$$

Remark 1.3. The collection of equations and structural hypotheses ((1.1a)–(1.1d))–((1.10a)–(1.10c)) will be referred to throughout the paper as model (P), or as the *general FENE-type dumbbell model with centre-of-mass diffusion*.

A noteworthy feature of equation (1.9) in the model (P) compared to classical Fokker–Planck equations for dumbbell models in the literature is the presence of the \underline{x} -dissipative centre-of-mass diffusion term $\varepsilon \Delta_x \psi$ on the right-hand side of the Fokker–Planck equation (1.9). We refer to Barrett and Süli [3] for the derivation of (1.9); see also the article by Schieber [28] concerning generalized dumbbell models with centre-of-mass diffusion, and the recent paper of Degond and Liu [14] for a careful justification of the presence of the centre-of-mass diffusion term through asymptotic analysis. In standard derivations of bead-spring models the centre-of-mass diffusion term is routinely omitted on the grounds that it is several orders of magnitude smaller than the other terms in the equation. Indeed, when the characteristic macroscopic length-scale $L_0 \approx 1$, (for example, $L_0 = \text{diam}(\Omega)$), Bhava *et al.* [10] estimate the ratio ℓ_0^2/L_0^2 to be in the range of about 10^{-9} to 10^{-7} . However, the omission of the term $\varepsilon \Delta_x \psi$ from (1.9) in the case of a heterogeneous solvent velocity $\underline{u}(\underline{x}, t)$ is a mathematically counterproductive model reduction. When $\varepsilon \Delta_x \psi$ is absent, (1.9) becomes a degenerate parabolic equation exhibiting hyperbolic behaviour with respect to (\underline{x}, t) . Since the study of weak solutions to the coupled problem requires one to work with velocity fields \underline{u} that have very limited Sobolev regularity (typically $\underline{u} \in L^\infty(0, T; \underline{L}^2(\Omega)) \cap L^2(0, T; \underline{H}_0^1(\Omega))$), one is then forced into the technically unpleasant framework of hyperbolically degenerate parabolic equations with rough transport coefficients (*cf.* Ambrosio [1] and DiPerna and Lions [15]). The resulting difficulties are further exacerbated by the fact that a typical spring force $\underline{F}(\underline{q})$ for a finitely extensible model (such as FENE) explodes as \underline{q} approaches ∂D ; see Remark 1.2 above. For these reasons, here we shall retain the centre-of-mass diffusion term in (1.9).

Lions and Masmoudi [24] proved the global existence of weak solutions for the simplified *corotational* FENE dumbbell model, *i.e.* with $\sigma(\underline{u}) = \nabla_x \underline{u}$ replaced by its skew-symmetric part $\frac{1}{2}(\nabla_x \underline{u} - (\nabla_x \underline{u})^T)$, and with

$\varepsilon = 0$; see also the work of Masmoudi [25]. Under very general assumptions on the finite-dimensional spaces used for the purpose of spatial discretization, including, in particular, classical conforming finite element spaces and spectral Galerkin subspaces, Barrett and Süli [5] showed the convergence of a (sub)sequence of numerical approximations to a weak solution of the coupled Navier–Stokes–Fokker–Planck system (P), for a large class of unbounded spring potentials, including the FENE potential, in the case of the simplified corotational model. Recently, Masmoudi [26] has extended the analysis of Lions and Masmoudi [24] to the noncorotational case. For a fuller literature survey on the mathematical analysis of FENE-type dumbbell models we refer the reader to Barrett and Süli [7]. In the rest of this section we concentrate on those references that are relevant to the finite element approximation developed and analyzed in this paper.

In Barrett and Süli [4] we showed the existence of global-in-time weak solutions to the general class of noncorotational FENE type dumbbell models (including the standard FENE dumbbell model) with centre-of-mass diffusion and microscopic cut-off (*cf.* (1.13) and (1.14) below) in the drag term

$$\nabla_q \cdot (\underline{\sigma}(u) \underline{q} \psi) = \nabla_q \cdot \left[\underline{\sigma}(u) \underline{q} M \left(\frac{\psi}{M} \right) \right]. \quad (1.12)$$

We observe that if ψ/M is bounded above then, for $L \in \mathbb{R}_{>0}$ sufficiently large, the drag term (1.12) is equal to

$$\nabla_q \cdot \left[\underline{\sigma}(u) \underline{q} M \beta^L \left(\frac{\psi}{M} \right) \right], \quad (1.13)$$

where $\beta^L \in C(\mathbb{R})$ is a cut-off function defined as

$$\beta^L(s) := \min(s, L). \quad (1.14)$$

It then follows that, for $L \gg 1$, any solution ψ of (1.9), such that ψ/M is bounded above, also satisfies

$$\frac{\partial \psi}{\partial t} + (\underline{u} \cdot \nabla_x) \psi + \nabla_q \cdot \left(\underline{\sigma}(u) \underline{q} M \beta^L \left(\frac{\psi}{M} \right) \right) = \varepsilon \Delta_x \psi + \frac{1}{2\lambda} \nabla_q \cdot \left(M \nabla_q \left(\frac{\psi}{M} \right) \right) \quad \text{in } \Omega \times D \times (0, T], \quad (1.15)$$

and the following boundary and initial conditions:

$$M \left[\frac{1}{2\lambda} \nabla_q \left(\frac{\psi}{M} \right) - \underline{\sigma}(u) \underline{q} \beta^L \left(\frac{\psi}{M} \right) \right] \cdot \frac{\underline{q}}{|\underline{q}|} = 0 \quad \text{on } \Omega \times \partial D \times (0, T], \quad (1.16a)$$

$$\varepsilon \nabla_x \psi \cdot \underline{n} = 0 \quad \text{on } \partial \Omega \times D \times (0, T], \quad (1.16b)$$

$$\psi(\cdot, \cdot, 0) = M(\cdot) \beta^L(\psi_0(\cdot, \cdot)/M(\cdot)) \geq 0 \quad \text{on } \Omega \times D. \quad (1.16c)$$

Clearly, if there exists $L > 0$ such that $0 \leq \psi_0 \leq LM$, then $M \beta^L(\psi_0/M) = \psi_0$. Henceforth $L > 1$ is assumed.

Remark 1.4. The coupled problem (1.1a)–(1.1d), (1.7), (1.8), (1.15), (1.16a)–(1.16c) will be referred to as model (P_L), or as the *general FENE-type dumbbell model with centre-of-mass diffusion and microscopic cut-off*, with cut-off parameter $L > 1$.

In order to highlight the dependence on L , in subsequent sections the solution to (1.15), (1.10a)–(1.10c) will be labelled ψ_L , and we work with the variable $\widehat{\psi}_L := \psi_L/M$. Due to the coupling of (1.15) to (1.1a)–(1.1d) through (1.7), the velocity and the pressure will also depend on L and we shall therefore denote them in subsequent sections by \underline{u}_L and p_L . As has been already emphasized earlier, the centre-of-mass diffusion coefficient $\varepsilon > 0$ is a physical parameter and is regarded as being fixed, so we do not highlight its presence in the model through our notation.

Barrett and Süli [8] constructed a Galerkin finite element approximation, and proved (sub)sequence convergence, to a weak solution of a system similar to (P_L), where $\widehat{\psi}_L$ in the convective term, in addition to the drag term, is replaced by $\beta^L(\widehat{\psi}_L)$. Finally, Barrett and Süli proved in [7, 9] the existence and exponential equilibration of global-in-time weak solutions to Navier–Stokes–Fokker–Planck systems for general classes of finitely extensible nonlinear elastic and Hookean-type bead-spring chains models.

After this brief literature survey, we now turn our attention to the description of the formal energy bounds on which the constructions of the temporally semidiscrete and fully-discrete approximations are based.

2. FORMAL ENERGY BOUNDS FOR (P) AND (P_{L,δ})

In this section we identify formally the energy structure for (P), and related regularized models. Before doing so, we note that the notation $|\cdot|$ will be used to signify one of the following. When applied to a real number x , $|x|$ will denote the absolute value of the number x ; when applied to a vector y , $|y|$ will stand for the Euclidean norm of the vector y ; and, when applied to a square matrix A , $|A|$ will signify the Frobenius norm, $[\text{tr}(A^T A)]^{\frac{1}{2}}$, of the matrix A , where, for a square matrix B , $\text{tr}(B)$ denotes the trace of B .

Multiplying (1.1a) by y , integrating over Ω , and noting (1.1b), (1.1c) yields that

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left[\int_{\Omega} |u|^2 dx \right] + \nu \int_{\Omega} |\nabla_x u|^2 dx - \int_{\Omega} f \cdot u dx &= - \int_{\Omega} \tau(M \widehat{\psi}) : \nabla_x u dx \\ &= -k \int_{\Omega} C(M \widehat{\psi}) : \nabla_x u dx, \end{aligned} \tag{2.1}$$

where $\widehat{\psi} := \psi/M$. Let $\mathcal{F}(s) := (\ln s - 1)s + 1$ for $s > 0$, with $\mathcal{F}(0) := 1$. Multiplying the Fokker–Planck equation (1.9) by $\mathcal{F}'(\widehat{\psi}) \equiv \ln \widehat{\psi}$, on assuming that $\widehat{\psi} > 0$, integrating over $\Omega \times D$ and noting (1.10a), (1.10b) and (1.1b), (1.1c) yields that

$$\begin{aligned} \frac{d}{dt} \left[\int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}) dq dx \right] + \frac{1}{2\lambda} \int_{\Omega \times D} M \nabla_q \widehat{\psi} \cdot \nabla_q [\mathcal{F}'(\widehat{\psi})] dq dx \\ + \varepsilon \int_{\Omega \times D} M \nabla_x \widehat{\psi} \cdot \nabla_x [\mathcal{F}'(\widehat{\psi})] dq dx &= \int_{\Omega \times D} M \widehat{\psi} [(\nabla_x u) q] \cdot \nabla_q [\mathcal{F}'(\widehat{\psi})] dq dx. \end{aligned} \tag{2.2}$$

It follows, on noting that $\mathcal{F}''(s) = s^{-1} > 0$ for $s > 0$ and hence that $\widehat{\psi} \nabla_q [\mathcal{F}'(\widehat{\psi})] = \nabla_q \widehat{\psi}$, (1.5), (1.1b) and $M = 0$ on ∂D that

$$\begin{aligned} \int_{\Omega \times D} M \widehat{\psi} [(\nabla_x u) q] \cdot \nabla_q [\mathcal{F}'(\widehat{\psi})] dq dx &= \int_{\Omega \times D} M [(\nabla_x u) q] \cdot \nabla_q \widehat{\psi} dq dx \\ &= \int_{\Omega \times D} M U' \left(\frac{1}{2} |q|^2 \right) q \cdot [(\nabla_x u) q] \widehat{\psi} dq dx \\ &= \int_{\Omega} C(M \widehat{\psi}) : \nabla_x u dx, \end{aligned} \tag{2.3}$$

on recalling (1.8). Combining (2.1)–(2.3), we obtain the following energy law for (P):

$$\begin{aligned} \frac{d}{dt} \left[\frac{1}{2} \int_{\Omega} |u|^2 dx + k \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}) dq dx \right] + \nu \int_{\Omega} |\nabla_x u|^2 dx + k\varepsilon \int_{\Omega \times D} M \widehat{\psi} |\nabla_x [\mathcal{F}'(\widehat{\psi})]|^2 dq dx \\ + \frac{k}{2\lambda} \int_{\Omega \times D} M \widehat{\psi} |\nabla_q [\mathcal{F}'(\widehat{\psi})]|^2 dq dx &= \int_{\Omega} f \cdot u dx. \end{aligned} \tag{2.4}$$

To make the above rigorous, and for computational purposes, we replace the convex function $\mathcal{F} \in C(\mathbb{R}_{\geq 0}) \cap C^\infty(\mathbb{R}_{>0})$ by its convex regularization $\mathcal{F}_\delta^L \in C^{2,1}(\mathbb{R})$ defined, for any $\delta \in (0, 1)$ and $L > 1$, as follows:

$$\mathcal{F}_\delta^L(s) := \begin{cases} \frac{s^2 - \delta^2}{2\delta} + (\ln \delta - 1)s + 1 & s \leq \delta, \\ \mathcal{F}(s) \equiv (\ln s - 1)s + 1 & \delta \leq s \leq L, \\ \frac{s^2 - L^2}{2L} + (\ln L - 1)s + 1 & L \leq s. \end{cases} \quad (2.5)$$

Hence, we have that

$$[\mathcal{F}_\delta^L]'(s) = \begin{cases} \frac{s}{\delta} + \ln \delta - 1 & s \leq \delta, \\ \ln s & \delta \leq s \leq L, \\ \frac{s}{L} + \ln L - 1 & L \leq s, \end{cases} \quad \text{and} \quad [\mathcal{F}_\delta^L]''(s) = \begin{cases} \delta^{-1} & s \leq \delta, \\ s^{-1} & \delta \leq s \leq L, \\ L^{-1} & L \leq s. \end{cases} \quad (2.6)$$

In addition, we introduce

$$\beta_\delta^L(s) := [[\mathcal{F}_\delta^L]''(s)]^{-1} = \begin{cases} \delta & s \leq \delta, \\ s & \delta \leq s \leq L, \\ L & L \leq s. \end{cases} \quad (2.7)$$

It follows from (2.7), for any sufficiently smooth $\widehat{\varphi}$, that

$$\beta_\delta^L(\widehat{\varphi}) \nabla_x ([\mathcal{F}_\delta^L]'(\widehat{\varphi})) = \nabla_x \widehat{\varphi} \quad \text{and} \quad \beta_\delta^L(\widehat{\varphi}) \nabla_q ([\mathcal{F}_\delta^L]'(\widehat{\varphi})) = \nabla_q \widehat{\varphi}. \quad (2.8)$$

Let $\{u_{L,\delta}, \widehat{\psi}_{L,\delta}\}$ solve problem $(P_{L,\delta})$, which is a regularization of the problem (P) , similar to (P_L) , where $\beta^L(\cdot)$ in (1.15) and (1.16a) is replaced by $\beta_\delta^L(\cdot)$. Multiplying the Fokker–Planck equation in $(P_{L,\delta})$ by $[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta})$, integrating over $\Omega \times D$, noting the boundary conditions and (2.8) yields, similarly to (2.2) and (2.3), that

$$\begin{aligned} \frac{d}{dt} \left[\int_{\Omega \times D} M \mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta}) dq dx \right] + \frac{1}{2\lambda} \int_{\Omega \times D} M \nabla_q \widehat{\psi}_{L,\delta} \cdot \nabla_q \left[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta}) \right] dq dx \\ + \varepsilon \int_{\Omega \times D} M \nabla_x \widehat{\psi}_{L,\delta} \cdot \nabla_x \left[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta}) \right] dq dx = \int_{\Omega} C(M \widehat{\psi}_{L,\delta}) : \nabla_x u_{L,\delta} dx. \end{aligned} \quad (2.9)$$

Combining (2.9) and the $(P_{L,\delta})$ version of (2.1), we obtain the following energy law for $(P_{L,\delta})$, a regularized analogue of (2.4):

$$\begin{aligned} \frac{d}{dt} \left[\frac{1}{2} \int_{\Omega} |u_{L,\delta}|^2 dx + k \int_{\Omega \times D} M \mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta}) dq dx \right] + \nu \int_{\Omega} |\nabla_x u_{L,\delta}|^2 dx \\ + k\varepsilon \int_{\Omega \times D} M \beta_\delta^L(\widehat{\psi}_{L,\delta}) |\nabla_x \left[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta}) \right]|^2 dq dx \\ + \frac{k}{2\lambda} \int_{\Omega \times D} M \beta_\delta^L(\widehat{\psi}_{L,\delta}) |\nabla_q \left[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta}) \right]|^2 dq dx = \int_{\Omega} f \cdot u_{L,\delta} dx. \end{aligned} \quad (2.10)$$

On noting that $[\mathcal{F}_\delta^L]'' \geq L^{-1}$, and

$$\min\{\mathcal{F}_\delta^L(s), s[\mathcal{F}_\delta^L]'(s)\} \geq \begin{cases} \frac{s^2}{2\delta} & \text{if } s \leq 0, \\ \frac{s^2}{4L} - C(L) & \text{if } s \geq 0, \end{cases} \quad (2.11)$$

one deduces from (2.10) that

$$\sup_{t \in (0,T)} \left[\int_{\Omega} |u_{L,\delta}|^2 dx \right] + \nu \int_{\Omega_T} |\nabla_x u_{L,\delta}|^2 dx dt + \delta^{-1} \sup_{t \in (0,T)} \left[\int_{\Omega \times D} M |[\widehat{\psi}_{L,\delta}]_-|^2 dq dx \right] \leq C(L). \quad (2.12)$$

In addition, one can show that

$$\begin{aligned} & \sup_{t \in (0, T)} \left[\int_{\Omega \times D} M |\widehat{\psi}_{L, \delta}|^2 \, dq \, dx \right] + \frac{1}{\lambda} \int_0^T \int_{\Omega \times D} M \left| \nabla_q \widehat{\psi}_{L, \delta} \right|^2 \, dq \, dx \, dt \\ & + \varepsilon \int_0^T \int_{\Omega \times D} M \left| \nabla_x \widehat{\psi}_{L, \delta} \right|^2 \, dq \, dx \, dt + \sup_{t \in (0, T)} \int_{\Omega} |C(M \widehat{\psi}_{L, \delta})|^2 \, dx \leq C(L, T). \end{aligned} \tag{2.13}$$

The above formal bounds can be made rigorous and the existence of a global-in-time weak solution $\{u_{L, \delta}, \widehat{\psi}_{L, \delta}\}$ to $(P_{L, \delta})$ can be established, see [4]. Moreover, one can take the limit $\delta \rightarrow 0_+$ in problem $(P_{L, \delta})$ to establish the existence of a global-in-time weak solution $\{u_L, \widehat{\psi}_L\}$ to problem (P_L) with $\widehat{\psi}_L \geq 0$ a.e. in $\Omega \times D \times (0, T)$. Once again, see [4].

The aim of this paper is to construct a finite element approximation, $(P_{L, \delta}^{\Delta t, h})$, of problem $(P_{L, \delta})$, which mimics the energy law (2.10) at a discrete level, and to show that a (sub)sequence of this approximation converges to a weak solution of $(P_L^{\Delta t})$, as the spatial discretization parameter h , as well as the regularization parameter δ , tend to zero. Here $(P_L^{\Delta t})$ is a time discretization of (P_L) . Barrett and Süli [7] showed that for a specific time discretization $(P_L^{\Delta t})$ a (sub)sequence of this approximation converges to a weak solution of (P) , as the cut-off parameter L tends to infinity with the time discretization parameter $\Delta t = o(L^{-1})$.

