Analysis of thresholding for codimension two motion by mean curvature: a gradient-flow approach

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Abstract

The Merriman-Bence-Osher (MBO) scheme, also known as thresholding or diffusion generated motion, is an efficient numerical algorithm for computing mean curvature flow (MCF). It is fairly well understood in the case of hypersurfaces. This paper establishes the first convergence proof of the scheme in codimension two. We concentrate on the case of the curvature motion of a filament (curve) in $\mathbb{R}^3$. Our proof is based on a new generalization of the minimizing movements interpretation for hypersurfaces (Esedoglu-Otto '15) by means of an energy that approximates the Dirichlet energy of the state function. As long as a smooth MCF exists, we establish uniform energy estimates for the approximations away from the smooth solution and prove convergence towards this MCF. The current result which holds in codimension two relies in a very crucial manner on a new sharp monotonicity formula for the thresholding energy. This is an improvement of an earlier approximate version.

Keywords: Mean curvature flow, Ginzburg-Landau equation, Thresholding, MBO scheme, Higher codimension, Diffusion generated motion, Filament motion, Vortex motion

Mathematical Subject Classification: 35A15, 65M12, 35B25, 35K08

1 Introduction

1.1 Motivation

This paper is devoted to the analysis of the thresholding scheme in codimension two which may model the motion of vortices (points) in the plane, filaments (curves) in three-dimensional space or two-dimensional surfaces in four dimensions. For the sake of definiteness we will mostly focus on the—from our point of view—most relevant case of a curve in $\mathbb{R}^3$. Important applications of curvature-driven motion of filaments in $\mathbb{R}^3$ include superconductivity (magnetic flux tubes in type-I superconductors move by curve-shortening flow), fluid dynamics (where the motion of vortex lines is described by *binormal* curvature flow), image processing (in particular for identifying vasculature in magnetic resonance angiography (MRA) images), and many more. Curiously, the curvature flow of a filament has also been used to define the curve-shortening flow of immersed planar curves past singularities [3].

The analysis of motion by mean curvature for a hypersurface has a long history, starting from the fundamental work of Brakke [11]. A range of techniques has later been developed to further the understanding of such geometric evolutions. These include singular perturbations [12, 13, 18, 27], the level set formulation [24, 14, 23], and variational time stepping or minimizing movements [2, 38]. However, for higher codimension curvature motions, there are relatively

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fewer results. We refer to the works [3, 48] for statements in the classical setting and [49, 50] for reviews of the current status. One reason is that the comparison principle which is used often in the hypersurface case is not applicable in higher codimension. However, variational techniques are quite versatile. The current paper uses a variational interpretation to analyze an efficient numerical scheme and prove its convergence to motion by mean curvature of curves in three dimensional space.

The idea of thresholding goes back to the 1992-paper [39] of Merriman, Bence and Osher treating the evolution of hypersurfaces by their mean curvature. The algorithm is henceforth often called the MBO scheme. It is a two-step time discretization procedure easily described as: Given an open set Ω_0 of $\mathbb{R}^d$ and a time-step size $h > 0$, a sequence of open subsets $\{\Omega_n\}_{n\geq 1}$ of $\mathbb{R}^d$ is generated by alternating between

1. solving the linear heat equation for time h, starting from the characteristic function of the set Ω_n:

$$\partial_t v = \Delta v, \quad \text{for } 0 < t < h, \quad v(x,0) = \chi_{\Omega_n}(x) = \begin{cases} 1, & x \in \Omega_n, \\ 0, & x \notin \Omega_n, \end{cases} \tag{1}$$

and

2. projecting the function $v(x,h)$ onto $\{0,1\}$ to obtain the new set Ω_{n+1}:

$$\Omega_{n+1} = \left\{ x : v(x,h) > \tfrac{1}{2} \right\}. \tag{2}$$

In the following, we will use u^n to denote χ_{Ω_n}, the state of the evolution at the n-th time step. The second procedure above is also called the *thresholding* step due to the use of the threshold value $\frac{1}{2}$. (Sometimes, the completely equivalent choice of $\{-1,1\}$-valued functions is used. In this case, u^n and Ω_n are related by $u^n = 2\chi_{\Omega_n} - 1$. Then the threshold value is 0 and the projection step above can be simply stated as $u^n = \frac{v}{|v|}$.) The sequence of sets $\{\Omega_n\}_{n\geq 0}$ is shown to converge to motion by mean curvature in the viscosity sense [22, 7]. These proofs rely very much on the comparison principle which is satisfied by the scheme above. See also [28, 29] for a generalization of the result for more general kernels.