The outline of this paper is as follows. In the next section, we introduce the necessary function spaces. In addition, we introduce the particular time discretization, $(P_L^{\Delta t})$, of (P_L) and state the relevant convergence results from Barrett and Süli [7]. In Section 4, we introduce our finite element approximation, $(P_{L, \delta}^{\Delta t, h})$, of problem $(P_{L, \delta})$ and show that a (sub)sequence of this approximation converges to a weak solution of $(P_L^{\Delta t})$, as the spatial discretization parameter h , as well as the regularization parameter δ , tend to zero. Hence combining this with the convergence result in Section 3, we obtain the desired result that a (sub)sequence of our finite element approximation $(P_{L, \delta}^{\Delta t, h})$ converges to a weak solution of (P) as first $h, \delta \rightarrow 0_+$ and then $L \rightarrow \infty$, with $\Delta t = o(L^{-1})$. In Section 5 we discuss possible extensions of our results. The paper closes with an Appendix, containing the proofs of some technical bounds required in the convergence analysis of the initialization of the scheme.

3. THE DISCRETE-IN-TIME APPROXIMATION $(P_L^{\Delta t})$

Let

$$\underline{H} := \{w \in \underline{L}^2(\Omega) : \nabla_x \cdot w = 0\} \quad \text{and} \quad \underline{V} := \{w \in \underline{H}_0^1(\Omega) : \nabla_x \cdot w = 0\}, \tag{3.1}$$

where the divergence operator $\nabla_x \cdot$ is to be understood in the sense of distributions on Ω . Let \underline{V}' be the dual of \underline{V} . More generally, let \underline{V}_σ denote the closure of the set of all divergence-free $\mathcal{C}_0^\infty(\Omega)$ functions in the norm of $\underline{H}_0^1(\Omega) \cap \underline{H}^\sigma(\Omega)$, $\sigma \geq 1$, equipped with the Hilbert space norm, denoted by $\|\cdot\|_{\underline{V}_\sigma}$, inherited from $\underline{H}^\sigma(\Omega)$, and let \underline{V}'_σ signify the dual space of \underline{V}_σ , with duality pairing $\langle \cdot, \cdot \rangle_{\underline{V}_\sigma}$. As Ω is a bounded Lipschitz domain, we have that $\underline{V}_1 = \underline{V}$ (cf. Temam [30], Chap. 1, Thm. 1.6). Similarly, $\langle \cdot, \cdot \rangle_{\underline{H}_0^1(\Omega)}$ will denote the duality pairing between $(\underline{H}_0^1(\Omega))'$ and $\underline{H}_0^1(\Omega)$. The norm on $(\underline{H}_0^1(\Omega))'$ will be that induced from taking $\|\nabla_x \cdot\|_{L^2(\Omega)}$ to be the norm on $\underline{H}_0^1(\Omega)$.

For later purposes, we recall the following well-known Gagliardo–Nirenberg inequality. Let $r \in [2, \infty)$ if $d = 2$, and $r \in [2, 6]$ if $d = 3$ and $\theta = d \left(\frac{1}{2} - \frac{1}{r}\right)$. Then, there is a constant $C = C(\Omega, r, d)$, such that, for all $\eta \in H^1(\Omega)$:

$$\|\eta\|_{L^r(\Omega)} \leq C \|\eta\|_{L^2(\Omega)}^{1-\theta} \|\eta\|_{H^1(\Omega)}^\theta. \tag{3.2}$$

Let $\mathcal{F} \in C(\mathbb{R}_{>0})$ be defined by $\mathcal{F}(s) := s(\log s - 1) + 1$, $s > 0$. As $\lim_{s \rightarrow 0_+} \mathcal{F}(s) = 1$, the function \mathcal{F} can be considered to be defined and continuous on $[0, \infty)$, where it is a nonnegative, strictly convex function with $\mathcal{F}(1) = 0$.

We recall our assumptions on the data:

$$\begin{aligned}
 \text{(A1)} \quad & \partial\Omega \in C^{0,1}; \quad D = B(0, r_D) \text{ with } r_D > 0 \text{ and } U \text{ satisfying (1.4a), (1.4b) with } \gamma > 1; \\
 & u_0 \in H; \quad \widehat{\psi}_0 := \frac{\psi_0}{M} \geq 0 \text{ a.e. on } \Omega \times D \quad \text{with } \mathcal{F}(\widehat{\psi}_0) \in L^1_M(\Omega \times D) \\
 & \text{and } \int_D M(q) \widehat{\psi}_0(x, q) \, dq = 1 \quad \text{for a.e. } x \in \Omega; \quad \text{and } f \in L^2(0, T; (H^1_0(\Omega))'). \quad (3.3)
 \end{aligned}$$

Here, $L^p_M(\Omega \times D)$, for $p \in [1, \infty)$, denotes the Maxwellian-weighted L^p space over $\Omega \times D$ with norm

$$\|\widehat{\varphi}\|_{L^p_M(\Omega \times D)} := \left\{ \int_{\Omega \times D} M |\widehat{\varphi}|^p \, dq \, dx \right\}^{\frac{1}{p}}.$$

Similarly, we introduce $L^p_M(D)$, the Maxwellian-weighted L^p space over D . Letting

$$\|\widehat{\varphi}\|_{H^1_M(\Omega \times D)} := \left\{ \int_{\Omega \times D} M \left[|\widehat{\varphi}|^2 + |\nabla_x \widehat{\varphi}|^2 + |\nabla_q \widehat{\varphi}|^2 \right] \, dq \, dx \right\}^{\frac{1}{2}}, \quad (3.4)$$

we then set

$$\widehat{X} \equiv H^1_M(\Omega \times D) := \left\{ \widehat{\varphi} \in L^1_{\text{loc}}(\Omega \times D) : \|\widehat{\varphi}\|_{H^1_M(\Omega \times D)} < \infty \right\}. \quad (3.5)$$

It is shown in Appendix C of [6] (the extended version of Barrett and Süli [7]) that

$$C^\infty(\overline{\Omega \times D}) \text{ is dense in } \widehat{X}. \quad (3.6)$$

In addition, we note that the embeddings

$$H^1_M(D) \hookrightarrow L^2_M(D), \quad (3.7a)$$

$$H^1_M(\Omega \times D) \equiv L^2(\Omega; H^1_M(D)) \cap H^1(\Omega; L^2_M(D)) \hookrightarrow L^2_M(\Omega \times D) \equiv L^2(\Omega; L^2_M(D)) \quad (3.7b)$$

are compact if $\gamma \geq 1$ in (1.4a), (1.4b); see Appendix D in [6]. Throughout we will assume that (3.3) hold, so that (1.6) and (3.7a), (3.7b) hold. We note for future reference that (1.8) and (1.6) yield that, for $\widehat{\varphi} \in L^2_M(\Omega \times D)$,

$$\int_\Omega |C(M \widehat{\varphi})|^2 \, dx = \int_\Omega \left| \int_D M \widehat{\varphi} U' q q^T \, dq \right|^2 \, dx \leq C \left(\int_{\Omega \times D} M |\widehat{\varphi}|^2 \, dq \, dx \right), \quad (3.8)$$

where C is a positive constant.

We now formulate our discrete-in-time approximation of problem (P_L) for a fixed parameter $L > 1$. For any $T > 0$ and $N \geq 1$, let $N \Delta t = T$ and $t_n = n \Delta t$, $n = 0, \dots, N$. To prove existence of a solution under minimal smoothness requirements on the initial datum u_0 (recall (3.3)), we introduce $u^0 = u^0(\Delta t) \in \mathcal{V}$, the unique solution of

$$\int_\Omega \left[u^0 \cdot v + \Delta t \nabla_x u^0 : \nabla_x v \right] \, dx = \int_\Omega u_0 \cdot v \, dx \quad \forall v \in \mathcal{V}; \quad (3.9)$$

and so

$$\int_\Omega \left[|u^0|^2 + \Delta t |\nabla_x u^0|^2 \right] \, dx \leq \int_\Omega |u_0|^2 \, dx \leq C. \quad (3.10)$$

In addition, we have that u^0 converges to u_0 weakly in H in the limit of $\Delta t \rightarrow 0_+$.

Analogously to defining u^0 for a given initial velocity field u_0 , we shall assign a certain ‘smoothed’ initial datum, $\widehat{\psi}^0 = \widehat{\psi}^0(L, \Delta t) \in H_M^1(\Omega \times D)$, to the initial datum $\widehat{\psi}_0$ such that

$$\int_{\Omega \times D} M \left[\widehat{\psi}^0 \widehat{\varphi} + \Delta t \left(\widetilde{\nabla}_x \widehat{\psi}^0 \cdot \widetilde{\nabla}_x \widehat{\varphi} + \widetilde{\nabla}_q \widehat{\psi}^0 \cdot \widetilde{\nabla}_q \widehat{\varphi} \right) \right] dq dx = \int_{\Omega \times D} M \beta^L(\widehat{\psi}_0) \widehat{\varphi} dq dx \quad \forall \widehat{\varphi} \in H_M^1(\Omega \times D). \tag{3.11}$$

For $p \in [1, \infty)$, let

$$\widehat{Z}_p := \left\{ \widehat{\varphi} \in L_M^p(\Omega \times D) : \widehat{\varphi} \geq 0 \text{ a.e. on } \Omega \times D \text{ and } \int_D M(q) \widehat{\varphi}(x, q) dq \leq 1 \text{ for a.e. } x \in \Omega \right\}. \tag{3.12}$$

It is proved in the appendix that there exists a unique $\widehat{\psi}^0 \in H_M^1(\Omega \times D)$ satisfying (3.11); furthermore,

$$\widehat{\psi}^0 \in \widehat{Z}_1; \quad \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}^0) dq dx + 4 \Delta t \int_{\Omega \times D} M \left[|\widetilde{\nabla}_x \sqrt{\widehat{\psi}^0}|^2 + |\widetilde{\nabla}_q \sqrt{\widehat{\psi}^0}|^2 \right] dq dx \leq \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}_0) dq dx; \tag{3.13a}$$

and

$$\widehat{\psi}^0 \equiv \beta^L(\widehat{\psi}_0) \rightarrow \widehat{\psi}_0 \text{ weakly in } L_M^1(\Omega \times D) \text{ as } L \rightarrow \infty \text{ and } \Delta t \rightarrow 0_+. \tag{3.13b}$$

It follows from (3.13a), (3.13b) and (1.14) that $\widehat{\psi}^0 \in \widehat{Z}_2$; in fact, $\widehat{\psi}^0 \in L^\infty(\Omega \times D) \cap H_M^1(\Omega \times D)$.

Our discrete-in-time approximation of (P_L) is then defined as follows.

(P_L^{Δt}) Let $u_L^0 := u^0 \in V$ and $\widehat{\psi}_L^0 := \widehat{\psi}^0 \in \widehat{Z}_2$. Then, for $n = 1, \dots, N$, given $(u_L^{n-1}, \widehat{\psi}_L^{n-1}) \in V \times \widehat{Z}_2$, find $(u_L^n, \widehat{\psi}_L^n) \in V \times (\widehat{X} \cap \widehat{Z}_2)$ such that

$$\begin{aligned} \int_{\Omega} \left[\frac{u_L^n - u_L^{n-1}}{\Delta t} + (u_L^{n-1} \cdot \widetilde{\nabla}_x) u_L^n \right] \cdot w dx + \nu \int_{\Omega} \widetilde{\nabla}_x u_L^n : \widetilde{\nabla}_x w dx \\ = \langle f^n, w \rangle_{H_0^1(\Omega)} - k \int_{\Omega} C(M \widehat{\psi}_L^n) : \widetilde{\nabla}_x w dx \quad \forall w \in V, \end{aligned} \tag{3.14a}$$

$$\begin{aligned} \int_{\Omega \times D} M \frac{\widehat{\psi}_L^n - \widehat{\psi}_L^{n-1}}{\Delta t} \widehat{\varphi} dq dx + \int_{\Omega \times D} M \left[\frac{1}{2\lambda} \widetilde{\nabla}_q \widehat{\psi}_L^n - [\sigma(u_L^n) q] \beta^L(\widehat{\psi}_L^n) \right] \cdot \widetilde{\nabla}_q \widehat{\varphi} dq dx \\ + \int_{\Omega \times D} M \left[\varepsilon \widetilde{\nabla}_x \widehat{\psi}_L^n - u_L^{n-1} \widehat{\psi}_L^n \right] \cdot \widetilde{\nabla}_x \widehat{\varphi} dq dx = 0 \quad \forall \widehat{\varphi} \in \widehat{X}; \end{aligned} \tag{3.14b}$$

where, for $t \in [t_{n-1}, t_n)$, and $n = 1, \dots, N$,

$$f^{\Delta t, +}(\cdot, t) = f^n(\cdot) := \frac{1}{\Delta t} \int_{t_{n-1}}^{t_n} f(\cdot, t) dt \in (H_0^1(\Omega))' \subset V'. \tag{3.15}$$

It follows from (3.3) and (3.15) that

$$\sum_{n=1}^N \Delta t \|f^n\|_{H^{-1}(\Omega)}^r \leq \int_0^T \|f\|_{H^{-1}(\Omega)}^r dt \leq C \quad \text{for any } r \in [1, 2], \tag{3.16a}$$

$$f^{\Delta t, +} \rightarrow f \text{ strongly in } L^2(0, T; (H_0^1(\Omega))') \text{ as } \Delta t \rightarrow 0_+. \tag{3.16b}$$

Note that as the test function w in (3.14a) is chosen to be divergence-free, the term containing the density ρ in the definition of $\underline{\tau}$ (cf. (1.7)) is eliminated from (3.14a).

In line with (3.16b), let

$$\underline{u}_L^{\Delta t}(\cdot, t) := \frac{t - t_{n-1}}{\Delta t} \underline{u}_L^n(\cdot) + \frac{t_n - t}{\Delta t} \underline{u}_L^{n-1}(\cdot), \quad t \in [t_{n-1}, t_n], \quad n = 1, \dots, N, \quad (3.17a)$$

$$\underline{u}_L^{\Delta t, +}(\cdot, t) := \underline{u}_L^n(\cdot), \quad \underline{u}_L^{\Delta t, -}(\cdot, t) := \underline{u}_L^{n-1}(\cdot), \quad t \in (t_{n-1}, t_n], \quad n = 1, \dots, N, \quad (3.17b)$$

and throughout we adopt the notation $\underline{u}_L^{\Delta t(\pm)}$, which means $\underline{u}_L^{\Delta t}$ with or without the superscripts \pm . Using the above notation, and introducing analogous notation for $\{\widehat{\psi}_L^n\}_{n=0}^N$, (3.14a), (3.14b) multiplied by Δt and summed for $n = 1, \dots, N$ can be restated as:

$$\begin{aligned} & \int_0^T \int_{\Omega} \left[\frac{\partial \underline{u}_L^{\Delta t}}{\partial t} + (\underline{u}_L^{\Delta t, -} \cdot \nabla_x) \underline{u}_L^{\Delta t, +} \right] \cdot \underline{w} \, dx \, dt + \nu \int_0^T \int_{\Omega} \nabla_x \underline{u}_L^{\Delta t, +} : \nabla_x \underline{w} \, dx \, dt \\ & = \langle \underline{f}^{\Delta t, +}, \underline{w} \rangle_{H_0^1(\Omega)} - k \int_{\Omega} C(M \widehat{\psi}_L^{\Delta t, +}) : \nabla_x \underline{w} \, dx \, dt \quad \forall \underline{w} \in L^1(0, T; V), \end{aligned} \quad (3.18a)$$

$$\begin{aligned} & \int_0^T \int_{\Omega \times D} M \frac{\partial \widehat{\psi}_L^{\Delta t}}{\partial t} \widehat{\varphi} \, dq \, dx \, dt + \int_0^T \int_{\Omega \times D} M \left[\frac{1}{2\lambda} \nabla_q \widehat{\psi}_L^{\Delta t, +} - [\sigma(\underline{u}_L^{\Delta t, +}) q] \beta^L(\widehat{\psi}_L^{\Delta t, +}) \right] \cdot \nabla_q \widehat{\varphi} \, dq \, dx \, dt \\ & + \int_0^T \int_{\Omega \times D} M \left[\varepsilon \nabla_x \widehat{\psi}_L^{\Delta t, +} - \underline{u}_L^{\Delta t, -} \widehat{\psi}_L^{\Delta t, +} \right] \cdot \nabla_x \widehat{\varphi} \, dq \, dx \, dt = 0 \quad \forall \widehat{\varphi} \in L^1(0, T; \widehat{X}). \end{aligned} \quad (3.18b)$$

The existence of solutions to problem (3.18a), (3.18b) is established in Lemma 3.3 in Barrett and Süli [7]. The following theorem is proved in [7], Theorem 6.1, for a bead-spring chain polymer model with $K \geq 1$ linearly coupled finitely extensible nonlinear elastic springs. Here we state it for the special case of $K = 1$, corresponding to the dumbbell model.

Theorem 3.1. *Suppose that the assumptions (3.3) hold. Then, there exists a subsequence of $\{(\underline{u}_L^{\Delta t}, \widehat{\psi}_L^{\Delta t})\}_{L>1}$ (not indicated) with $\Delta t = o(L^{-1})$, and a pair of functions $(\underline{u}, \widehat{\psi})$ such that*

$$\underline{u} \in L^\infty(0, T; \underline{L}^2(\Omega)) \cap L^2(0, T; V) \cap H^1(0, T; V'_\sigma), \quad \sigma \geq \frac{1}{2}d, \quad \sigma > 1,$$

and

$$\widehat{\psi} \in L^1(0, T; L^1_M(\Omega \times D)) \cap H^1(0, T; M^{-1}(H^s(\Omega \times D))'), \quad s > 1 + d,$$

with $\widehat{\psi} \geq 0$ a.e. on $\Omega \times D \times [0, T]$,

$$\rho(\underline{x}, t) := \int_D M(q) \widehat{\psi}(\underline{x}, q, t) \, dq = 1 \quad \text{for a.e. } (\underline{x}, t) \in \Omega \times [0, T], \quad (3.19)$$

whereby $\widehat{\psi} \in L^\infty(0, T; L^1_M(\Omega \times D))$; and finite relative entropy and Fisher information, i.e.,

$$\mathcal{F}(\widehat{\psi}) \in L^\infty(0, T; L^1_M(\Omega \times D)) \quad \text{and} \quad \sqrt{\widehat{\psi}} \in L^2(0, T; H^1_M(\Omega \times D)), \quad (3.20)$$

such that, as $L \rightarrow \infty$ (and thereby $\Delta t \rightarrow 0_+$),

$$\underline{u}_L^{\Delta t(\pm)} \rightharpoonup \underline{u} \quad \text{weak}^* \text{ in } L^\infty(0, T; \underline{L}^2(\Omega)), \quad (3.21a)$$

$$\underline{u}_L^{\Delta t(\pm)} \rightharpoonup \underline{u} \quad \text{weakly in } L^2(0, T; V), \quad (3.21b)$$

$$\underline{u}_L^{\Delta t(\pm)} \rightarrow \underline{u} \quad \text{strongly in } L^2(0, T; \underline{L}^r(\Omega)), \quad (3.21c)$$

$$\frac{\partial \underline{u}_L^{\Delta t}}{\partial t} \rightharpoonup \frac{\partial \underline{u}}{\partial t} \quad \text{weakly in } L^2(0, T; V'_\sigma), \quad (3.21d)$$

where $r \in [1, \infty)$ if $d = 2$ and $r \in [1, 6)$ if $d = 3$; and

$$M^{\frac{1}{2}} \nabla_x \sqrt{\widehat{\psi}_L^{\Delta t(\pm)}} \rightharpoonup M^{\frac{1}{2}} \nabla_x \sqrt{\widehat{\psi}} \quad \text{weakly in} \quad L^2(0, T; L^2(\Omega \times D)), \quad (3.22a)$$

$$M^{\frac{1}{2}} \nabla_q \sqrt{\widehat{\psi}_L^{\Delta t(\pm)}} \rightharpoonup M^{\frac{1}{2}} \nabla_q \sqrt{\widehat{\psi}} \quad \text{weakly in} \quad L^2(0, T; L^2(\Omega \times D)), \quad (3.22b)$$

$$M \frac{\partial \widehat{\psi}_L^{\Delta t}}{\partial t} \rightharpoonup M \frac{\partial \widehat{\psi}}{\partial t} \quad \text{weakly in} \quad L^2(0, T; (H^s(\Omega \times D))'), \quad (3.22c)$$

$$\widehat{\psi}_L^{\Delta t(\pm)} \rightarrow \widehat{\psi} \quad \text{strongly in} \quad L^p(0, T; L^1_M(\Omega \times D)), \quad (3.22d)$$

for all $p \in [1, \infty)$; and,

$$\nabla_x \cdot C(M \widehat{\psi}_L^{\Delta t,+}) \rightharpoonup \nabla_x \cdot C(M \widehat{\psi}) \quad \text{weakly in} \quad L^2(0, T; V'_\sigma). \quad (3.22e)$$

The pair $(\underline{u}, \widehat{\psi})$ is a global weak solution to problem (P), in the sense that

$$\begin{aligned} & - \int_0^T \int_\Omega \underline{u} \cdot \frac{\partial w}{\partial t} \, dx \, dt + \int_0^T \int_\Omega \left[\left[(\underline{u} \cdot \nabla_x) \underline{u} \right] \cdot w + \nu \nabla_x \underline{u} : \nabla_x w \right] \, dx \, dt \\ & = \int_\Omega \underline{u}_0(x) \cdot w(x, 0) \, dx + \int_0^T \left[\langle \underline{f}, w \rangle_{H^1_0(\Omega)} - k \int_\Omega C(M \widehat{\psi}) : \nabla_x w \, dx \right] \, dt \\ & \quad \forall w \in W^{1,1}(0, T; V_\sigma) \text{ s.t. } w(\cdot, T) = 0, \end{aligned} \quad (3.23)$$

and

$$\begin{aligned} & - \int_0^T \int_{\Omega \times D} M \widehat{\psi} \frac{\partial \widehat{\varphi}}{\partial t} \, dq \, dx \, dt + \int_0^T \int_{\Omega \times D} M \left[\varepsilon \nabla_x \widehat{\psi} - \underline{u} \widehat{\psi} \right] \cdot \nabla_x \widehat{\varphi} \, dq \, dx \, dt \\ & + \frac{1}{2\lambda} \int_0^T \int_{\Omega \times D} M \nabla_q \widehat{\psi} \cdot \nabla_q \widehat{\varphi} \, dq \, dx \, dt - \int_0^T \int_{\Omega \times D} M \left[\underline{\sigma}(\underline{u}) q \right] \widehat{\psi} \cdot \nabla_q \widehat{\varphi} \, dq \, dx \, dt \\ & = \int_{\Omega \times D} \widehat{\psi}_0(x, q) \widehat{\varphi}(x, q, 0) \, dq \, dx \quad \forall \widehat{\varphi} \in W^{1,1}(0, T; H^s(\Omega \times D)) \text{ s.t. } \widehat{\varphi}(\cdot, \cdot, T) = 0. \end{aligned} \quad (3.24)$$

In addition, the function \underline{u} is weakly continuous as a mapping from $[0, T]$ to \underline{H} , and $\widehat{\psi}$ is weakly continuous as a mapping from $[0, T]$ to $L^1_M(\Omega \times D)$. The weak solution $(\underline{u}, \widehat{\psi})$ satisfies the following energy inequality for a.e. $t \in [0, T]$:

$$\begin{aligned} & \|\underline{u}(t)\|^2 + \nu \int_0^t \|\nabla_x \underline{u}(s)\|^2 \, ds + 2k \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}(t)) \, dq \, dx \\ & + 8k\varepsilon \int_0^t \int_{\Omega \times D} M |\nabla_x \sqrt{\widehat{\psi}}|^2 \, dq \, dx \, ds + \frac{2k}{\lambda} \int_0^t \int_{\Omega \times D} M |\nabla_q \sqrt{\widehat{\psi}}|^2 \, dq \, dx \, ds \\ & \leq \|\underline{u}_0\|^2 + \frac{1}{\nu} \int_0^t \|\underline{f}(s)\|_{(H^1_0(\Omega))'}^2 \, ds + 2k \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}_0) \, dq \, dx, \end{aligned} \quad (3.25)$$

with $\mathcal{F}(s) = s(\log s - 1) + 1$, $s \geq 0$.

4. FINITE ELEMENT APPROXIMATION $(P_{L,\delta}^{\Delta t,h})$

Let us denote the measure of a bounded open region $\omega \subset \mathbb{R}^d$ by $\underline{m}(\omega)$. We make the following assumption on Ω and the partitions of Ω and D .

(A2) For ease of exposition, we shall assume that Ω is a convex polytope. Let $\{\mathcal{T}_h^x\}_{h>0}$ be a quasiuniform family of partitions of Ω into disjoint open nonobtuse simplices κ_x , so that

$$\overline{\Omega} \equiv \bigcup_{\kappa_x \in \mathcal{T}_h^x} \overline{\kappa_x} \quad \text{with} \quad h_{\kappa_x} := \text{diam}(\kappa_x), \quad h_x := \max_{\kappa_x \in \mathcal{T}_h^x} h_{\kappa_x} \leq \text{diam}(\Omega) h \quad \text{and} \quad \underline{m}(\kappa_x) \geq C h^d.$$

Let $\{\mathcal{T}_h^q\}_{h>0}$ be a quasiuniform family of partitions of $D \equiv B(0, r_D)$, $r_D > 0$, into disjoint open nonobtuse simplices κ_q , with possibly one curved edge on ∂D when $d = 2$, or one curved face on ∂D when $d = 3$, so that

$$\overline{D} \equiv \bigcup_{\kappa_q \in \mathcal{T}_h^q} \overline{\kappa_q} \quad \text{with} \quad h_{\kappa_q} := \text{diam}(\kappa_q), \quad h_q := \max_{\kappa_q \in \mathcal{T}_h^q} h_{\kappa_q} \leq \text{diam}(D) h \quad \text{and} \quad \underline{m}(\kappa_q) \geq C h^d.$$

A ‘‘simplex’’ κ_q with a curved edge/face is nonobtuse if it is convex and the enclosed simplex with the same vertices is nonobtuse, in the sense that all of its dihedral angles are $\leq \pi/2$. It follows from the above that

$$\frac{h_x}{h_q} + \frac{h_q}{h_x} \leq C \quad \text{as} \quad h \rightarrow 0_+. \quad (4.1)$$

We note that such nonobtuse simplicial partitions of Ω and D are easily constructed in the case $d = 2$. For the construction of nonobtuse three-dimensional simplicial partitions we refer to the papers of Korotov and Krížek [22, 23] for example; the reader should note, however, that in [22] the authors use the term *acute* when they mean *nonobtuse*. Elsewhere in the computational geometry literature the term *acute* is reserved for a simplicial partition where all dihedral angles of any simplex in the partition are $< \pi/2$, which is a more restrictive requirement (especially in the case of $d = 3$) than what we assume here; see, for example, the articles of Brandts *et al.* [11], Eppstein *et al.* [16], and Itoh and Zamfirescu [18], and references therein. Nonobtuse simplicial partitions are sometimes also called *weakly acute* (*cf.* [29], p. 363).

We adopt the standard notation for L^2 inner products:

$$(\eta_1, \eta_2)_\Omega := \int_\Omega \eta_1 \eta_2 \, dx \quad \forall \eta_i \in L^2(\Omega) \quad \text{and} \quad (\eta_1, \eta_2)_{\Omega \times D} := \int_{\Omega \times D} \eta_1 \eta_2 \, dq \, dx \quad \forall \eta_i \in L^2(\Omega \times D), \quad (4.2)$$

which are naturally extended to vector/matrix functions.

Let \mathbb{P}_k^x and \mathbb{P}_k^q denote polynomials of degree less than or equal to k in x and q , respectively. We approximate the pressure and velocity with the lowest order Taylor–Hood element; that is,

$$R_h := \{\eta_h \in C(\overline{\Omega}) : \eta_h|_{\kappa_x} \in \mathbb{P}_1^x \quad \forall \kappa_x \in \mathcal{T}_h^x\}, \quad (4.3a)$$

$$\underline{W}_h := \{w_h \in [C(\overline{\Omega})]^d : w_h|_{\kappa_x} \in [\mathbb{P}_2^x]^d \quad \forall \kappa_x \in \mathcal{T}_h^x \text{ and } w_h = 0 \text{ on } \partial\Omega\} \subset [H_0^1(\Omega)]^d, \quad (4.3b)$$

$$\underline{V}_h := \{v_h \in \underline{W}_h : (\nabla_x \cdot v_h, \eta_h)_\Omega = 0 \quad \forall \eta_h \in R_h\}. \quad (4.3c)$$

It is well-known that R_h and \underline{W}_h satisfy the inf-sup condition: there exists $c_0 \in \mathbb{R}_{>0}$ such that

$$\sup_{w_h \in \underline{W}_h} \frac{(\nabla_x \cdot w_h, r_h)_\Omega}{\|w_h\|_{H^1(\Omega)}} \geq c_0 \|r_h\|_{L^2(\Omega)} \quad \forall r_h \in R_h, \quad (4.4)$$

see *e.g.* [12], Section VI.6. Hence for all $v \in \underline{V}$, there exists a sequence $\{v_h\}_{h>0}$, with $v_h \in \underline{V}_h$, such that

$$\lim_{h \rightarrow 0_+} \|v - v_h\|_{H^1(\Omega)} = 0. \quad (4.5)$$

For the approximation of the advection term in the Navier–Stokes equation we note that, for all $v \in \underline{V}$ and $w, z \in \underline{H}^1(\Omega)$, we have that

$$((v \cdot \nabla_x) w, z)_\Omega \equiv \frac{1}{2} \left[((v \cdot \nabla_x) w, z)_\Omega - ((v \cdot \nabla_x) z, w)_\Omega \right]. \quad (4.6)$$

In addition, the choice $w = z$ leads to both sides of (4.6) vanishing. Obviously, as $V_h \not\subset V$, the discrete analogue of the above does not hold; that is, it is *not* generally true that, for all $v_h \in V_h$, $w_h, z_h \in W_h$,

$$((v_h \cdot \nabla_x)w_h, z_h)_\Omega \equiv \frac{1}{2} \left[((v_h \cdot \nabla_x)w_h, z_h)_\Omega - ((v_h \cdot \nabla_x)z_h, w_h)_\Omega \right]. \tag{4.7}$$

We note that the right-hand side of (4.7) vanishes if $w_h = z_h$, which is not necessarily true for the left-hand side. Hence, we use the right-hand side form of (4.7) for the approximation of the advection term in the Navier–Stokes equation.

To approximate \widehat{X} , we first introduce

$$\widehat{X}_h^x := \{\widehat{\varphi}_h^x \in C(\overline{\Omega}) : \widehat{\varphi}_h^x|_{\kappa_x} \in \mathbb{P}_1^x \quad \forall \kappa_x \in \mathcal{T}_h^x\} \subset W^{1,\infty}(\Omega), \tag{4.8a}$$

$$\widehat{X}_h^q := \{\widehat{\varphi}_h^q \in C(\overline{D}) : \widehat{\varphi}_h^q|_{\kappa_q} \in \mathbb{P}_1^q \quad \forall \kappa_q \in \mathcal{T}_h^q\} \subset W^{1,\infty}(D). \tag{4.8b}$$

We then set

$$\widehat{X}_h := \widehat{X}_h^x \otimes \widehat{X}_h^q \subset \widehat{X}. \tag{4.9}$$

We note from (4.3a), (4.3c), (4.8a) and (4.9) that, for any $v_h \in V_h$ and any $q \in \overline{D}$,

$$(\nabla_x \cdot v_h, \widehat{\varphi}_h(\cdot, q))_\Omega = 0 \quad \forall \widehat{\varphi}_h \in \widehat{X}_h. \tag{4.10}$$

We note that for (4.10) to hold in general, we require that $\widehat{X}_h^x \subseteq R_h$.

We introduce the interpolation operators $\pi_h^x : C(\overline{\Omega}) \rightarrow \widehat{X}_h^x$ and $\pi_h^q : C(\overline{D}) \rightarrow \widehat{X}_h^q$ such that

$$\pi_h^x \widehat{\varphi}^x(P_j^x) = \widehat{\varphi}^x(P_j^x), \quad j = 1, \dots, I^x, \quad \text{and} \quad \pi_h^q \widehat{\varphi}^q(P_j^q) = \widehat{\varphi}^q(P_j^q), \quad j = 1, \dots, I^q, \tag{4.11}$$

where $\{P_j^x\}_{j=1}^{I^x}$ and $\{P_j^q\}_{j=1}^{I^q}$ are the nodes (vertices) of \mathcal{T}_h^x and \mathcal{T}_h^q , respectively. The associated basis functions are

$$\chi_i^x \in \widehat{X}_h^x \quad \text{such that} \quad \chi_i^x(P_j^x) = \delta_{ij} \quad \text{for } i, j = 1, \dots, I^x, \tag{4.12a}$$

$$\text{and} \quad \chi_i^q \in \widehat{X}_h^q \quad \text{such that} \quad \chi_i^q(P_j^q) = \delta_{ij} \quad \text{for } i, j = 1, \dots, I^q. \tag{4.12b}$$

We introduce also $\pi_h : C(\overline{\Omega \times D}) \rightarrow \widehat{X}_h$ such that

$$(\pi_h \widehat{\varphi})(P_i^x, P_j^q) = \widehat{\varphi}(P_i^x, P_j^q) \quad \text{for } i = 1, \dots, I^x, \quad j = 1, \dots, I^q. \tag{4.13}$$

Of course, we have that $\pi_h \equiv \pi_h^x \pi_h^q \equiv \pi_h^q \pi_h^x$. The vector versions of the above interpolation operators are

$$\widetilde{\pi}_h^x : [C(\overline{\Omega})]^d \rightarrow [\widehat{X}_h^x]^d, \quad \widetilde{\pi}_h^q : [C(\overline{D})]^d \rightarrow [\widehat{X}_h^q]^d, \quad \text{and} \quad \widetilde{\pi}_h : [C(\overline{\Omega \times D})]^d \rightarrow [\widehat{X}_h]^d. \tag{4.14}$$

We require also the local interpolation operators

$$\begin{aligned} \pi_{h,\kappa_x}^x &\equiv \pi_h^x|_{\kappa_x}, & \pi_{h,\kappa_q}^q &\equiv \pi_h^q|_{\kappa_q}, & \pi_{h,\kappa_x \times \kappa_q} &\equiv \pi_h|_{\kappa_x \times \kappa_q}, & \widetilde{\pi}_{h,\kappa_x}^x &\equiv \widetilde{\pi}_h^x|_{\kappa_x}, \\ \widetilde{\pi}_{h,\kappa_q}^q &\equiv \widetilde{\pi}_h^q|_{\kappa_q} & \text{and} & & \widetilde{\pi}_{h,\kappa_x \times \kappa_q} &\equiv \widetilde{\pi}_h|_{\kappa_x \times \kappa_q} & & \forall \kappa_x \in \mathcal{T}_h^x, \quad \forall \kappa_q \in \mathcal{T}_h^q. \end{aligned} \tag{4.15}$$

For any $\widehat{\varphi}_h \in \widehat{X}_h$, there exist $[\widetilde{\Xi}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, \underline{q})$, $[\widetilde{\Xi}_{L,\delta}^q(\widehat{\varphi}_h)](\underline{x}, \underline{q}) \in \mathbb{R}^{d \times d}$ for a.e. $(\underline{x}, \underline{q}) \in \Omega \times D$ such that on $\kappa_x \times \kappa_q$, for all $\kappa_x \in \mathcal{T}_h^x$, $\kappa_q \in \mathcal{T}_h^q$,

$$\widetilde{\Xi}_{L,\delta}^x(\widehat{\varphi}_h) \in [\mathbb{P}_1^x]^{d \times d} \quad \text{and} \quad \mathfrak{T}_{h,\kappa_x \times \kappa_q} \left[\widetilde{\Xi}_{L,\delta}^x(\widehat{\varphi}_h) \nabla_x (\pi_h [(\mathcal{F}_\delta^L)'(\widehat{\varphi}_h)]) \right] = \nabla_x \widehat{\varphi}_h; \tag{4.16a}$$

$$\widetilde{\Xi}_{L,\delta}^q(\widehat{\varphi}_h) \in [\mathbb{P}_1^q]^{d \times d} \quad \text{and} \quad \mathfrak{T}_{h,\kappa_x \times \kappa_q} \left[\widetilde{\Xi}_{L,\delta}^q(\widehat{\varphi}_h) \nabla_q (\pi_h [(\mathcal{F}_\delta^L)'(\widehat{\varphi}_h)]) \right] = \nabla_q \widehat{\varphi}_h. \tag{4.16b}$$