Thresholding for a filament in $\mathbb{R}^3$, due to Ruuth, Merriman, Xin, and Osher [45], is just as simple to describe as the hypersurface case. Consider an $\mathbb{R}^2$- or complex-valued function u defined on $\mathbb{R}^3$ such that it has length one almost everywhere, or equivalently a measurable function $u : \mathbb{R}^3 \to \mathbb{S}^1$. Given a curve $\Gamma \subset \mathbb{R}^3$, it is fairly straightforward to construct a function u such that it "winds around" Γ with winding number equal to one, see Section 2.2 and Appendix 5.2. The curve is also the set where u is "singular" (see Fig. 1). The thresholding scheme in this case is very similar to the one for hypersurfaces. In the first step, as in (1), we diffuse the predecessor u^{n-1}, which is a unit vector field. The second step (2) is replaced by projecting v onto $\mathbb{S}^1$:

$$u^{n+1}(x) = \frac{v(x,h)}{|v(x,h)|}. \tag{3}$$

The main result of the present paper is the convergence of the above algorithm to the mean curvature flow of Γ. A heuristic argument, using asymptotic expansions is given in [45]. We will also briefly describe the underlying formal computation in Appendix 5.1. To the best of our knowledge, our work is the first convergence proof of the thresholding scheme in higher codimension.

We spend a moment here to interpret the above thresholding scheme from the point of view of Ginzburg-Landau functionals and their gradient flows. These concepts appear often in the study of phase transition and interface motions. The functional has the form

$$\mathcal{F}_\varepsilon(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{\varepsilon^2}W(u)\,dx \tag{4}$$

where $u : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}^m$ is the phase function and $W : \mathbb{R}^m \to \mathbb{R}_+$ is a (non-negative) potential function which vanishes on some prescribed set. In the above, $\varepsilon \ll 1$ is a small positive number. The gradient flow of $\mathcal{F}_\varepsilon$ (in the L^2-sense) is given by

$$\partial_t u_\varepsilon = \Delta u_\varepsilon - \frac{1}{\varepsilon^2}\nabla_u W(u_\varepsilon) \left(= -\frac{\partial \mathcal{F}_\varepsilon(u)}{\partial u}\right). \tag{5}$$

A direct computation gives the following energy dissipation law:

$$\frac{d}{dt}\mathcal{F}_\varepsilon(u_\varepsilon) = -\int |\partial_t u_\varepsilon|^2\,dx. \tag{6}$$

For both stationary and dynamic considerations, the singular limit $\varepsilon \to 0$ is one of the key questions to investigate.

By setting different values for the dimensions of the ambient space and the range, the functional can model various geometric objects. For example, to model hypersurfaces and their motions, one may take $m = 1$, i.e., u is scalar-valued and $W(u) = (1 - u^2)^2$. In this case, W vanishes on the discrete set $\{-1, 1\}$. The energy is usually called the Cahn-Hilliard functional, whose dynamics (5) are known as the Allen-Cahn equation due to their first appearance in the materials science literature [1]. The typical behavior is that the function u_ε will partition the ambient space into two domains Ω_- and Ω_+ on which u_ε takes values roughly equal to 1 and -1 separated by a narrow transition layer of width $O(\varepsilon)$. Hence in the limit $\varepsilon \to 0$ this layer forms a sharp interface which can be described precisely as a minimal surface in the stationary regime or it evolves according to MCF in the dynamical case. We refer to [43] for a heuristic illustration which has been proved rigorously in various mathematical settings—see the beginning of this introduction. If $n = m = 2$, the function u_ε is defined on (a subset of) $\mathbb{R}^2$ and takes values in $\mathbb{R}^2$, or equivalently is *complex-valued.* A common choice for the potential function is $W(u) = (1-|u|^2)^2$ so that the zero set of W is the unit circle $\mathbb{S}^1$. Hence any u_ε with reasonably low functional energy value $\mathcal{F}_\varepsilon(u_\varepsilon)$ has point-wise norm approximately equal to one. In this case, by topological reasoning, u_ε can have points (vortices) as its singular (defect) sets. Such functionals are widely used in the modeling and analysis of vortices, their dynamics and interaction in superconductivity phenomena (see [8, 46]). Next, if we take $n = 3$ and $m = 2$, i.e., u_ε is a complex valued function defined on (a subset of) $\mathbb{R}^3$, and the same potential function $W(u) = (1-|u|^2)^2$, then u_ε can incorporate curves as its singular sets, see Figure 1. This is also used in the modeling of vortex lines in superconductivity as well as superfluids [42, 41]. Even more generally, the zero set of W can consist of disjoint Riemannian manifolds. Then the dynamics (5) can model harmonic heat flows [44, 37]. The above description clearly demonstrates the range of applicability of the functional (4) and explains the intensive mathematical activities surrounding it. We defer to Section 1.3 for more recent references of related work.