Hence (4.16a), (4.16b) are discrete analogues of the relations (2.8). We now give the construction of $\underline{\underline{\Xi}}_{L,\delta}^x(\cdot)$ and $\underline{\underline{\Xi}}_{L,\delta}^q(\cdot)$. Given $\widehat{\varphi}_h \in \widehat{X}_h$, $\kappa_x \in \mathcal{T}_h^x$ with vertices $\{P_{i_j}^x\}_{j=0}^d$ and $\kappa_q \in \mathcal{T}_h^q$ with vertices $\{P_{i_j}^q\}_{j=0}^d$, then for a fixed vertex $P_{i_k}^q$ of κ_q let $[\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, P_{i_k}^q) \in \mathbb{R}^{d \times d}$ for $\underline{x} \in \kappa_x$ be diagonal with entries, for $j = 1, \dots, d$,

$$[\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)]_{jj}(\underline{x}, P_{i_k}^q) = \begin{cases} \frac{\varphi_j - \varphi_0}{[\mathcal{F}_\delta^L]'(\varphi_j) - [\mathcal{F}_\delta^L]'(\varphi_0)} & \text{if } \varphi_j := \widehat{\varphi}_h(P_{i_j}^x, P_{i_k}^q) \neq \varphi_0 := \widehat{\varphi}_h(P_{i_0}^x, P_{i_k}^q), \\ \frac{1}{[\mathcal{F}_\delta^L]''(\varphi_j)} = \beta_\delta^L(\varphi_j) & \text{if } \varphi_j = \varphi_0. \end{cases} \quad (4.17)$$

Let $\{\underline{e}_i\}_{i=1}^d$ be the orthonormal vectors in \mathbb{R}^d , such that the j^{th} component of \underline{e}_i is δ_{ij} , $i, j = 1, \dots, d$. Let $\tilde{\kappa}$ be the standard reference simplex in \mathbb{R}^d with vertices $\{\tilde{P}_i\}_{i=0}^d$, where \tilde{P}_0 is the origin and $\tilde{P}_i = \underline{e}_i$, $i = 1, \dots, d$. Let $B_{\kappa_x} \in \mathbb{R}^{d \times d}$ be such that the affine mapping $\mathcal{B}_{\kappa_x} : \underline{y} \in \mathbb{R}^d \mapsto P_{k_0}^x + B_{\kappa_x} \underline{y}$ maps the vertex \tilde{P}_j to $P_{i_j}^x$, $j = 0, \dots, d$, and hence $\tilde{\kappa}$ to κ_x . For any $\widehat{\varphi}_h^x \in \widehat{X}_h$, let $\widehat{\varphi}_{h,y}^x(\underline{x}) \equiv \widehat{\varphi}_h^x(\mathcal{B}_{\kappa_x} \underline{y})$ for all $\underline{y} \in \tilde{\kappa}$. Hence it follows that

$$\nabla_x \widehat{\varphi}_h^x = [B_{\kappa_x}^T]^{-1} \nabla_y \widehat{\varphi}_{h,y}^x. \quad (4.18)$$

Therefore, for $k = 0, \dots, d$,

$$[\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, P_{i_k}^q) = [B_{\kappa_x}^T]^{-1} [\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, P_{i_k}^q) B_{\kappa_x}^T \quad (4.19)$$

is such that

$$[\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)] \nabla_x (\pi_h [[\mathcal{F}_\delta^L]'(\widehat{\varphi}_h)]) (\underline{x}, P_{i_k}^q) = \nabla_x \widehat{\varphi}_h(\underline{x}, P_{i_k}^q) \quad \forall \underline{x} \in \kappa_x. \quad (4.20)$$

Finally, on recalling (4.12b), we set

$$[\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, \underline{q}) = \sum_{k=0}^d [\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, P_{i_k}^q) \chi_{i_k}^q(\underline{q}) \quad \forall \underline{x} \in \kappa_x, \quad \forall \underline{q} \in \kappa_q. \quad (4.21)$$

Hence $\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)$ satisfies (4.16a). A similar construction yields $\underline{\underline{\Xi}}_{L,\delta}^q(\widehat{\varphi}_h)$ satisfying (4.16b). The only difference is for those κ_{q_i} with a curved side or face: the corresponding linear mapping \mathcal{B}_{κ_q} maps $\tilde{\kappa}$ to the *enclosed* simplex with the same vertices as κ_q , where vertex \tilde{P}_j of $\tilde{\kappa}$ is mapped to $P_{i_j}^q$ of κ_q , $j = 0, \dots, d$.

As \mathcal{T}_h^x , \mathcal{T}_h^q are quasiuniform partitions, we have from (4.21), (4.19) and (4.17), and their $\underline{\underline{\Xi}}_\delta^q$ counterparts, that, for all $\widehat{\varphi}_h \in \widehat{X}_h$,

$$\|\underline{\underline{\Xi}}_{L,\delta}^x(\widehat{\varphi}_h)\|_{L^\infty(\Omega \times D)}^2 + \|\underline{\underline{\Xi}}_{L,\delta}^q(\widehat{\varphi}_h)\|_{L^\infty(\Omega \times D)}^2 \leq C L^2. \quad (4.22)$$

We note that the construction of $\underline{\underline{\Xi}}_{L,\delta}^x(\cdot)$ and $\underline{\underline{\Xi}}_{L,\delta}^q(\cdot)$ satisfying (4.16a), (4.16b) is an extension of ideas used in *e.g.* [2, 17] for the finite element approximation of fourth-order degenerate nonlinear parabolic equations, such as the thin film equation.

We will require also a discrete analogue of

$$\widehat{\varphi} \nabla_x ([\mathcal{F}_\delta^L]'(\widehat{\varphi})) = \nabla_x (G_\delta^L(\widehat{\varphi})) \quad (4.23)$$

for any sufficiently smooth $\widehat{\varphi}$, where $G_\delta^L \in C^{0,1}(\mathbb{R})$ is defined by

$$G_\delta^L(s) := \begin{cases} \frac{s^2}{2\delta} + \frac{\delta-L}{2} & s \leq \delta, \\ s - \frac{L}{2} & \delta \leq s \leq L, \\ \frac{s^2}{2L} & L \leq s; \end{cases} \quad (4.24)$$

and so $[G_\delta^L]'(s) = s/\beta_\delta^L(s) = s[\mathcal{F}_\delta^L]''(s)$. For later purposes, let

$$H_\delta^L(s) := G_\delta^L([\mathcal{F}_\delta^L]')^{-1}(s) = \begin{cases} \frac{\delta}{2}(s+1-\log\delta)^2 + \frac{\delta-L}{2} & s \leq \log\delta, \\ e^s - \frac{L}{2} & \log\delta \leq s \leq \log L, \\ \frac{L}{2}(s+1-\log L)^2 & \log L \leq s. \end{cases} \tag{4.25}$$

Hence it follows that

$$[H_\delta^L]'([\mathcal{F}_\delta^L]'(s)) = s. \tag{4.26}$$

We now introduce a discrete analogue of (4.23). For any $\widehat{\varphi}_h \in \widehat{X}_h$, there exists $[\underline{A}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, \underline{q}) \in \mathbb{R}^{d \times d}$ for a.e. $(\underline{x}, \underline{q}) \in \Omega \times D$ such that on $\kappa_x \times \kappa_q$, for all $\kappa_x \in \mathcal{T}_h^x$, $\kappa_q \in \mathcal{T}_h^q$,

$$\underline{A}_{L,\delta}^x(\widehat{\varphi}_h) \in [\mathbb{P}_1^q]^{d \times d} \quad \text{and} \quad \pi_{h,\kappa_x \times \kappa_q} \left[\underline{A}_{L,\delta}^x(\widehat{\varphi}_h) \nabla_x (\pi_h([\mathcal{F}_\delta^L]'(\widehat{\varphi}_h))) \right] = \nabla_x (\pi_h[G_\delta^L(\widehat{\varphi}_h)]). \tag{4.27}$$

We now give the construction of $\underline{A}_{L,\delta}^x(\cdot)$. Given $\widehat{\varphi}_h \in \widehat{X}_h$, $\kappa_x \in \mathcal{T}_h^x$ with vertices $\{\underline{P}_{i_j}^x\}_{j=0}^d$ and $\kappa_q \in \mathcal{T}_h^q$ with vertices $\{\underline{P}_{i_k}^q\}_{k=0}^d$, then for a fixed vertex $\underline{P}_{i_k}^q$ of κ_q , let $[\widetilde{\underline{A}}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, \underline{P}_{i_k}^q) \in \mathbb{R}^{d \times d}$ for $\underline{x} \in \kappa_x$ be diagonal with entries, for $j = 1, \dots, d$,

$$[\widetilde{\underline{A}}_{L,\delta}^x(\widehat{\varphi}_h)]_{jj}(\underline{x}, \underline{P}_{i_k}^q) = \begin{cases} \frac{G_\delta^L(\varphi_j) - G_\delta^L(\varphi_0)}{[\mathcal{F}_\delta^L]'(\varphi_j) - [\mathcal{F}_\delta^L]'(\varphi_0)} & \text{if } \varphi_j := \widehat{\varphi}_h(\underline{P}_{i_j}^x, \underline{P}_{i_k}^q) \neq \varphi_0 := \widehat{\varphi}_h(\underline{P}_{i_0}^x, \underline{P}_{i_k}^q), \\ \frac{[G_\delta^L]'(\varphi_j)}{[\mathcal{F}_\delta^L]''(\varphi_j)} = \varphi_j & \text{if } \varphi_j = \varphi_0, \end{cases} \tag{4.28}$$

where we have noted (4.25) and (4.26). We then define $[\underline{A}_{L,\delta}^x(\widehat{\varphi}_h)](\underline{x}, \underline{q})$ via (4.19) and (4.21) with $\widetilde{\underline{\Xi}}_{L,\delta}^x$ and $\underline{\Xi}_{L,\delta}^x$ replaced by $\widetilde{\underline{A}}_{L,\delta}^x$ and $\underline{A}_{L,\delta}^x$, respectively. As \mathcal{T}_h^x is quasi-uniform, it follows similarly to (4.22), on noting (4.28), (4.25) and (4.26) that, for all $\widehat{\varphi}_h \in \widehat{X}_h$,

$$\|\underline{A}_{L,\delta}^x(\widehat{\varphi}_h)\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \leq C \|\widehat{\varphi}_h\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \quad \forall \kappa_x \in \mathcal{T}_h^x, \quad \forall \kappa_q \in \mathcal{T}_h^q. \tag{4.29}$$

As the partitions \mathcal{T}_h^x and \mathcal{T}_h^q are nonobtuse, we deduce (see, for example, [13] Chap. 3, Bibliography and Comments on Sect. 3.3; and Sect. 4 in the paper of Brandts *et al.* [11]) that

$$\nabla_x \chi_i^x \cdot \nabla_x \chi_j^x \leq 0 \quad \text{on } \kappa_x \quad i \neq j, \quad i, j = 1, \dots, I^x, \quad \forall \kappa_x \in \mathcal{T}_h^x; \tag{4.30a}$$

$$\text{and} \quad \nabla_q \chi_i^q \cdot \nabla_q \chi_j^q \leq 0 \quad \text{on } \kappa_q \quad i \neq j, \quad i, j = 1, \dots, I^q, \quad \forall \kappa_q \in \mathcal{T}_h^q. \tag{4.30b}$$

Our next lemma can be seen as a generalization of a result in Section 2.4.2 of [27].

Lemma 4.1. *Suppose that the partitions \mathcal{T}_h^x and \mathcal{T}_h^q are nonobtuse and let $g \in C^{0,1}(\mathbb{R})$ be monotonic increasing with Lipschitz constant g_{Lip} ; then, for all $\kappa_x \in \mathcal{T}_h^x$ and $\kappa_q \in \mathcal{T}_h^q$ and for all $\widehat{\varphi}_h \in \widehat{X}_h$,*

$$\begin{aligned} & \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\left| \nabla_x (\pi_{h,\kappa_x \times \kappa_q}[g(\widehat{\varphi}_h)]) \right|^2 \right] \text{d}\underline{q} \text{d}\underline{x} \\ & \leq g_{\text{Lip}} \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\nabla_x \widehat{\varphi}_h \cdot \nabla_x (\pi_{h,\kappa_x \times \kappa_q}[g(\widehat{\varphi}_h)]) \right] \text{d}\underline{q} \text{d}\underline{x}; \end{aligned} \tag{4.31a}$$

and

$$\begin{aligned} & \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\left| \nabla_q (\pi_{h,\kappa_x \times \kappa_q}[g(\widehat{\varphi}_h)]) \right|^2 \right] \text{d}\underline{q} \text{d}\underline{x} \\ & \leq g_{\text{Lip}} \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\nabla_q \widehat{\varphi}_h \cdot \nabla_q (\pi_{h,\kappa_x \times \kappa_q}[g(\widehat{\varphi}_h)]) \right] \text{d}\underline{q} \text{d}\underline{x}. \end{aligned} \tag{4.31b}$$

Proof. We shall prove (4.31a); the proof of (4.31b) is analogous. Suppose that $\widehat{\varphi}_h \in \widehat{X}_h$ and let $\kappa_x \in \mathcal{T}_h^x$ and $\kappa_q \in \mathcal{T}_h^q$. Then, letting $G(\underline{x}, \underline{q}) := \pi_{h, \kappa_q}^q [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))]$, we have that

$$\pi_{h, \kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))] = \pi_{h, \kappa_x}^x \pi_{h, \kappa_q}^q [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))] = \pi_{h, \kappa_x}^x G(\underline{x}, \underline{q}) = \sum_{j=0}^d G(P_{k_j}^x, \underline{q}) \chi_{k_j}^x(\underline{x}), \quad (\underline{x}, \underline{q}) \in \kappa_x \times \kappa_q,$$

where $\{\chi_{k_j}^x\}_{j=0}^d$ are the $d+1$ vertices of the d -dimensional simplex κ_x and $\chi_{k_j}^x$, $j = 0, \dots, d$, are the linear Lagrange element-basis-functions associated with κ_x . Hence, on expanding $\widehat{\varphi}_h|_{\kappa_x}$ in terms of the same basis, we have that

$$\begin{aligned} \nabla_x \widehat{\varphi}_h(\underline{x}, \underline{q}) \cdot \nabla_x (\pi_{h, \kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))]) &= \sum_{i=0}^d \sum_{j=0}^d \left[\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) G(P_{k_j}^x, \underline{q}) \nabla_x \chi_{k_i}^x(\underline{x}) \cdot \nabla_x \chi_{k_j}^x(\underline{x}) \right] \\ &= \sum_{i=0}^d \left(\sum_{0 \leq j < i} + \sum_{j=i} + \sum_{i < j \leq d} \right) \left[\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) G(P_{k_j}^x, \underline{q}) \nabla_x \chi_{k_i}^x(\underline{x}) \cdot \nabla_x \chi_{k_j}^x(\underline{x}) \right] \\ &= \sum_{i=1}^d \sum_{0 \leq j < i} \left[\left(\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) G(P_{k_j}^x, \underline{q}) + \widehat{\varphi}_h(P_{k_j}^x, \underline{q}) G(P_{k_i}^x, \underline{q}) \right) \nabla_x \chi_{k_i}^x(\underline{x}) \cdot \nabla_x \chi_{k_j}^x(\underline{x}) \right] \\ &\quad + \sum_{i=0}^d \left[\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) G(P_{k_i}^x, \underline{q}) |\nabla_x \chi_{k_i}^x(\underline{x})|^2 \right] \quad \forall (\underline{x}, \underline{q}) \in \kappa_x \times \kappa_q. \end{aligned} \quad (4.32)$$

As $\sum_{j=0}^d \chi_{k_j}^x(\underline{x}) \equiv 1$ on κ_x , it follows that $\nabla_x \chi_{k_i}^x = -\sum_{j \neq i} \nabla_x \chi_{k_j}^x$, and so $|\nabla_x \chi_{k_i}^x|^2 = -\sum_{j \neq i} \nabla_x \chi_{k_i}^x \cdot \nabla_x \chi_{k_j}^x$. Thus, on substitution into the last term in (4.32), we have that, for all $(\underline{x}, \underline{q}) \in \kappa_x \times \kappa_q$,

$$\begin{aligned} \nabla_x \widehat{\varphi}_h(\underline{x}, \underline{q}) \cdot \nabla_x (\pi_{h, \kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))]) \\ = -\frac{1}{2} \sum_{i=0}^d \sum_{j=0}^d \left[\left(G(P_{k_i}^x, \underline{q}) - G(P_{k_j}^x, \underline{q}) \right) \left(\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) - \widehat{\varphi}_h(P_{k_j}^x, \underline{q}) \right) \nabla_x \chi_{k_i}^x(\underline{x}) \cdot \nabla_x \chi_{k_j}^x(\underline{x}) \right]. \end{aligned} \quad (4.33)$$

Similarly to (4.33), we have that

$$|\nabla_x (\pi_{h, \kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))])|^2 = -\frac{1}{2} \sum_{i=0}^d \sum_{j=0}^d \left[\left(G(P_{k_i}^x, \underline{q}) - G(P_{k_j}^x, \underline{q}) \right)^2 \nabla_x \chi_{k_i}^x(\underline{x}) \cdot \nabla_x \chi_{k_j}^x(\underline{x}) \right]. \quad (4.34)$$

Now, for all $\underline{q} \in \kappa_q$,

$$\begin{aligned} \pi_{h, \kappa_q}^q \left[\left(G(P_{k_i}^x, \underline{q}) - G(P_{k_j}^x, \underline{q}) \right) \left(\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) - \widehat{\varphi}_h(P_{k_j}^x, \underline{q}) \right) \right] \\ = \pi_{h, \kappa_q}^q \left[\left(\pi_{h, \kappa_q}^q [g(\widehat{\varphi}_h(P_{k_i}^x, \underline{q}))] - \pi_{h, \kappa_q}^q [g(\widehat{\varphi}_h(P_{k_j}^x, \underline{q}))] \right) \left(\widehat{\varphi}_h(P_{k_i}^x, \underline{q}) - \widehat{\varphi}_h(P_{k_j}^x, \underline{q}) \right) \right] \\ \geq \frac{1}{g_{\text{Lip}}} \pi_{h, \kappa_q}^q \left[\left(g(\widehat{\varphi}_h(P_{k_i}^x, \underline{q})) - g(\widehat{\varphi}_h(P_{k_j}^x, \underline{q})) \right)^2 \right] \\ = \frac{1}{g_{\text{Lip}}} \pi_{h, \kappa_q}^q \left[\left(G(P_{k_i}^x, \underline{q}) - G(P_{k_j}^x, \underline{q}) \right)^2 \right]. \end{aligned} \quad (4.35)$$

On applying π_{h,κ_q}^q to both sides of (4.33) and (4.34), noting (4.35), and (4.34) corresponding to $i = j$ are equal to zero, we deduce that, for all $(\underline{x}, \underline{q}) \in \kappa_x \times \kappa_q$,

$$\pi_{h,\kappa_q}^q \left[\nabla_x \widehat{\varphi}_h(\underline{x}, \underline{q}) \cdot \nabla_x (\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))]) \right] \geq \frac{1}{g_{\text{Lip}}} \pi_{h,\kappa_q}^q \left| \nabla_x (\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h(\underline{x}, \underline{q}))]) \right|^2.$$

By applying π_{h,κ_x}^x to both sides of this inequality, multiplying by the (nonnegative) function M and then integrating over $\kappa_x \times \kappa_q$ we arrive at (4.31a) on recalling that $\pi_{h,\kappa_x}^x \pi_{h,\kappa_q}^q = \pi_{h,\kappa_x \times \kappa_q}$. As we have noted above, the proof of (4.31b) is analogous. \square

Corollary 4.2. *Suppose that the partitions \mathcal{T}_h^x and \mathcal{T}_h^q are nonobtuse and let g be defined and strictly monotonic increasing on \mathbb{R} such that g^{-1} , the inverse function of g , is Lipschitz continuous on \mathbb{R} , with Lipschitz constant $(g^{-1})_{\text{Lip}}$; then, for all $\kappa_x \in \mathcal{T}_h^x$ and $\kappa_q \in \mathcal{T}_h^q$ and for all $\widehat{\varphi}_h \in \widehat{X}_h$,*

$$\int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\left| \nabla_x \widehat{\varphi}_h \right|^2 \right] \underset{\sim}{\underset{\sim}{\leq}} (g^{-1})_{\text{Lip}} \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\nabla_x \widehat{\varphi}_h \cdot \nabla_x (\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h)]) \right] \underset{\sim}{\underset{\sim}{\text{d}q \text{ d}x};} \tag{4.36a}$$

and

$$\int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\left| \nabla_q \widehat{\varphi}_h \right|^2 \right] \underset{\sim}{\underset{\sim}{\leq}} (g^{-1})_{\text{Lip}} \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} \left[\nabla_q \widehat{\varphi}_h \cdot \nabla_q (\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h)]) \right] \underset{\sim}{\underset{\sim}{\text{d}q \text{ d}x}.} \tag{4.36b}$$

Proof. These inequalities follow on replacing g in Lemma 4.1 by g^{-1} ; $\widehat{\varphi}_h$ by $\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h)]$; and noting that

$$\pi_{h,\kappa_x \times \kappa_q} \left[g^{-1}(\pi_{h,\kappa_x \times \kappa_q} [g(\widehat{\varphi}_h|_{\kappa_x \times \kappa_q})]) \right] = \widehat{\varphi}_h|_{\kappa_x \times \kappa_q} \quad \forall \widehat{\varphi}_h \in \widehat{X}_h.$$

That completes the proof. \square

Given initial data u_0 and $\widehat{\psi}_0$ satisfying (3.3), we choose $u_{L,\delta,h}^0 \in V_h$ and $\widehat{\psi}_{L,\delta,h}^0 \in \widehat{X}_h$ as the unique solutions of, respectively,

$$(u_{L,\delta,h}^0, v_h)_\Omega + \Delta t (\nabla_x u_{L,\delta,h}^0, \nabla_x v_h)_\Omega = (u_0, v_h)_\Omega \quad \forall v_h \in V_h, \tag{4.37a}$$

$$(M, \pi_h [\widehat{\psi}_{L,\delta,h}^0, \widehat{\varphi}_h])_{\Omega \times D} + \Delta t (M, \pi_h [\nabla_x \widehat{\psi}_{L,\delta,h}^0 \cdot \nabla_x \widehat{\varphi}_h + \nabla_q \widehat{\psi}_{L,\delta,h}^0 \cdot \nabla_q \widehat{\varphi}_h])_{\Omega \times D} = (M \beta^L(\widehat{\psi}_0), \widehat{\varphi}_h)_{\Omega \times D} \quad \forall \widehat{\varphi}_h \in \widehat{X}_h. \tag{4.37b}$$

It follows from (4.37a), (4.37b) that

$$\int_\Omega \left[|u_{L,\delta,h}^0|^2 + \Delta t |\nabla_x u_{L,\delta,h}^0|^2 \right] \underset{\sim}{\text{d}x} \leq \int_\Omega |u_0|^2 \underset{\sim}{\text{d}x} \leq C, \quad 0 \leq \widehat{\psi}_{L,\delta,h}^0(x, q) \leq L \quad \forall (x, q) \in \overline{\Omega \times D}$$

and

$$\int_{\Omega \times D} M \pi_h \left[|\widehat{\psi}_{L,\delta,h}^0|^2 + \Delta t \left(|\nabla_x \widehat{\psi}_{L,\delta,h}^0|^2 + |\nabla_q \widehat{\psi}_{L,\delta,h}^0|^2 \right) \right] \underset{\sim}{\text{d}q \text{ d}x} \leq \int_{\Omega \times D} M L^2 = C(L). \tag{4.38}$$

Here in deriving the lower bound on $\widehat{\psi}_{L,\delta,h}^0$ we choose $\widehat{\varphi}_h = \pi_h[\widehat{\psi}_{L,\delta,h}^0]_-$ in (4.37b) and note (4.31a), (4.31b). Similarly, in deriving the upper bound, we note that (4.37b) holds with $\widehat{\psi}_{L,\delta,h}^0$ and $\beta^L(\widehat{\psi}_0)$ replaced by $L - \widehat{\psi}_{L,\delta,h}^0$ and $L - \beta^L(\widehat{\psi}_0)$, respectively, and choose $\widehat{\varphi}_h = \pi_h[L - \widehat{\psi}_{L,\delta,h}^0]_-$.

Our finite element approximation of $(P_L^{\Delta t})$ is defined as follows:

$(P_{L,\delta}^{\Delta t,h})$ For $n = 1, \dots, N$, given $(u_{L,\delta,h}^{n-1}, \widehat{\psi}_{L,\delta,h}^{n-1}) \in \underline{V}_h \times \widehat{X}_h$, find $(u_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n) \in \underline{V}_h \times \widehat{X}_h$ such that

$$\begin{aligned} & \left(\frac{u_{L,\delta,h}^n - u_{L,\delta,h}^{n-1}}{\Delta t}, \widetilde{w}_h \right)_{\Omega} + \nu (\nabla_x u_{L,\delta,h}^n, \nabla_x \widetilde{w}_h)_{\Omega} + \frac{1}{2} \left[((u_{L,\delta,h}^{n-1} \cdot \nabla_x) u_{L,\delta,h}^n, \widetilde{w}_h)_{\Omega} - ((u_{L,\delta,h}^{n-1} \cdot \nabla_x) \widetilde{w}_h, u_{L,\delta,h}^n)_{\Omega} \right] \\ & = \langle f^n, \widetilde{w}_h \rangle_{H_0^1(\Omega)} - k (C(M \widehat{\psi}_{L,\delta,h}^n), \nabla_x \widetilde{w}_h)_{\Omega} \quad \forall \widetilde{w}_h \in \underline{V}_h, \end{aligned} \quad (4.39a)$$

$$\begin{aligned} & \left(M, \pi_h \left[\frac{\widehat{\psi}_{L,\delta,h}^n - \widehat{\psi}_{L,\delta,h}^{n-1}}{\Delta t} \widehat{\varphi}_h + \varepsilon \nabla_x \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_x \widehat{\varphi}_h + \frac{1}{2\lambda} \nabla_q \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_q \widehat{\varphi}_h \right] \right)_{\Omega \times D} \\ & = \left(M (\nabla_x u_{L,\delta,h}^n) q, \pi_h \left[\underline{\Xi}_{L,\delta}^q(\widehat{\psi}_{L,\delta,h}^n) \nabla_q \widehat{\varphi}_h \right] \right)_{\Omega \times D} + \left(M u_{L,\delta,h}^n, \pi_h \left[A_{L,\delta}^x(\widehat{\psi}_{L,\delta,h}^n) \nabla_x \widehat{\varphi}_h \right] \right)_{\Omega \times D} \\ & \quad \forall \widehat{\varphi}_h \in \widehat{X}_h; \end{aligned} \quad (4.39b)$$

where for ease of notation, we write π_h and $\underline{\pi}_h$ in (4.39b) whereas it should really be $\pi_{h,\kappa_x \times \kappa_q}$ and $\underline{\pi}_{h,\kappa_x \times \kappa_q}$, respectively, on each $\kappa_x \times \kappa_q$ of $\Omega \times D$. We note that these interpolation operators play a crucial role in (4.39b) in obtaining a discrete version of (2.9). For example, we can exploit the results (4.16b), (4.27) and (4.31a), (4.31b) on choosing the test function $\widehat{\varphi}_h = \pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]$.

Remark 4.3. The only difference between the full discretization, $(P_L^{\Delta t,h})$, of (P_L) stated in (4.39a), (4.39b) and that in Barrett and Süli [8], (4.32a), (4.32b), is that $A_{L,\delta}^x$ in (4.39b) is replaced by $\underline{\Xi}_{L,\delta}^x$. Recall that solutions of the approximation in [8] are shown to (sub)sequence converge, as $h, \Delta t, \delta \rightarrow 0_+$, to a weak solution of a system similar to (P_L) , where $\widehat{\psi}_L$ in the convective term, in addition to the drag term, is replaced by $\beta^L(\widehat{\psi}_L)$. Moreover, we were unable to pass to the limit $L \rightarrow \infty$ in [8]. Whereas, in this paper we will show that solutions of (4.39a), (4.39b) (sub)sequence converge to a weak solution of $(P_L^{\Delta t})$ as $h, \delta \rightarrow 0_+$. Then we can appeal to the convergence result, Theorem 3.1 from [7], to show that a (sub)sequence of our finite approximation $(P_{L,\delta}^{\Delta t,h})$ converges to a weak solution of (P) as first $h, \delta \rightarrow 0_+$ and then $L \rightarrow \infty$, with $\Delta t = o(L^{-1})$.

We note that the approximations $u_{L,\delta,h}^n$ and $\widehat{\psi}_{L,\delta,h}^n$ at time level t_n to the velocity field and the scaled probability distribution satisfy a coupled nonlinear system, (4.39a), (4.39b). We will show existence of a solution to (4.39a), (4.39b) below, see Theorem 4.6, via a Brouwer fixed point theorem. First, assuming existence, we show that $(P_{L,\delta}^{\Delta t,h})$ satisfies a discrete analogue of the energy equality (2.10). For all the following lemmas and theorems we assume that the assumptions (A1) and (A2) hold.

Lemma 4.4. For $n = 1, \dots, N$, a solution $(u_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n) \in \underline{V}_h \times \widehat{X}_h$ of (4.39a), (4.39b), if it exists, satisfies

$$\begin{aligned} & \frac{1}{2} \left[\|u_{L,\delta,h}^n\|_{L^2(\Omega)}^2 + \|u_{L,\delta,h}^n - u_{L,\delta,h}^{n-1}\|_{L^2(\Omega)}^2 \right] + k (M, \pi_h[\mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta,h}^n)])_{\Omega \times D} + \Delta t \nu \| \nabla_x u_{L,\delta,h}^n \|_{L^2(\Omega)}^2 \\ & + \Delta t k \left(M, \pi_h \left[\varepsilon \nabla_x \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_x (\pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]) + \frac{1}{2\lambda} \nabla_q \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_q (\pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]) \right] \right)_{\Omega \times D} \\ & \leq \frac{1}{2} \|u_{L,\delta,h}^{n-1}\|_{L^2(\Omega)}^2 + k (M, \pi_h[\mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta,h}^{n-1})])_{\Omega \times D} + \Delta t \langle f^n, u_{L,\delta,h}^n \rangle_{H_0^1(\Omega)} \\ & \leq \frac{1}{2} \|u_{L,\delta,h}^{n-1}\|_{L^2(\Omega)}^2 + k (M, \pi_h[\mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta,h}^{n-1})])_{\Omega \times D} + \Delta t \left[\frac{\nu}{2} \| \nabla_x u_{L,\delta,h}^n \|_{L^2(\Omega)}^2 + C \| f^n \|_{H^{-1}(\Omega)}^2 \right]. \end{aligned} \quad (4.40)$$

Proof. On choosing $w_h = u_{L,\delta,h}^n$ in (4.39a), it follows that

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} \left[|u_{L,\delta,h}^n|^2 + |u_{L,\delta,h}^n - u_{L,\delta,h}^{n-1}|^2 - |u_{L,\delta,h}^{n-1}|^2 \right] dx + \Delta t \nu \int_{\Omega} |\nabla_x u_{L,\delta,h}^n|^2 dx \\ & = \Delta t \left[\langle f^n, u_{L,\delta,h}^n \rangle_{H_0^1(\Omega)} - k (C(M \widehat{\psi}_{L,\delta,h}^n), \nabla_x u_{L,\delta,h}^n)_{\Omega} \right], \end{aligned} \quad (4.41)$$

where we have noted the simple identity

$$2(s_1 - s_2)s_1 = s_1^2 + (s_1 - s_2)^2 - s_2^2 \quad \forall s_1, s_2 \in \mathbb{R}. \tag{4.42}$$

Next, on choosing $\widehat{\varphi}_h = \pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]$ in (4.39b), and noting the convexity of \mathcal{F}_δ^L , (4.16b), (4.27), (1.5), (4.10) and (1.8), we have that

$$\begin{aligned} & (M, \pi_h[\mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta,h}^n) - \mathcal{F}_\delta^L(\widehat{\psi}_{L,\delta,h}^{n-1})])_{\Omega \times D} \\ & + \Delta t \left(M, \pi_h \left[\varepsilon \nabla_x \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_x (\pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]) + \frac{1}{2\lambda} \nabla_q \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_q (\pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]) \right] \right)_{\Omega \times D} \\ & \leq (M \nabla_x \underline{u}_{L,\delta,h}^n, q, \nabla_q \widehat{\psi}_{L,\delta,h}^n)_{\Omega \times D} + (M \underline{u}_{L,\delta,h}^n, \nabla_x (\pi_h[G_\delta^L(\widehat{\psi}_{L,\delta,h}^n)]))_{\Omega \times D} \\ & = (M U'(\frac{1}{2}|q|^2) q \cdot [(\nabla_x \underline{u}_{L,\delta,h}^n) q], \widehat{\psi}_{L,\delta,h}^n)_{\Omega \times D} - (M \nabla_x \cdot \underline{u}_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n)_{\Omega \times D} \\ & \quad - (M \nabla_x \cdot \underline{u}_{L,\delta,h}^n, \pi_h[G_\delta^L(\widehat{\psi}_{L,\delta,h}^n)])_{\Omega \times D} \\ & = (C(M \widehat{\psi}_{L,\delta,h}^n), \nabla_x \underline{u}_{L,\delta,h}^n)_{\Omega}. \end{aligned} \tag{4.43}$$

Combining (4.41) and (4.43) yields the first inequality (4.40). The second inequality follows from using the Cauchy–Schwarz inequality, Young’s inequality, and a Poincaré inequality. \square

Remark 4.5. On noting (4.36a), (4.36b), the last term on the left-hand side of the first inequality in (4.40) is nonnegative, and this is exploited in the existence result in Theorem 4.6 and the stability analysis in Lemma 4.10 below. In the case of a bead-spring chain with $K \geq 1$ coupled springs, the q term becomes

$$\Delta t \left(M, \pi_h \left[\frac{1}{2\lambda} \sum_{i=1}^K \sum_{j=1}^K A_{ij} \nabla_{q_j} \widehat{\psi}_{L,\delta,h}^n \cdot \nabla_{q_i} (\pi_h[[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L,\delta,h}^n)]) \right] \right)_{\Omega \times D}, \tag{4.44}$$

where $A = (A_{ij})_{i,j=1}^K \in \mathbb{R}^{d \times d}$ is the symmetric and positive definite *Rouse matrix*. Unfortunately, we do not know at the moment how to guarantee the nonnegativity of this term, except when $K = 1$, or if $K \geq 1$ and the symmetric positive definite Rouse matrix A is *diagonal*, corresponding to the case of K decoupled dumbbells. When A is an arbitrary symmetric positive definite matrix, a natural idea is to perform a diagonalization $A = OLO^T$, where O is an orthogonal $d \times d$ matrix whose column vectors are the orthonormal eigenvectors of A , and L is a positive definite diagonal $d \times d$ matrix, with the eigenvalues of A along its diagonal; and perform the change of variable $\widehat{q} := O^T q$. Such an orthogonal transformation will, however, map the high-dimensional configuration domain D into a domain $O^T D$ that is no longer of a Cartesian-product form, and the construction of a weakly acute triangulation, which is essential for our argument so as to ensure the nonnegativity of the finite element approximation to $\widehat{\psi}$ on the transformed version of D , is not at all obvious. Hence our restriction in this paper to the case of a dumbbell ($K = 1$) model, instead of a general bead-spring chain ($K \geq 1$).

We now show using a Brouwer fixed point theorem that there exists a solution $(\underline{u}_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n)$ at time level t_n to (4.39a), (4.39b).