Note that the gradient flow dynamics (5) can be formally solved by *operator splitting*, alternating the following two steps:

$$\text{(i) linear diffusion: } \partial_t u_\varepsilon = \Delta u_\varepsilon; \quad \text{(ii) fast reaction: } \partial_t u_\varepsilon = -\frac{1}{\varepsilon^2}\nabla_u W(u_\varepsilon). \tag{7}$$

The key idea of [39] is to replace Step (ii) by instantly projecting u_ε onto the zero set of W. Referring to the description at the beginning, we have that for the hypersurface case, u_ε is projected onto $\{-1, 1\}$ while for the filament case, u_ε is projected onto $\mathbb{S}^1$. We remark that this projection step clearly generalizes to the case when W vanishes on more general sets, for example multiple disconnected copies of $\mathbb{S}^N$.

Similar to the Ginzburg-Landau equation (5), MCF also has a gradient-flow structure. Indeed, it is the L^2-gradient flow of the area functional. This suggests to analyze the dynamics using variational methods. Such an approach has been implemented in [2, 38] for the MCF of hypersurfaces. De Giorgi [16] formalized this idea in a more general setting, which is now often called minimizing movements. We refer the reader to [4] for a more contemporary exposition. The key idea of such a method is to discretize the evolution in time (with time step $h > 0$) and obtain the state u^n at the n-th time step by minimizing the functional

$$E(u) + \frac{1}{2h} d^2(u, u^{n-1}) \tag{8}$$

where E is the energy of the state, d is the distance or metric compatible to the gradient structure of E, and u^{n-1} is the state at the previous time step. The overall effect of minimizing (8) is that the energy decreases according to some dissipation mechanism. Furthermore, the sequence of minimizers u^n formally satisfies the implicit time discretization scheme for the gradient flow of E

$$\frac{u^n - u^{n-1}}{h} = -\nabla E(u^n). \tag{9}$$

The limit as $h \to 0$ of the sequence $\{u^n\}_{n\geq 0}$ thus obtained is then called a minimizing movements for E. We emphasize here that the definition of the metric d which provides appropriate dissipation mechanism is just as important as the energy E itself. In fact, if the metric d on the state space is the induced distance of some Riemannian metric (via shortest paths), then ∇E appearing in (9) is the gradient of the functional E w.r.t. this Riemannian metric.

The compatibility of the thresholding scheme to the above gradient-flow structure in form of a minimizing movements interpretation was first made by Esedoḡlu and Otto in the work [20]. In the hypersurface case, they constructed an energy that approximates—or more precisely, Γ-converges to—the interfacial area. Their approach also allows them to handle multi-phase systems with a broad class of surface tensions. This generalization has been an open problem for several decades. Based on this minimizing movements principle, the work [32] provides a rigorous analysis of the scheme in the dynamical setting and gives a convergence proof to motion by mean curvature in the multi-phase case. We will comment more on these related works in §1.2 and §1.3.

Interpreting thresholding as a minimizing movements scheme has practical implications as well. We will see that in our case of codimension two, the minimizing movements principle furnishes a generalization of the scheme to incorporate Dirichlet or Neumann boundary conditions as well as a chemical potential leading to a pinning effect. An advantage of the current approach is that the same Gaussian kernel works with very minor modification. Hence numerical efficiency is not affected. In the next section, we will briefly describe the basis of our method of proof in the filament case.

1.2 Idea of proof

The protagonist in the present work is the approximate energy

$$E_h(u) = \frac{1}{h} \int (1 - u \cdot G_h * u)\, dx \tag{10}$$

defined for any unit vector fields $u\colon \mathbb{R}^3 \to \mathbb{S}^1$; here G_h denotes the heat kernel in $\mathbb{R}^3$ evaluated at time h, i.e., a Gaussian kernel of variance $2h$. Note that the counterpart of (10) in the hypersurface case [20] is given by

$$F_h(\chi) = \frac{1}{\sqrt{h}} \int (1-\chi)\, G_h * \chi \, dx, \quad \text{where } \chi\colon \mathbb{R}^3 \to \{0,1\}. \tag{11}$$

There is a fundamental difference between them. The energy F_h measures the heat transfer from the set $\{\chi = 1\}$ into its complement $\{\chi = 0\}$ which is roughly equal to the $(d-1)$-dimensional area or measure of the boundary of $\{\chi = 1\}$. This can be rigorously justified by that F_h Γ-converges to $c_0\mathcal{H}^{n-1}(\partial\{\chi = 1\})$ for some constant c_0 [20, Prop. A.1]. On the other hand, the energy E_h measures the distance of the diffused vector field $G_{h/2} * u$ to the sphere $\mathbb{S}^1$, i.e., it quantifies in how far it fails to be a unit vector field. Writing E_h as a weighted average of squared finite difference quotients (Lemma 2.7 (40)) shows its natural connection to the Dirichlet energy. This can also be phrased in terms of the Γ-convergence of $\frac{1}{2}E_h$ to the Dirichlet energy $\frac{1}{2}\int |\nabla u|^2 dx$.

The basis of our analysis is a minimizing movements interpretation of thresholding in our context of higher codimension. In resemblance to (8), given the state u^{n-1} at the $(n-1)$-st step, the state u^n is found by minimizing the functional

$$\frac{1}{2}E_h(u) + \frac{1}{2h} \left\| G_{\frac{h}{2}} * (u - u^{n-1}) \right\|_{L^2}^2 \tag{12}$$

(see Lemma 2.4 below). The minimization principle (12) is in accordance with the gradient flow structure of the (harmonic map) heat flow, which is the L^2-gradient flow of the Dirichlet energy.

From (12), we immediately obtain some energy dissipation relation (Lemma 2.9), which serves well as an a priori estimate. However this estimate fails to fully capture the limiting dynamics as $h \to 0$. To understand this well known fact, let us give some background on minimizing movements. While at first glance, a gradient flow $\partial_t u = -\nabla E(u)$ seems to need a smooth Riemannian structure, it is clear that the minimization problem (8) makes sense in any metric space. This is the basis of De Giorgi's theory to define gradient flows in metric spaces: It is easy to see that the solution of a smooth gradient flow is characterized by the optimal rate of energy dissipation $\frac{d}{dt}E(u) \le -\frac{1}{2}|\partial_t u|^2 - \frac{1}{2}|\nabla E(u)|^2$ (since then equality holds in Young's and Cauchy's inequality).

It is worth noting that the energy dissipation rate $\frac{d}{dt}E(u) \le -|\nabla E(u)|^2$ (or $\frac{d}{dt}E(u) \le -|\partial_t u|^2$, respectively) is necessary but by no means does it characterize the solution. Because of the degeneracy in the case of mean curvature flow however, it is more convenient to measure this rate only in terms of gradient of the area functional, i.e., the mean curvature. To then capture all information, one needs to monitor localized versions of the energy. Then under certain regularity conditions, this family of energy dissipation inequalities indeed characterizes the MCF.

When deriving either of these energy dissipation relations for limits of minimizing movements schemes, another technical difficulty appears: The a priori bound obtained from comparing u^n to its predecessor in (8) fails to be sharp by a factor $\frac{1}{2}$. However, this can be cured by considering the nonlinear interpolation between u^{n-1} and u^n, choosing $u^{(n-1)+\lambda}$ to be a minimizer of $E(u) + \frac{1}{2\lambda h}d^2(u, u^{n-1})$. This interpolation was first proposed by De Giorgi and has been used recently for the localized energies of thresholding by Otto and the first author [33].