Theorem 4.6. *Given $(\underline{u}_{L,\delta,h}^{n-1}, \widehat{\psi}_{L,\delta,h}^{n-1}) \in \mathcal{V}_h \times \widehat{X}_h$ and for any time step $\Delta t > 0$, there exists at least one solution $(\underline{u}_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n) \in \mathcal{V}_h \times \widehat{X}_h$ to (4.39a), (4.39b).*

Proof. We define the inner product $((\cdot, \cdot))$ on the Hilbert space $\mathcal{V}_h \times \widehat{X}_h$ as follows:

$$((\underline{u}_h, \widehat{\psi}_h), (\underline{w}_h, \widehat{\varphi}_h)) := (\underline{u}_h, \underline{w}_h)_\Omega + (M, \pi_h[\widehat{\psi}_h \widehat{\varphi}_h])_{\Omega \times D} \quad \forall (\underline{u}_h, \widehat{\psi}_h), (\underline{w}_h, \widehat{\varphi}_h) \in \mathcal{V}_h \times \widehat{X}_h.$$

Given $(\underline{u}_{L,\delta,h}^{n-1}, \widehat{\psi}_{L,\delta,h}^{n-1}) \in \underline{V}_h \times \widehat{X}_h$, let $\mathcal{H} : \underline{V}_h \times \widehat{X}_h \rightarrow \underline{V}_h \times \widehat{X}_h$ be such that, for any $(\underline{u}_h, \widehat{\psi}_h) \in \underline{V}_h \times \widehat{X}_h$,

$$\begin{aligned} ((\mathcal{H}(\underline{u}_h, \widehat{\psi}_h), (w_h, \widehat{\varphi}_h))) &:= \left(\frac{u_h - u_{L,\delta,h}^{n-1}}{\Delta t}, w_h \right)_{\Omega} + \nu (\nabla_{\approx} u_h, \nabla_x w_h)_{\Omega} - \langle f^n, w_h \rangle_{H_0^1(\Omega)} \\ &+ k (C(M \widehat{\psi}_h), \nabla_x w_h)_{\Omega} + \frac{1}{2} \left[((u_{L,\delta,h}^{n-1} \cdot \nabla_x) u_h, w_h)_{\Omega} - ((u_{L,\delta,h}^{n-1} \cdot \nabla_x) w_h, u_h)_{\Omega} \right] \\ &+ \left(M, \pi_h \left[\frac{\widehat{\psi}_h - \widehat{\psi}_{L,\delta,h}^{n-1}}{\Delta t} \widehat{\varphi}_h + \varepsilon \nabla_x \widehat{\psi}_h \cdot \nabla_x \widehat{\varphi}_h + \frac{1}{2\lambda} \nabla_q \widehat{\psi}_h \cdot \nabla_q \widehat{\varphi}_h \right] \right)_{\Omega \times D} \\ &- \left(M (\nabla_x u_h) q, \pi_h \left[\underline{\Xi}_{L,\delta}^q(\widehat{\psi}_h) \nabla_q \widehat{\varphi}_h \right] \right)_{\Omega \times D} - \left(M u_h, \pi_h \left[\underline{\Lambda}_{L,\delta}^x(\widehat{\psi}_h) \nabla_x \widehat{\varphi}_h \right] \right)_{\Omega \times D} \\ &\forall (w_h, \widehat{\varphi}_h) \in V_h \times \widehat{X}_h. \end{aligned} \quad (4.45)$$

We note that a solution $(\underline{u}_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n)$ to (4.39a), (4.39b), if it exists, corresponds to a zero of \mathcal{H} ; that is,

$$((\mathcal{H}(\underline{u}_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n), (w_h, \widehat{\varphi}_h))) = 0 \quad \forall (w_h, \widehat{\varphi}_h) \in V_h \times \widehat{X}_h. \quad (4.46)$$

On noting the construction of $\underline{\Lambda}_{\delta}^x$ and $\underline{\Xi}_{\delta}^q$, it is easily deduced that the mapping \mathcal{H} is continuous.

For any $(\underline{u}_h, \widehat{\psi}_h) \in \underline{V}_h \times \widehat{X}_h$, by choosing $(w_h, \widehat{\varphi}_h) = (\underline{u}_h, \pi_h[[\mathcal{F}_{\delta}^L]'(\widehat{\psi}_h)])$, we obtain analogously to (4.40), on noting (4.31a), (4.31b) and neglecting some nonnegative terms, that

$$\begin{aligned} ((\mathcal{H}(\underline{u}_h, \widehat{\psi}_h), (\underline{u}_h, \pi_h[[\mathcal{F}_{\delta}^L]'(\widehat{\psi}_h)]))) &\geq \frac{1}{\Delta t} \left[\frac{1}{2} \left(\|\underline{u}_h\|_{L^2(\Omega)}^2 - \|\underline{u}_{L,\delta,h}^{n-1}\|_{L^2(\Omega)}^2 \right) \right. \\ &\quad \left. + k (M, \pi_h[\mathcal{F}_{\delta}^L(\widehat{\psi}_h) - \mathcal{F}_{\delta}^L(\widehat{\psi}_{L,\delta,h}^{n-1})])_{\Omega \times D} \right] + \frac{\nu}{2} \|\nabla_x \underline{u}_h\|_{L^2(\Omega)}^2 - C \|f^n\|_{H^{-1}(\Omega)}^2. \end{aligned} \quad (4.47)$$

The rest of the proof follows exactly the argument in the proof of Theorem 4.2 in [8]. \square

In order to establish a stability result for our approximation $(P_{L,\delta}^{\Delta t,h})$, we need first to prove a number of auxiliary results. Applying Jensen's inequality, we have that, for all $\kappa_x \in \mathcal{T}_x^h$ with vertices $\{x_{i_j}^x\}_{j=0}^d$,

$$\begin{aligned} |[\pi_{h,\kappa_x}^x \widehat{\varphi}^x](x)|^2 &= \left| \sum_{j=0}^d \widehat{\varphi}^x(P_{i_j}^x) \chi_{i_j}^x(x) \right|^2 \leq \sum_{j=0}^d [\widehat{\varphi}^x(P_{i_j}^x)]^2 \chi_{i_j}^x(x) = [\pi_{h,\kappa_x}^x [(\widehat{\varphi}^x)^2]](x) \\ &\forall x \in \kappa_x, \quad \forall \widehat{\varphi}^x \in C(\overline{\kappa_x}), \end{aligned} \quad (4.48a)$$

where we have used (4.12a) and that $\chi_{i_j}^x$ are nonnegative, and $\sum_{j=0}^d \chi_{i_j}^x(x) = 1$ for all $x \in \kappa_x$. Similarly, we have for all $\kappa_x \in \mathcal{T}_x^h$, $\kappa_q \in \mathcal{T}_q^h$ that

$$|[\pi_{h,\kappa_q}^q \widehat{\varphi}^q](q)|^2 \leq [\pi_{h,\kappa_q}^q [(\widehat{\varphi}^q)^2]](q) \quad \forall q \in \kappa_q, \quad \forall \widehat{\varphi}^q \in C(\overline{\kappa_q}), \quad (4.48b)$$

$$|[\pi_{h,\kappa_x \times \kappa_q} \widehat{\varphi}](x, q)|^2 \leq [\pi_{h,\kappa_x \times \kappa_q} [\widehat{\varphi}^2]](x, q) \quad \forall (x, q) \in \kappa_x \times \kappa_q, \quad \forall \widehat{\varphi} \in C(\overline{\kappa_x \times \kappa_q}), \quad (4.48c)$$

$$|[\pi_{h,\kappa_x \times \kappa_q} \widehat{\varphi}](x, q)|^2 \leq [\pi_{h,\kappa_x \times \kappa_q} [|\widehat{\varphi}|^2]](x, q) \quad \forall (x, q) \in \kappa_x \times \kappa_q, \quad \forall \widehat{\varphi} \in [C(\overline{\kappa_x \times \kappa_q})]^d. \quad (4.48d)$$

In addition, for all $\kappa_x \in \mathcal{T}_x^h$, $\kappa_q \in \mathcal{T}_q^h$ and for all $\widehat{\varphi}, \widehat{\eta} \in C(\overline{\kappa_x \times \kappa_q})$, $\widehat{\varphi}, \widehat{\eta} \in [C(\overline{\kappa_x \times \kappa_q})]^d$ the following inequalities are easily deduced for any $\eta \in \mathbb{R}_{>0}$:

$$|[\pi_{h,\kappa_x \times \kappa_q} [\widehat{\varphi} \widehat{\eta}]](x, q)| \leq \frac{1}{2} [\pi_{h,\kappa_x \times \kappa_q} [\eta \widehat{\varphi}^2 + \eta^{-1} \widehat{\eta}^2]](x, q) \quad \forall (x, q) \in \kappa_x \times \kappa_q, \quad (4.49a)$$

$$\text{and} \quad |[\pi_{h,\kappa_x \times \kappa_q} [\widehat{\varphi} \cdot \widehat{\eta}]](x, q)| \leq \frac{1}{2} [\pi_{h,\kappa_x \times \kappa_q} [\eta |\widehat{\varphi}|^2 + \eta^{-1} |\widehat{\eta}|^2]](x, q) \quad \forall (x, q) \in \kappa_x \times \kappa_q. \quad (4.49b)$$

The following interpolation stability results are easily established, using the mean value theorem, for all $\kappa_x \in \mathcal{T}_h^x$ and $\kappa_q \in \mathcal{T}_h^q$, respectively:

$$\|\nabla_x \pi_{h,\kappa_x}^x \widehat{\varphi}^x\|_{L^\infty(\kappa_x)} \leq d \|\nabla_x \widehat{\varphi}^x\|_{L^\infty(\kappa_x)} \quad \forall \widehat{\varphi}^x \in W^{1,\infty}(\kappa_x), \tag{4.50a}$$

$$\|\nabla_q \pi_{h,\kappa_q}^q \widehat{\varphi}^q\|_{L^\infty(\kappa_q)} \leq d \|\nabla_q \widehat{\varphi}^q\|_{L^\infty(\kappa_q)} \quad \forall \widehat{\varphi}^q \in W^{1,\infty}(\kappa_q); \tag{4.50b}$$

furthermore,

$$\begin{aligned} \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2}{\partial x_i \partial q_j} \pi_{h,\kappa_x \times \kappa_q} \widehat{\varphi} \right\|_{L^\infty(\kappa_x \times \kappa_q)} &= \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial}{\partial x_i} \pi_{h,\kappa_x}^x \left[\frac{\partial}{\partial q_j} \pi_{h,\kappa_q}^q \widehat{\varphi} \right] \right\|_{L^\infty(\kappa_x \times \kappa_q)} \\ &\leq \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2}{\partial x_i \partial q_j} \widehat{\varphi} \right\|_{L^\infty(\kappa_x \times \kappa_q)} \quad \forall \widehat{\varphi} \in W^{2,\infty}(\kappa_x \times \kappa_q). \end{aligned} \tag{4.51}$$

We recall the following well-known approximation results for all $\kappa_x \in \mathcal{T}_h^x$ and $\kappa_q \in \mathcal{T}_h^q$: for $m = 0$ or 1 and $s = 1$ or 2 , we have that

$$\|(I - \pi_{h,\kappa_x}^x) \widehat{\varphi}^x\|_{W^{m,\infty}(\kappa_x)} \leq C h_x^{s-m} |\widehat{\varphi}^x|_{W^{s,\infty}(\kappa_x)} \quad \forall \widehat{\varphi}^x \in W^{s,\infty}(\kappa_x), \tag{4.52a}$$

$$\|(I - \pi_{h,\kappa_q}^q) \widehat{\varphi}^q\|_{W^{m,\infty}(\kappa_q)} \leq C h_q^{s-m} |\widehat{\varphi}^q|_{W^{s,\infty}(\kappa_q)} \quad \forall \widehat{\varphi}^q \in W^{s,\infty}(\kappa_q). \tag{4.52b}$$

Similarly, since $I - \pi_{h,\kappa_x \times \kappa_q} \equiv (I - \pi_{h,\kappa_x}^x) + (I - \pi_{h,\kappa_q}^q) \pi_{h,\kappa_x}^x$, it follows from (4.52a), (4.52b) that

$$\|(I - \pi_{h,\kappa_x \times \kappa_q}) \widehat{\varphi}\|_{W^{m,\infty}(\kappa_x \times \kappa_q)} \leq C (h_x^{s-m} + h_q^{s-m}) |\widehat{\varphi}|_{W^{s,\infty}(\kappa_x \times \kappa_q)} \quad \forall \widehat{\varphi} \in W^{s,\infty}(\kappa_x \times \kappa_q). \tag{4.53}$$

Hence, on noting (3.6) and (4.53), for all $\widehat{\varphi} \in \widehat{X}$, there exists a sequence $\{\widehat{\varphi}_h\}_{h>0}$, with $\widehat{\varphi}_h \in \widehat{X}_h$, such that

$$\lim_{h \rightarrow 0_+} \|\widehat{\varphi} - \widehat{\varphi}_h\|_{\widehat{X}} = 0. \tag{4.54}$$

We require the following inverse bounds for all $\widehat{\varphi}_h^x \in \mathbb{P}_1^x$, $\widehat{\varphi}_h^q \in \mathbb{P}_1^q$ and for all $\kappa_x^* \subset \kappa_x \in \mathcal{T}_h^x$, $\kappa_q^* \subset \kappa_q \in \mathcal{T}_h^q$ with $\underline{m}(\kappa_x) \leq C \underline{m}(\kappa_x^*)$, $\underline{m}(\kappa_q) \leq C \underline{m}(\kappa_q^*)$:

$$\|\widehat{\varphi}_h^x\|_{L^\infty(\kappa_x)}^2 \leq C [\underline{m}(\kappa_x^*)]^{-1} \int_{\kappa_x^*} |\widehat{\varphi}_h^x|^2 dx, \tag{4.55a}$$

$$\|\widehat{\varphi}_h^q\|_{L^\infty(\kappa_q)}^2 \leq C [\underline{m}(\kappa_q^*)]^{-1} \int_{\kappa_q^*} |\widehat{\varphi}_h^q|^2 dq, \tag{4.55b}$$

$$\int_{\kappa_x^*} |\nabla_x \widehat{\varphi}_h^x|^2 dx \leq C h_x^{-2} \int_{\kappa_x^*} |\widehat{\varphi}_h^x|^2 dx \leq C h_x^{-2} \int_{\kappa_x^*} \pi_{h,\kappa_x}^x [|\widehat{\varphi}_h^x|^2] dx, \tag{4.55c}$$

$$\int_{\kappa_q^*} |\nabla_q \widehat{\varphi}_h^q|^2 dq \leq C h_q^{-2} \int_{\kappa_q^*} |\widehat{\varphi}_h^q|^2 dq \leq C h_q^{-2} \int_{\kappa_q^*} \pi_{h,\kappa_q}^q [|\widehat{\varphi}_h^q|^2] dq. \tag{4.55d}$$

The bounds (4.55a), (4.55b) are standard inverse bounds in the case $\kappa_x^* \equiv \kappa_x$ and $\kappa_q^* \equiv \kappa_q$. The results are easily generalized to $\kappa_x^* \subset \kappa_x$ and $\kappa_q^* \subset \kappa_q$ under the stated conditions, since then $\|\widehat{\varphi}_h^x\|_{L^\infty(\kappa_x)} \leq C \|\widehat{\varphi}_h^x\|_{L^\infty(\kappa_x^*)}$ and $\|\widehat{\varphi}_h^q\|_{L^\infty(\kappa_q)} \leq C \|\widehat{\varphi}_h^q\|_{L^\infty(\kappa_q^*)}$. The first inequalities in (4.55c), (4.55d) then follow immediately from (4.55a), (4.55b), respectively; whereas the second inequalities in (4.55c), (4.55d) follow from (4.48a), (4.48b), respectively. The following bounds follow immediately from (4.55a), (4.55b) under the same stated conditions:

$$\int_{\kappa_x^*} \pi_{h,\kappa_x}^x [|\widehat{\varphi}_h^x|^2] dx \leq C \int_{\kappa_x^*} |\widehat{\varphi}_h^x|^2 dx \quad \text{and} \quad \int_{\kappa_q^*} \pi_{h,\kappa_q}^q [|\widehat{\varphi}_h^q|^2] dq \leq C \int_{\kappa_q^*} |\widehat{\varphi}_h^q|^2 dq. \tag{4.56}$$

In addition, we require the following weighted bounds.

Lemma 4.7. For all $\kappa_q \in \mathcal{T}_q^h$ and for all $\widehat{\varphi}_h^q \in \mathbb{P}_1^q$ we have that

$$\int_{\kappa_q} M |\nabla_q \widehat{\varphi}_h^q|^2 dq \leq C h_q^{-2} \int_{\kappa_q} M |\widehat{\varphi}_h^q|^2 dq \leq C h_q^{-2} \int_{\kappa_q} M \pi_{h,\kappa_q}^q [|\widehat{\varphi}_h^q|^2] dq, \quad (4.57a)$$

$$\int_{\kappa_q} M \pi_{h,\kappa_q}^q [|\widehat{\varphi}_h^q|^2] dq \leq \left(\int_{\kappa_q} M dq \right) \|\widehat{\varphi}_h^q\|_{L^\infty(\kappa_q)}^2 \leq C \int_{\kappa_q} M |\widehat{\varphi}_h^q|^2 dq. \quad (4.57b)$$

Proof. See the proof of Lemma 4.3 in [8]. \square

Lemma 4.8. For all $\kappa_x \in \mathcal{T}_h^x$, $\kappa_q \in \mathcal{T}_h^q$ and for all $\widehat{\eta}_h, \widehat{\varphi}_h \in \widehat{X}_h$ we have that

$$\begin{aligned} & \left| \int_{\kappa_x \times \kappa_q} M (I - \pi_{h,\kappa_x \times \kappa_q}) [\nabla_q \widehat{\eta}_h \cdot \nabla_q \widehat{\varphi}_h] dq dx \right| \\ & \leq C h_x \left(\int_{\kappa_x \times \kappa_q} M |\nabla_q \widehat{\eta}_h|^2 dq dx \right)^{\frac{1}{2}} \left(\sum_{i=1}^d \sum_{j=1}^d \int_{\kappa_x \times \kappa_q} M \left| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial x_j} \right|^2 dq dx \right)^{\frac{1}{2}}, \end{aligned} \quad (4.58a)$$

$$\begin{aligned} & \left| \int_{\kappa_x \times \kappa_q} M (I - \pi_{h,\kappa_x \times \kappa_q}) [\nabla_x \widehat{\eta}_h \cdot \nabla_x \widehat{\varphi}_h] dq dx \right| \\ & \leq C h_q \left(\int_{\kappa_x \times \kappa_q} M |\nabla_x \widehat{\eta}_h|^2 dq dx \right)^{\frac{1}{2}} \left(\sum_{i=1}^d \sum_{j=1}^d \int_{\kappa_x \times \kappa_q} M \left| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial x_j} \right|^2 dq dx \right)^{\frac{1}{2}}, \end{aligned} \quad (4.58b)$$

and

$$\begin{aligned} \left| \int_{\kappa_x \times \kappa_q} M (I - \pi_{h,\kappa_x \times \kappa_q}) [\widehat{\eta}_h \widehat{\varphi}_h] dq dx \right| & \leq C h_x^2 \left(\int_{\kappa_x \times \kappa_q} M |\nabla_x \widehat{\eta}_h|^2 dq dx \right)^{\frac{1}{2}} \left(\int_{\kappa_x \times \kappa_q} M |\nabla_x \widehat{\varphi}_h|^2 dq dx \right)^{\frac{1}{2}} \\ & \quad + C h_q^2 \left(\int_{\kappa_x \times \kappa_q} M |\nabla_q \widehat{\eta}_h|^2 dq dx \right)^{\frac{1}{2}} \left(\int_{\kappa_x \times \kappa_q} M |\nabla_q \widehat{\varphi}_h|^2 dq dx \right)^{\frac{1}{2}}. \end{aligned} \quad (4.58c)$$