A nice feature of the current line of proof is that the technical difficulty if interpolating the state functions can be omitted as the precise prefactor of the metric term has no importance in our main estimate. However, the estimate is still delicate in the sense that the prefactors of two other term need to match in order to cancel a diverging term. This will be guaranteed by a new monotonicity formula.

The foremost obstacle in the case of codimension two is the fact that the Dirichlet energy is not uniformly bounded near the filament which is exactly the place where the u^n becomes singular. In fact $E_h(u^n)$ blows up with rate $|\log h|$ near the filament. For remedy, we introduce a *localized* version of E_h (Definition 2.3 (23)). The localization is taken to be a truncated version of the the squared distance function $d^2(\cdot, \Gamma_t)$ to the actual solution of the filament MCF. The importance of distance function was first pointed out by De Giorgi [17]. Later on, Ambrosio and Soner [5] have used this idea to characterize higher codimensional geometric flows in terms of their distance function. The work of Lin [36] further takes advantage of the properties of the squared distance function to derive a localized energy dissipation law for the the complex Ginzburg-Landau equation. (A more detailed description will be given at the beginning of Section 2.3.) Inspired by this last work, exploiting the properties of the squared distance function, in particular (34)–(37), we can similarly establish that the localized thresholding energy is uniformly bounded (Proposition 2.6) so that the location of the singular set of u^n exactly coincides with Γ_t.

Yet another new ingredient in the filament case is that we need to capture two equations: (i) the motion law of the filament—the set where u is singular and (ii) the evolution of the phase of u *away* from the filament. The latter is due to the extra degree of freedom in the zero set $\mathbb{S}^1$ of W. To this end, we will derive two Euler-Lagrange equations (Lemma 2.10 (50)–(51)) for u^n by considering *inner* and *outer* variations of u^n (48)–(49). Note that for the thresholding scheme in the hypersurface case, the limiting description is simply described by the MCF of the interface Γ. The state variable u is identically equal to $+1$ and -1 away from Γ.

Last but not the least, a sharp monotonicity formula (Lemma 2.8) for the thresholding energy (as a function of the time step h) is used in a very crucial way. It is an improved version of an earlier "approximate monotonicity" formula due to Esedoğlu-Otto in [20]. So far it is only proved in codimension two and does not carry over immediately the the hypersurface case. In the hindsight, this is related to the fact that for complex-valued u, in the Ginzburg-Landau functional (4), for typical functions, the Dirichlet energy dominates the potential term. On the other hand, for the scalar version (Allen-Cahn equation), there is equipartition of energy, i.e., the energy is equally distributed between the two terms. It will be interesting to investigate the monotonicity formula in a more general setting.

1.3 Related work

Here we describe some related work on the analysis of thresholding scheme and some of its generalizations.

As mentioned before, the use of thresholding scheme for hypersurfaces has a long history, initiated by the work of Merriman, Bence, and Osher [39]. Soon after, rigorous proofs of convergence are given in Evans [22] and Barles and Georgelin [7]. As these proofs are entirely based on the comparison principle, they are basically restricted to the special case of a single hypersurface. Several recent works on thresholding scheme have overcome this restriction. Esedoğlu and Otto's minimizing movements interpretation [20] generalized the scheme to arbitrary surface tensions and led to a series of conditional convergence results which are not based on the comparison principle but on the gradient-flow structure of MCF (of networks of interfaces). Under the assumption that the total energy of the approximations converge to those of the limit, Otto and the first author proved that the limit solves a distributional formulation of motion by mean curvature, also in case of networks of hypersurfaces [32]. (See also [34] for a proof of a similar result for a multi-phase Allen-Cahn system.) Swartz and the first author extended these methods to incorporate external forces and volume constraints [35]. Only recently, a *local* minimality property of thresholding in the case of (networks of) hypersurfaces has been observed and used by Otto and the first author to prove that under the same assumption, this limit is also a unit-density Brakke flow [33]. There the precise dissipation rate is fundamental in proving Brakke's inequality and the authors use De Giorgi's variational interpolations to obtain the precise constant.

The incorporation of anisotroy in the curvature motion is also of interest, both mathematically and practically, due to again the simplicity of thresholding. One of the earliest work in this regard is [29]. It starts from a given (positive) convolution kernel and identity the anisotropy. The "inverse problem"—the construction of kernels for prescribed anisotropy—is considered in [10, 19]. A technically difficult aspect is that in general the kernel must be necessarily non-positive. Hence the traditional proof of convergence is again not applicable in a straightforward way. Regarding this, another line of proof is constructed by Swartz and the second author [47]. This last work proves, by constructing an appropriate ansatz, consistency and stability statements and a convergence rate of the scheme without using the comparison principle. Though currently it only considers the case of classical isotropic MCF, at the conceptual level, it can be applicable to a more general situation.

Departing from the hypersurface case, in relation to the current paper, we emphasize here work related to the motion of a filament in $\mathbb{R}^3$ which has codimension two. The convergence of the Ginzburg-Landau dynamics to MCF when classical solution exists was proved in [31] and [36]. The work [6] extended the result to varifold convergence under the assumption that the density of the limit measure is bounded from below. This assumption was finally eliminated in the work [9]. A counter-part of the motion law (5) is the consideration of Schrödinger dynamics of (4), written as $i\partial_t u_\varepsilon = \partial_u \mathcal{F}_\varepsilon(u)$. Heuristic asymptotics lead to a limit singular measure that coincides with a filament evolving according to curvature motion along the *bi-normal* $\mathbf{B}$ to the curve. There are many interesting open questions concerning this motion, regarding well-posedness and approximation algorithms. We refer to [30] for a recent survey of this model.

Last but not the least, the very recent work Osting and Wang [40] discovered the same minimizing movements principle of the scheme [45] as ours and used it to generalize the scheme from unit vector fields to matrix fields in $O(n)$, i.e., "unit" matrix fields w.r.t. the Frobenius norm. Furthermore, they provide promising numerical tests of this extension. While the limit $h \to 0$ is not studied there, it seems that our convergence analysis, as described in Section 4.3 should apply to this case as well. In the absence of singularities, the proof might simplify in the sense that one only needs to consider outer variations as in the case of Section 4.3. It might also be interesting to consider and classify the singularity structures that can appear.

1.4 Structure of the paper

In the next Section 2, we state our main convergence result §2.1 and some remarks about it §2.2. Then in §2.3 we list all the technical lemmas to be used. We highlight here the (localized) minimizing movements principles Lemma 2.4, (localized) energy dissipation law Proposition 2.6, the sharp monotonicity lemma 2.8, and the two Euler-Lagrange equations for the minimizers during each time step Lemma 2.10. These are all proved in Section 3 which forms the bulk of the paper. In Section 4, we discuss further insights from the variational viewpoint, namely boundary conditions, vortex motion in two dimensions and the less singular harmonic map heat flow in higher dimensions.

2 Mean curvature flow of a filament in $\mathbb{R}^3$

Throughout the paper we will assume that a smooth mean curvature flow of an embedded curve Γ_t starting from Γ_0 exists up to some time $T > 0$. The flow can be expressed in terms of a parametrization $\gamma(\cdot, t)$ such that $\Gamma_t = \gamma([0,1], t)$, where

$$\gamma : [0,1] \times [0,T) \longrightarrow \mathbb{R}^3, \tag{13}$$

and it satisfies

$$\frac{\partial}{\partial t}\gamma(\theta, t) = \kappa_{\gamma(\theta,t)} \mathbf{N}_{\gamma(\theta,t)}, \quad \gamma([0,1], 0) = \Gamma_0. \tag{14}$$