Proof. See the proof of Lemma 4.5 in [8]. \square

Lemma 4.9. For all $\kappa_x \in \mathcal{T}_h^x$, $\kappa_q \in \mathcal{T}_h^q$ and for all $\widehat{\eta}_h, \widehat{\varphi}_h \in \widehat{X}_h$ we have that

$$\int_{\kappa_x \times \kappa_q} M \left| (I - \pi_{h,\kappa_x \times \kappa_q}) [\Xi_{L,\delta}^q(\widehat{\eta}_h) \nabla_q \widehat{\varphi}_h] \right|^2 dq dx \leq C(L) h_x^2 \sum_{i=1}^d \sum_{j=1}^d \int_{\kappa_x \times \kappa_q} M \left| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial x_j} \right|^2 dq dx, \quad (4.59a)$$

$$\begin{aligned} & \int_{\kappa_x \times \kappa_q} M \left| (I - \pi_{h,\kappa_x \times \kappa_q}) [A_{L,\delta}^x(\widehat{\eta}_h) \nabla_x \widehat{\varphi}_h] \right|^2 dq dx \\ & \leq C h_q^2 \left(\int_{\kappa_x \times \kappa_q} M |\widehat{\eta}_h|^2 dq dx \right) \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial x_j} \right\|_{L^\infty(\kappa_x \times \kappa_q)}^2. \end{aligned} \quad (4.59b)$$

Proof. The bound (4.59a) is proved in Lemma 4.6 in [8]. We adapt the proof there to prove (4.59b). As $A_{L,\delta}^x(\widehat{\eta}_h) \in [\mathbb{P}_1^q]^{d \times d}$ and $\nabla_x \widehat{\varphi}_h \in [\mathbb{P}_1^q]^d$ on $\kappa_x \times \kappa_q$, it follows from (4.52b), a standard inverse bound on κ_q , (4.29) and (4.57b)

that

$$\begin{aligned}
 & \int_{\kappa_x \times \kappa_q} M \left| (I - \pi_{h, \kappa_x \times \kappa_q}) [A_{L, \delta}^x(\widehat{\eta}_h)] \nabla_x \widehat{\varphi}_h \right|_{\approx}^2 dq dx \\
 & \leq C h_q^4 \left(\int_{\kappa_x \times \kappa_q} M dq dx \right) \left(\sum_{i=1}^d \sum_{j=1}^d \left\| \nabla_q [A_{L, \delta}^x(\widehat{\eta}_h)]_{ij} \right\|_{L^\infty(\kappa_q)}^2 \right) \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial q_j} \right\|_{L^\infty(\kappa_q)}^2 \\
 & \leq C h_q^2 \left(\int_{\kappa_x \times \kappa_q} M dq dx \right) \left(\sum_{i=1}^d \sum_{j=1}^d \left\| [A_{L, \delta}^x(\widehat{\eta}_h)]_{ij} \right\|_{L^\infty(\kappa_q)}^2 \right) \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial q_j} \right\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \\
 & \leq C h_q^2 \left(\int_{\kappa_x \times \kappa_q} M dq dx \right) \|\widehat{\eta}_h\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial q_j} \right\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \\
 & \leq C h_q^2 \underline{m}(\kappa_x) \left\| \int_{\kappa_q} M(\widehat{\eta}_h(x, q))^2 dq \right\|_{L^\infty(\kappa_x)} \sum_{i=1}^d \sum_{j=1}^d \left\| \frac{\partial^2 \widehat{\varphi}_h}{\partial x_i \partial q_j} \right\|_{L^\infty(\kappa_x \times \kappa_q)}^2. \tag{4.60}
 \end{aligned}$$

Hence, the desired result (4.59b) follows from (4.60) on applying a standard inverse bound over κ_x . □

We are now in a position to prove the following stability result for $(P_{L, \delta}^{\Delta t, h})$.

Lemma 4.10. *A solution $\{(u_{L, \delta, h}^n, \widehat{\psi}_{L, \delta, h}^n)\}_{n=1}^N$ of $(P_{L, \delta}^{\Delta t, h})$ satisfies the following stability bounds:*

$$\begin{aligned}
 & \max_{n=1, \dots, N} \|u_{L, \delta, h}^n\|_{L^2(\Omega)}^2 + \max_{n=1, \dots, N} (M, \pi_h [\mathcal{F}_\delta^L(\widehat{\psi}_{L, \delta, h}^n)])_{\Omega \times D} + \sum_{n=1}^N \Delta t \|\nabla_x u_{L, \delta, h}^n\|_{L^2(\Omega)}^2 \\
 & + \sum_{n=1}^N \Delta t \left((M, \pi_h [\nabla_x \widehat{\psi}_{L, \delta, h}^n \cdot \nabla_x (\pi_h [[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L, \delta, h}^n)]) + \nabla_q \widehat{\psi}_{L, \delta, h}^n \cdot \nabla_q (\pi_h [[\mathcal{F}_\delta^L]'(\widehat{\psi}_{L, \delta, h}^n)])])_{\Omega \times D} \right) \\
 & \leq C \left[\|u_{L, \delta, h}^0\|_{L^2(\Omega)}^2 + (M, \pi_h [\mathcal{F}_\delta^L(\widehat{\psi}_{L, \delta, h}^0)])_{\Omega \times D} + \sum_{n=1}^n \Delta t \|f^n\|_{H^{-1}(\Omega)}^2 \right] \leq C(L), \tag{4.61a}
 \end{aligned}$$

and

$$\begin{aligned}
 & \max_{n=1, \dots, N} (M, |\widehat{\psi}_{L, \delta, h}^n|^2)_{\Omega \times D} + \delta^{-1} \max_{n=1, \dots, N} (M, \pi_h [|\widehat{\psi}_{L, \delta, h}^n|_-^2])_{\Omega \times D} + \sum_{n=1}^N \Delta t (M, |\nabla_q \widehat{\psi}_{L, \delta, h}^n|^2 + |\nabla_x \widehat{\psi}_{L, \delta, h}^n|^2)_{\Omega \times D} \\
 & + \max_{n=1, \dots, N} \left[\int_{\Omega} |C(M \widehat{\psi}_{L, \delta, h}^n)|^2 dx \right] \leq C(L). \tag{4.61b}
 \end{aligned}$$

Proof. Summing (4.40) from $n = 1, \dots, m$, for $m = 1, \dots, N$, yields the desired result (4.61a) on noting (4.31a), (4.31b), (4.38), (2.5) and (3.16a).

The first and second bounds in (4.61b) follow immediately from the second bound in (4.61a), (2.11) and (4.48c). The third bound in (4.61b) follows directly from the fourth bound in (4.61a), Corollary 4.2 on taking $\widehat{\varphi}_h = \widehat{\psi}_{L, \delta, h}^n$ and $g = [\mathcal{F}_\delta^L]'$ in (4.36a), (4.36b), and noting that this g is strictly monotonic increasing on \mathbb{R} and its inverse map g^{-1} is Lipschitz continuous on \mathbb{R} , with Lipschitz constant L , and (4.48d). Finally, the fourth bound in (4.61b) follows immediately from the first bound in (4.61b) and (3.8). □

Before proving a convergence result for $(P_{L, \delta}^{\Delta t, h})$, we need the following lemma.

Lemma 4.11. For all $\kappa_x \in \mathcal{T}_h^x$, $\kappa_q \in \mathcal{T}_h^q$ and for all $\widehat{\varphi}_h \in \widehat{X}_h$ we have that

$$\int_{\kappa_x \times \kappa_q} M |\Xi_{L,\delta}^q(\widehat{\varphi}_h) - \beta^L(\widehat{\varphi}_h) I|^2 dq dx \leq C \left(\delta^2 + h_q^2 \int_{\kappa_x \times \kappa_q} M |\nabla_q \widehat{\varphi}_h|^2 dq dx + \int_{\kappa_x \times \kappa_q} M \pi_{h,\kappa_x \times \kappa_q} [[\widehat{\varphi}_h]_-]^2 dq dx \right), \quad (4.62a)$$

$$\int_{\kappa_x \times \kappa_q} M |\Lambda_{L,\delta}^x(\widehat{\varphi}_h) - \widehat{\varphi}_h I|^2 dq dx \leq C h_x^2 \int_{\kappa_x \times \kappa_q} M |\nabla_x \widehat{\varphi}_h|^2 dq dx. \quad (4.62b)$$

Proof. The bound (4.62a) is proved in Lemma 4.9 in [8]. We adapt the proof there to prove (4.62b). We have from the $\widetilde{\Lambda}_{L,\delta}^x$ version of (4.19), (4.28), (4.25), (4.26) and (4.57b) that

$$\begin{aligned} \int_{\kappa_x \times \kappa_q} M |\Lambda_{L,\delta}^x(\widehat{\varphi}_h) - \widehat{\varphi}_h I|^2 dq dx &\leq C \left(\int_{\kappa_x \times \kappa_q} M dq dx \right) \|\widetilde{\Lambda}_{L,\delta}^x(\widehat{\varphi}_h) - \widehat{\varphi}_h I\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \\ &\leq C h_x^2 \left(\int_{\kappa_x \times \kappa_q} M dq dx \right) \|\nabla_x \widehat{\varphi}_h\|_{L^\infty(\kappa_x \times \kappa_q)}^2 \\ &\leq C h_x^2 \int_{\kappa_x \times \kappa_q} M |\nabla_x \widehat{\varphi}_h|^2 dq dx, \end{aligned} \quad (4.63)$$

and hence the desired result (4.62b). \square

We are now in a position to prove the following convergence result for $(P_{L,\delta}^{\Delta t,h})$.

Theorem 4.12. Firstly, the initial data of $(P_{L,\delta}^{\Delta t,h})$ are such that, as $\delta, h \rightarrow 0_+$,

$$\widetilde{u}_{L,\delta,h}^0 \rightarrow \widetilde{u}^0 = \widetilde{u}_L^0 \quad \text{strongly in } \widetilde{L}^2(\Omega), \quad (4.64a)$$

$$M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^0 \rightarrow M^{\frac{1}{2}} \widehat{\psi}^0 = M^{\frac{1}{2}} \widehat{\psi}_L^0 \quad \text{strongly in } L^2(\Omega \times D). \quad (4.64b)$$

Secondly, there exists a subsequence (not indicated) of $\{(u_{L,\delta,h}^n, \widehat{\psi}_{L,\delta,h}^n)\}_{\delta>0,h>0}$, and functions $\underline{u}_L^n \in \mathcal{V}$ and $\widehat{\psi}_L^n \in \widehat{X} \cap \widehat{Z}_2$, $n = 1, \dots, N$, such that, as $\delta, h \rightarrow 0_+$,

$$\widetilde{u}_{L,\delta,h}^n \rightarrow \widetilde{u}_L^n \quad \text{weakly in } \widetilde{H}^1(\Omega), \quad (4.65a)$$

$$\widetilde{u}_{L,\delta,h}^n \rightarrow \widetilde{u}_L^n \quad \text{strongly in } \widetilde{L}^r(\Omega), \quad (4.65b)$$

and

$$M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^n \rightarrow M^{\frac{1}{2}} \widehat{\psi}_L^n \quad \text{weakly in } L^2(\Omega \times D), \quad (4.66a)$$

$$M^{\frac{1}{2}} \nabla_q \widehat{\psi}_{L,\delta,h}^n \rightarrow M^{\frac{1}{2}} \nabla_q \widehat{\psi}_L^n \quad \text{weakly in } L^2(\Omega \times D), \quad (4.66b)$$

$$M^{\frac{1}{2}} \nabla_x \widehat{\psi}_{L,\delta,h}^n \rightarrow M^{\frac{1}{2}} \nabla_x \widehat{\psi}_L^n \quad \text{weakly in } L^2(\Omega \times D), \quad (4.66c)$$

$$M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^n \rightarrow M^{\frac{1}{2}} \widehat{\psi}_L^n \quad \text{strongly in } L^2(\Omega \times D), \quad (4.66d)$$

$$M^{\frac{1}{2}} \Xi_{L,\delta}^q(\widehat{\psi}_{L,\delta,h}^n) \rightarrow M^{\frac{1}{2}} \beta^L(\widehat{\psi}_L^n) I \quad \text{strongly in } L^2(\Omega \times D), \quad (4.66e)$$

$$M^{\frac{1}{2}} \Lambda_{L,\delta}^x(\widehat{\psi}_{L,\delta,h}^n) \rightarrow M^{\frac{1}{2}} \widehat{\psi}_L^n I \quad \text{strongly in } L^2(\Omega \times D), \quad (4.66f)$$

$$C(M \widehat{\psi}_{L,\delta,h}^n) \rightarrow C(M \widehat{\psi}_L^n) \quad \text{strongly in } L^2(\Omega); \quad (4.66g)$$

where $r \in [1, \infty)$ if $d = 2$ and $r \in [1, 6)$ if $d = 3$.

Furthermore, $\{(u_L^n, \widehat{\psi}_L^n)\}_{n=1}^N$ solves $(P_L^{\Delta t})$, (3.14a), (3.14b).

Proof. It follows from (4.38) that a subsequence of $\{u_{L,\delta,h}^0\}_{\delta>0,h>0}$ converges strongly in $L^2(\Omega)$, weakly in $H^1(\Omega)$, to some element $u^* \in H^1(\Omega)$, as $\delta, h \rightarrow 0_+$. It follows from passing to the limit $\delta, h \rightarrow 0_+$ in (4.37a), and noting (4.5) and (3.9) that $u^* = u^0$. In addition, the whole sequence $\{u_{L,\delta,h}^0\}_{\delta>0,h>0}$ converges as u^0 is the unique solution of (3.9). Hence we have the desired result (4.64a).

The bounds (4.38) and (4.48c), (4.48d) yield that

$$\int_{\Omega \times D} M \left[|\widehat{\psi}_{L,\delta,h}^0|^2 + \Delta t \left(|\nabla_x \widehat{\psi}_{L,\delta,h}^0|^2 + |\nabla_q \widehat{\psi}_{L,\delta,h}^0|^2 \right) \right] dq dx \leq C(L). \tag{4.67}$$

Therefore there exists a subsequence of $\{M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^0\}_{\delta>0,h>0}$ such that $M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^0$ converges weakly in $L^2(\Omega \times D)$ to some element $M^{\frac{1}{2}} \widehat{\psi}^* \in L^2(\Omega \times D)$, and $M^{\frac{1}{2}} \nabla_q \widehat{\psi}_{L,\delta,h}^0, M^{\frac{1}{2}} \nabla_x \widehat{\psi}_{L,\delta,h}^0$ converge weakly in $\underline{L}^2(\Omega \times D)$ to some elements $\widehat{g}_1^*, \widehat{g}_2^* \in \underline{L}^2(\Omega \times D)$, respectively, as $\delta, h \rightarrow 0_+$. To show that $\widehat{g}_1^* = M^{\frac{1}{2}} \nabla_q \widehat{\psi}^*$ and $\widehat{g}_2^* = M^{\frac{1}{2}} \nabla_x \widehat{\psi}^*$, see the proof of Lemma 3.3 in [7]. In addition, the compact embedding result (3.7b) yields that this subsequence of $\{M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^0\}_{\delta>0,h>0}$ is such that $M^{\frac{1}{2}} \widehat{\psi}_{L,\delta,h}^0$ converges strongly in $L^2(\Omega \times D)$ to $\widehat{\psi}^*$ as $\delta, h \rightarrow 0_+$. We can then pass to the limit $\delta, h \rightarrow 0_+$ in (4.37b) with $\widehat{\varphi}_h = \pi_h \widehat{\varphi}$ for any function $\widehat{\varphi} \in C^\infty(\overline{\Omega \times D})$ on noting (4.58a)–(4.58c), (4.50a), (4.50b), (4.51), (3.11) and (3.6) to obtain that $\widehat{\psi}^* = \widehat{\psi}^0$. Once again the whole sequence converges as $\widehat{\psi}^0$ is the unique solution of (3.11). Hence we have the desired result (4.64b).

The result (4.65a) follows immediately from the bound (4.61a). The denseness of $\bigcup_{h>0} R_h$ in $L^2(\Omega)$ and (4.3c) yield that $u_L^n \in \mathcal{V}$. The strong convergence result (4.65b) for $u_{L,\delta,h}^n$ follows immediately on noting that $\mathcal{V} \subset H_0^1(\Omega)$ is compactly embedded in $\underline{L}^r(\Omega)$ for the stated values of r .

The result (4.66a) follows directly from the first bound in (4.61b). It follows immediately from the bound on the second term on the left-hand side of (4.61b) that (4.66b) holds for some limit $g \in \underline{L}^2(\Omega \times D)$. To show that $g = M^{\frac{1}{2}} \nabla_q \widehat{\psi}_L^n$, once again see the proof of Lemma 3.3 in [7]. A similar argument proves (4.66c). The strong convergence result (4.66d) for $\widehat{\psi}_{L,\delta,h}^{\Delta t}$ follows immediately from (3.7b). The desired results (4.66e), (4.66f) follow directly from (4.62a), (4.62b), the second and third bounds in (4.61b) and (4.66d). The desired result (4.66g) follows immediately from (4.66d), (1.8) and (3.8). Finally, the nonnegativity of $\widehat{\psi}_L^n$ follows from (4.66d) and the second bound in (4.61b).

It remains to prove that $\{(u_L^n, \widehat{\psi}_L^n)\}_{n=1}^N$ solves $(P_L^{\Delta t})$, (3.14a), (3.14b). It follows from (4.5), (4.64a), (4.65a), (4.65b), (4.66g) and (4.6) that we may pass to the limit $\delta, h \rightarrow 0_+$ in (4.39a) to obtain that $\{(u_L^n, \underline{C}(M \widehat{\psi}_L^n))\}_{n=1}^N$, with $u_L^n \in \mathcal{V}$ and $\underline{C}(M \widehat{\psi}_L^n) \in \underline{L}^2(\Omega)$, satisfy (3.14a).