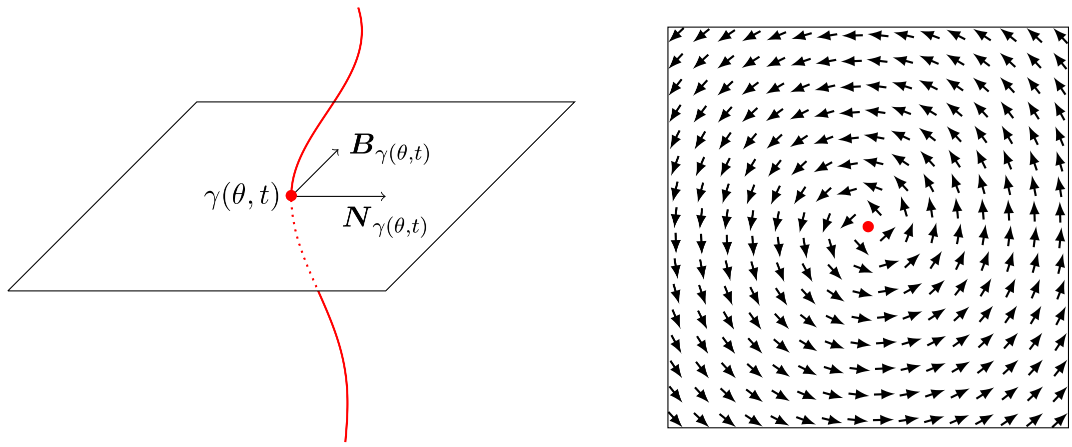

Figure 1: Left: A filament in $\mathbb{R}^3$ with a horizontal slice of $\mathbb{R}^3$. Right: The initial conditions u^0 on the depicted slice "wind" around the filament.

The boundary conditions at $\theta = 0$ and $\theta = 1$ will be specified later. In the above, κ denotes the curvature of Γ_t at $\theta \in [0,1]$ and $\mathbf{N}$ is unit normal vector pointing in direction of the derivative of the unit tangent vector. Although $\mathbf{N}$ is not defined when $\kappa = 0$, the product $\kappa\mathbf{N}$ is always well-defined. Note that short-time existence has been established in a very general framework by Gage and Hamilton [25, Section 2]. See also Huisken-Polden [26] for solving the equation using a graph coordinate system and [49, 50] for reviews of higher codimensional mean curvature flows.

We will state the algorithm of the thresholding scheme in terms of the heat kernel on $\mathbb{R}^d$,

$$G_h(z) = \frac{1}{(4\pi h)^{d/2}} \exp\Big(-\frac{|z|^2}{4h}\Big) \tag{15}$$

which is the solution operator of the linear heat equation and it solves

$$\partial_h G - \Delta G = 0, \quad G_0 = \delta_0. \tag{16}$$

Some basic facts about G_h will be collected at the beginning of Section 3.

We now present the algorithm for the filament thresholding scheme and our main convergence result. In order not to be distracted by boundary conditions, we will work with periodic boundary condition. Recall that in this setting, the configuration or "state" of the algorithm at each time step is given by an $\mathbb{R}^2$- or $\mathbb{C}$-valued function u defined on $\mathbb{T}^3$. To be more precise, after each projection step, u has unit length, i.e., it is $\mathbb{S}^1$-valued.

2.1 Main result

Algorithm 2.1. *Given a time-step size $h > 0$ and the configuration $u^{n-1} : \mathbb{T}^3 \to \mathbb{S}^1$ at time $t = (n-1)h$, construct the configuration u^n at time $t = nh$ by the following two operations:*

1. *Diffusion: convolve u^{n-1} with the heat kernel, i.e., set $v^n := G_h * u^{n-1}$;*
2. *Projection: project v^n onto the unit sphere, i.e., set $u^n := \frac{v^n}{|v^n|}$.*

We denote by u^h the piecewise constant interpolation in time of the functions $u^0, u^1, \ldots$ defined by

$$u^h(x,t) := u^n(x) \quad \text{for } t \in [nh, (n+1)h). \tag{17}$$

We also define the following backward in time finite difference quotient for any time dependent function v,

$$\partial_t^h v := \frac{v(t) - v(t-h)}{h}. \tag{18}$$

Our main result is the following convergence of u^h to a filament moving by its mean curvature.