It follows from (4.64b), (4.66a)–(4.66f), (4.65a), (4.65b), (4.58a)–(4.58c), (4.59a), (4.59b), (4.61b), (4.50a), (4.50b), (4.51) and (4.52a), (4.52b) that we may pass to the limit $\delta, h \rightarrow 0_+$ in (4.39b) with $\widehat{\varphi}_h = \pi_h \widehat{\varphi}$ to obtain equation (3.14b) for any function $\widehat{\varphi} \in C^\infty(\overline{\Omega \times D})$. The desired result (3.14b) then follows from recalling (3.6). \square

Therefore combining Theorems 4.12 and 3.1 we obtain the desired result that a (sub)sequence of our finite element approximation $(P_{L,\delta}^{\Delta t,h})$ converges to a weak solution of (P) as first $h, \delta \rightarrow 0_+$ and then $L \rightarrow \infty$, with $\Delta t = o(L^{-1})$ under our stated assumptions (A1) and (A2).

5. CONCLUDING REMARKS

The aim of this paper has been to develop a fully-discrete, convergent numerical method for the approximate solution of a general class of Navier–Stokes–Fokker–Planck systems, in the case of finitely extensible nonlinear elastic spring potentials, under minimal regularity hypotheses on the data. The numerical solutions defined by the method satisfy an energy inequality analogous to the one obeyed by weak solutions to the Navier–Stokes–Fokker–Planck system. The dumbbell model considered in the paper is a special case of a bead-spring chain model involving $K \geq 1$ linearly linked springs. As we have noted in Remark 4.5, in the general case of $K \geq 1$

the last term on the left-hand side of the first inequality in (4.40) term becomes (4.44). Unfortunately, we do not know at the moment how to guarantee the nonnegativity of this term, except when $K = 1$ (dumbbell model), or if $K \geq 1$ and the symmetric positive definite Rouse matrix A is *diagonal*, corresponding to the case of K decoupled dumbbells, which is why we have been forced to confine ourselves here to the dumbbell model ($K = 1$). If a family of finite element triangulations of $D = D_1 \times \cdots \times D_K$ could be identified over which the term (4.44) remains nonnegative for $K > 1$, then the convergence of a fully-discrete method analogous to the one considered here in the case of $K = 1$ could be proved for all $K \geq 1$ in an identical manner.

The Galerkin approximation (4.39b) is posed over the $2d$ -dimensional spatial domain $\Omega \times D$, with $d = 2$ or $d = 3$. A possible practical approach to its implementation might be based on operator-splitting, following the computational strategy advocated in the papers [19, 20], for example; see also [21]. We note however that the schemes that were analyzed in [19–21] were shown to converge for the Fokker–Planck equation considered in isolation, *i.e.* with the velocity field \underline{u} given and assumed to be sufficiently smooth. It is not known if those schemes would still converge if the Fokker–Planck equation were coupled to the Navier–Stokes system, and only the minimal regularity hypotheses on the data stated in (3.3), which guarantee the existence of weak solutions to the coupled system, were assumed. In contrast, the numerical approximations generated by the method proposed here have been proved to converge to a weak solution of the coupled Navier–Stokes–Fokker–Planck system under those minimal regularity assumptions on the data.

APPENDIX A. THE PROOFS OF (3.13a), (3.13b)

The arguments in this section follow the proofs in Barrett and Süli [7], Section 6.1. Given any $L > 1$, $\Delta t \in (0, 1)$ and an initial datum $\widehat{\psi}_0$ satisfying the conditions in (3.3), the existence of a unique solution $\widehat{\psi}^0 = \widehat{\psi}^0(L, \Delta t) \in H_M^1(\Omega \times D)$ to (3.11) follows directly from the Lax–Milgram theorem. We shall show that $\widehat{\psi}^0$ satisfies (3.13a), (3.13b). We begin by establishing the properties listed under (3.13a).

On taking $\widehat{\varphi} = [\widehat{\psi}^0]_- \in H_M^1(\Omega \times D)$ in (3.11) and noting that $\beta^L(\widehat{\psi}_0) \geq 0$ a.e. on $\Omega \times D$, it follows that

$$\int_{\Omega \times D} M \left[|[\widehat{\psi}^0]_-|^2 + \Delta t \left(|\nabla_{\underline{x}} [\widehat{\psi}^0]_-|^2 + |\nabla_{\underline{q}} [\widehat{\psi}^0]_-|^2 \right) \right] d\underline{q} d\underline{x} \leq 0, \quad (\text{A.1})$$

whereby $[\widehat{\psi}^0]_- = 0$ a.e. on $\Omega \times D$. Thus we deduce that $\widehat{\psi}^0 \geq 0$ a.e. on $\Omega \times D$.

We introduce also the following closed linear subspace of $\widehat{X} = H_M^1(\Omega \times D)$:

$$H^1(\Omega) \otimes 1(D) := \left\{ \widehat{\varphi} \in H_M^1(\Omega \times D) : \widehat{\varphi}(\cdot, \underline{q}^*) = \widehat{\varphi}(\cdot, \underline{q}^{**}) \quad \forall \underline{q}^*, \underline{q}^{**} \in D \right\}. \quad (\text{A.2})$$

Next we define

$$\gamma(\underline{x}) := \int_D M(\underline{q}) \widehat{\psi}^0(\underline{x}, \underline{q}) d\underline{q} \quad \text{and} \quad \zeta(\underline{x}) := \int_D M(\underline{q}) \beta^L(\widehat{\psi}_0(\underline{x}, \underline{q})) d\underline{q},$$

and we take $\widehat{\varphi} = \phi \in H^1(\Omega) \otimes 1(D)$ in (3.11). Hence,

$$\int_{\Omega} \gamma \phi d\underline{x} + \Delta t \int_{\Omega} \nabla_{\underline{x}} \gamma \cdot \nabla_{\underline{x}} \phi d\underline{x} = \int_{\Omega} \zeta \phi d\underline{x} \quad \forall \phi \in H^1(\Omega), \quad (\text{A.3})$$

and therefore, on subtracting $\int_{\Omega} \phi d\underline{x}$ from both sides of (A.3) and rearranging, also

$$\int_{\Omega} (1 - \gamma) \phi d\underline{x} + \Delta t \int_{\Omega} \nabla_{\underline{x}} (1 - \gamma) \cdot \nabla_{\underline{x}} \phi d\underline{x} = \int_{\Omega} (1 - \zeta) \phi d\underline{x} \quad \forall \phi \in H^1(\Omega). \quad (\text{A.4})$$

Since, thanks to (3.3) and (1.14), we have that $0 \leq \beta^L(\widehat{\psi}_0(\underline{x}, \underline{q})) \leq \widehat{\psi}_0(\underline{x}, \underline{q})$ for a.e. $(\underline{x}, \underline{q}) \in \Omega \times D$, it follows that $\zeta(\underline{x}) \geq 0$ and $1 - \zeta(\underline{x}) \geq 0$ for a.e. $\underline{x} \in \Omega$. Hence, on taking $\phi = [\gamma]_- \in H^1(\Omega)$ in (A.3) and $\phi = [1 - \gamma]_- \in H^1(\Omega)$

in (A.4), respectively, we deduce that $[\gamma(\underline{x})]_- = 0$ and $[1 - \gamma(\underline{x})]_- = 0$ for a.e. $x \in \Omega$. Consequently, $\gamma(x) \in [0, 1]$ for a.e. $x \in \Omega$, and therefore $\widehat{\psi}^0 \in \widehat{Z}_2 \subset \widehat{Z}_1$, as has been claimed in (3.13a).

Next, on taking $\widehat{\varphi} = \mathcal{F}'(\widehat{\psi}^0 + \alpha)$ in (3.11) with $\alpha > 0$, and then passing to the limit $\alpha \rightarrow 0_+$, we deduce, in the same manner as in the proof of inequality (6.11) in [7], that

$$\int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}^0) \, d\widetilde{q} \, d\widetilde{x} + 4 \Delta t \int_{\Omega \times D} M \left[|\nabla_x \sqrt{\widehat{\psi}^0}|^2 + |\nabla_q \sqrt{\widehat{\psi}^0}|^2 \right] \, d\widetilde{q} \, d\widetilde{x} \leq \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}_0) \, d\widetilde{q} \, d\widetilde{x}. \tag{A.5}$$

That completes the proof of (3.13a). It remains to prove (3.13b).

Noting that (3.11) holds with $\widehat{\psi}^0$ and $\beta^L(\widehat{\psi}_0)$ replaced by $L - \widehat{\psi}^0$ and $L - \beta^L(\widehat{\psi}_0)$, respectively, and choosing $\widehat{\varphi} = [L - \widehat{\psi}^0]_-$ yields, similarly to (A.1), that $[L - \widehat{\psi}^0]_- = 0$ a.e. on $\Omega \times D$. Hence, we have that $\widehat{\psi}^0 \equiv \beta^L(\widehat{\psi}_0)$.

Proceeding in the same way as in the argument leading to (6.23) in [7], now with $K = 1$, we deduce from (3.11), (A.5) and as $\widehat{\psi}^0 \in \widehat{Z}_1$ that

$$\left| \int_{\Omega \times D} M (\widehat{\psi}^0 - \beta^L(\widehat{\psi}_0)) \widehat{\varphi} \, d\widetilde{q} \, d\widetilde{x} \right| \leq (\Delta t)^{\frac{1}{2}} \left(\int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}_0) \, d\widetilde{q} \, d\widetilde{x} \right)^{\frac{1}{2}} \left(\int_{\Omega} \left[\|\nabla_x \widehat{\varphi}\|_{L^\infty(D)}^2 + \|\nabla_q \widehat{\varphi}\|_{L^\infty(D)}^2 \right] \, d\widetilde{x} \right)^{\frac{1}{2}} \tag{A.6}$$

for all $\widehat{\varphi} \in H^1(\Omega; L^\infty(D)) \cap L^2(\Omega; W^{1,\infty}(D))$ and therefore in particular for all $\widehat{\varphi} \in H^s(\Omega \times D)$ with $s > 1 + d$. As the last two factors on the right-hand side of (A.6) are independent of L and Δt , we can pass to the limit $L \rightarrow \infty$ and $\Delta t \rightarrow 0_+$ on both sides of (A.6) to deduce that $\widehat{\psi}^0 - \beta^L(\widehat{\psi}_0) \rightarrow 0$ weakly in $M^{-1}(H^s(\Omega \times D))'$, $s > 1 + d$, as $L \rightarrow \infty$ and $\Delta t \rightarrow 0_+$.

As $\widehat{\psi}_0 \geq \beta^L(\widehat{\psi}_0)$ and therefore $\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0) = [\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0)]_+$, it follows from (1.14) that

$$\left| \int_{\Omega \times D} M (\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0)) \widehat{\varphi} \, d\widetilde{q} \, d\widetilde{x} \right| \leq \left(\int_{\Omega \times D} M [\widehat{\psi}_0 - L]_+ \, d\widetilde{q} \, d\widetilde{x} \right) \|\widehat{\varphi}\|_{L^\infty(\Omega \times D)} \tag{A.7}$$

for all $\widehat{\varphi} \in L^\infty(\Omega \times D)$. Further, since (3.3) implies that $\widehat{\psi}_0 \in \widehat{Z}_1$, using (1.14) again we have that

$$0 \leq \int_{\widehat{\psi}_0 \geq L} M L \, d\widetilde{q} \, d\widetilde{x} \leq \int_{\Omega \times D} M \beta^L(\widehat{\psi}_0) \, d\widetilde{q} \, d\widetilde{x} \leq \int_{\Omega \times D} M \widehat{\psi}_0 \, d\widetilde{q} \, d\widetilde{x} \leq |\Omega|. \tag{A.8}$$

On noting that \mathcal{F} is nonnegative and monotonic increasing on $[1, \infty)$, and that $\mathcal{F}(s) \in [0, 1]$ for $s \in [0, 1]$, we deduce from (3.3) that

$$\begin{aligned} \int_{\Omega \times D} M \mathcal{F}([\widehat{\psi}_0 - L]_+) \, d\widetilde{q} \, d\widetilde{x} &= \int_{\widehat{\psi}_0 \in [0, L+1)} M \mathcal{F}([\widehat{\psi}_0 - L]_+) \, d\widetilde{q} \, d\widetilde{x} + \int_{\widehat{\psi}_0 \geq L+1} M \mathcal{F}([\widehat{\psi}_0 - L]_+) \, d\widetilde{q} \, d\widetilde{x} \\ &\leq \int_{\Omega \times D} M \, d\widetilde{q} \, d\widetilde{x} + \int_{\Omega \times D} M \mathcal{F}(\widehat{\psi}_0) \, d\widetilde{q} \, d\widetilde{x} \leq C. \end{aligned} \tag{A.9}$$

Let us recall the logarithmic Young’s inequality

$$r s \leq r \log r - r + e^s \quad \text{for all } r, s \in \mathbb{R}_{\geq 0}. \tag{A.10}$$

This follows from the Fenchel–Young inequality:

$$r s \leq g^*(r) + g(s) \quad \text{for all } r, s \in \mathbb{R},$$

involving the convex function $g : s \in \mathbb{R} \mapsto g(s) \in (-\infty, +\infty]$ and its convex conjugate g^* , with $g(s) = e^s$ and

$$g^*(r) = \begin{cases} +\infty & \text{if } r < 0, \\ 0 & \text{if } r = 0, \\ r(\log r - 1) & \text{if } r > 0; \end{cases}$$

with the resulting inequality then restricted to $\mathbb{R}_{\geq 0}$. It immediately follows from (A.10) that $rs \leq \mathcal{F}(r) + e^s$ for all $r, s \in \mathbb{R}_{\geq 0}$.

Applying the last inequality with $r = [\widehat{\psi}_0 - L]_+$ and $s = \log L$, we have that

$$[\widehat{\psi}_0 - L]_+ (\log L) \leq \mathcal{F}([\widehat{\psi}_0 - L]_+) + L. \quad (\text{A.11})$$

The bounds (A.8), (A.9) (noting that the integrand of the left-most integral in (A.9) is nonnegative) and (A.11) then imply that

$$\begin{aligned} \int_{\Omega \times D} M [\widehat{\psi}_0 - L]_+ \, \underset{\sim}{dq} \, \underset{\sim}{dx} &= \int_{\widehat{\psi}_0 \geq L} M [\widehat{\psi}_0 - L]_+ \, \underset{\sim}{dq} \, \underset{\sim}{dx} \\ &\leq \frac{1}{\log L} \left[\int_{\widehat{\psi}_0 \geq L} M \mathcal{F}([\widehat{\psi}_0 - L]_+) \, \underset{\sim}{dq} \, \underset{\sim}{dx} + \int_{\widehat{\psi}_0 \geq L} M L \, \underset{\sim}{dq} \, \underset{\sim}{dx} \right] \leq \frac{C}{\log L}. \end{aligned} \quad (\text{A.12})$$

On substituting (A.12) into the right-hand side of (A.7), we have that, for any $\widehat{\varphi} \in L^\infty(\Omega \times D)$ (and therefore, by Sobolev embedding, also for any $\widehat{\varphi} \in H^s(\Omega \times D)$ with $s > d$),

$$\lim_{L \rightarrow \infty} \left| \int_{\Omega \times D} M (\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0)) \widehat{\varphi} \, \underset{\sim}{dq} \, \underset{\sim}{dx} \right| \leq \left(\lim_{L \rightarrow \infty} \int_{\Omega \times D} M [\widehat{\psi}_0 - L]_+ \, \underset{\sim}{dq} \, \underset{\sim}{dx} \right) \|\widehat{\varphi}\|_{L^\infty(\Omega \times D)} = 0. \quad (\text{A.13})$$

Therefore, we have that $\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0)$ converges to 0, weakly in $M^{-1}(H^s(\Omega \times D))'$ for $s > d$, as $L \rightarrow \infty$. Consequently, also $\widehat{\psi}_0 - \beta^L(\widehat{\psi}_0)$ converges to 0, weakly in $M^{-1}(H^s(\Omega \times D))'$ for $s > 1 + d$, as $L \rightarrow \infty$. On recalling that $\widehat{\psi}^0 - \beta^L(\widehat{\psi}_0)$ converges to 0, weakly in $M^{-1}(H^s(\Omega \times D))'$ for $s > 1 + d$, as $L \rightarrow \infty$ and $\Delta t \rightarrow 0_+$, we then deduce by subtracting that

$$\widehat{\psi}^0 = \widehat{\psi}^0(L, \Delta t) \rightarrow \widehat{\psi}_0 \quad \text{weakly in } M^{-1}(H^s(\Omega \times D))' \text{ for } s > 1 + d, \quad \text{as } L \rightarrow \infty \text{ and } \Delta t \rightarrow 0_+.$$

Noting (3.13a) and the fact that $\mathcal{F}(r)/r \rightarrow \infty$ as $r \rightarrow \infty$, we deduce from de la Vallée-Poussin's theorem that the family $\{\widehat{\psi}^0(L, \Delta t)\}_{L>1, \Delta t>0}$ is uniformly integrable in $L^1_M(\Omega \times D)$. Hence, by the Dunford–Pettis theorem, the family $\{\widehat{\psi}^0(L, \Delta t)\}_{L>1, \Delta t>0}$ is weakly relatively compact in $L^1_M(\Omega \times D)$. Consequently, one can extract a subsequence $\{\widehat{\psi}^0(L_k, \Delta t_k)\}_{k=1}^\infty$ that converges weakly in $L^1_M(\Omega \times D)$; however the uniqueness of the weak limit together with the weak convergence of the (entire) sequence $\{\widehat{\psi}^0 = \widehat{\psi}^0(L, \Delta t)\}_{L>1, \Delta t>0}$ to $\widehat{\psi}_0$ in $M^{-1}(H^s(\Omega \times D))'$, $s > 1 + d$, as $L \rightarrow \infty$ and $\Delta t \rightarrow 0_+$, established in the previous paragraph, then implies that the (entire) sequence $\{\widehat{\psi}^0 = \widehat{\psi}^0(L, \Delta t)\}_{L>1, \Delta t>0}$ converges to $\widehat{\psi}_0$ weakly in $L^1_M(\Omega \times D)$, as $L \rightarrow \infty$ and $\Delta t \rightarrow 0_+$, on noting that $L^1_M(\Omega \times D)$ is (continuously) embedded in $M^{-1}(H^s(\Omega \times D))'$ for $s > 1 + d$ (cf. the discussion following Thm. 5.1 in [7] with $K = 1$). As $\widehat{\psi}^0 \equiv \beta^L(\widehat{\psi}_0)$, that completes the proof of (3.13b).

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