Theorem 2.2. *Let Γ_t, $t \in [0,T)$ be a filament evolving smoothly by mean curvature flow* (13)-(14) *in $\mathbb{T}^3$ and assume that the initial conditions for Algorithm 2.1 are well-prepared in the sense of Definition 2.5. Then the approximate solutions u^h* (17) *obtained by Algorithm 2.1 converge as $h \downarrow 0$ to Γ_t in the following sense.*

For every sequence u^h, there exists a subsequence (still denoted by u^h) and a vector field $u \in H^1_{loc}((\mathbb{T}^3 \times (0,T)) \setminus \Gamma; \mathbb{S}^1)$ such that

$$u^h \to u \qquad \text{in } L^2(\mathbb{T}^3 \times (0,T)), \tag{19}$$

$$\nabla G_h * u^h \rightharpoonup \nabla u \qquad \text{in } L^2_{loc}((\mathbb{T}^3 \times (0,T)) \setminus \Gamma), \quad \text{and} \tag{20}$$

$$\partial_t^h (G_h * u^h) \rightharpoonup \partial_t u \qquad \text{in } L^2_{loc}((\mathbb{T}^3 \times (0,T)) \setminus \Gamma). \tag{21}$$

In the limit $h \to 0$, the vorticity set concentrates only on Γ_t in the sense that the Dirichlet energy of u stays bounded away from Γ_t. Furthermore, u solves the harmonic map heat flow equation away from Γ.

We pause to elaborate the above statement. Further explanation and remarks will be given in Section 2.2.

Our paper crucially makes use of the following energy functional and its localized version.

Definition 2.3 (Thresholding energy)**.** Let $h > 0$. For any unit vector field, $u : \mathbb{T}^3 \to \mathbb{S}^1$, we define the energies

$$E_h(u) := \frac{1}{h} \int (1 - u \cdot G_h * u)\, dx. \tag{22}$$

and its localized version, which is defined for any $\psi : \mathbb{T}^3 \to \mathbb{R}$ as:

$$E_h(u, \psi) := \frac{1}{h} \int \psi\, (1 - u \cdot G_h * u)\, dx. \tag{23}$$

As to be seen later in Lemma 2.7, the above functionals approximate the Dirichlet energy $\int |\nabla u|^2 dx$ of u.

The following lemma is the basis of our analysis. It states that—similar to thresholding for hypersurfaces, cf. [20],—also in our case of higher codimension, thresholding can be interpreted as a minimizing movements scheme. Furthermore, the lemma establishes a localized version of this minimizing movements interpretation similar to the one for hypersurfaces in [33].

Lemma 2.4. *Each time step $u^{n-1} \mapsto u^n = \frac{G_h * u^{n-1}}{|G_h * u^{n-1}|}$ of the thresholding scheme (Algorithm 2.1) is equivalent to minimizing*

$$E_h(u) + \frac{1}{h} \int \left(u - u^{n-1}\right) \cdot G_h * \left(u - u^{n-1}\right) dx \tag{24}$$

among all $u \colon \mathbb{T}^3 \to \mathbb{R}^2$ with $|u| \le 1$ a.e. In particular, we have the following energy-dissipation estimate for the piecewise constant interpolation u^h (17)*,*

$$E_h(u^h(T)) + \int_0^T \int \left|G_{h/2} * \partial_t^h u^h\right|^2 dx\, dt \le E_h(u^0). \tag{25}$$

Furthermore, for any non-negative test function $\psi \geq 0$, u^n minimizes the following localized version of (24),

$$E_h(u,\psi) + \frac{1}{h}\int \psi\left(u-u^{n-1}\right)\cdot G_h * \left(u-u^{n-1}\right)dx + \frac{1}{h}\int \left(u-u^{n-1}\right)\cdot [G_h*,\psi]\, u^{n-1}\,dx \quad (26)$$

among all $u\colon \mathbb{T}^3 \to \mathbb{R}^2$ with $|u| \leq 1$ a.e.

The analogy of the energy dissipation law (25) for (26) with appropriate choice of the localization function ψ is the key technical result of our approach and will be stated in Proposition 2.6.

In the formula (26), note the appearance of the commutator $[G_h*,\psi]$ between the convolution with G_h and multiplication by ψ which is defined as:

$$[G_h*,\psi]f = G_h * (\psi f) - \psi(G_h * f). \quad (27)$$

Definition 2.5. The initial datum $u^0\colon \mathbb{T}^3 \setminus \Gamma_0 \to \mathbb{S}^1$ is called well-prepared if the following two conditions hold:

1. the approximate energies blow up logarithmically: there exist constants $0 < c < C < \infty$ such that
$$c\,|\log h| \leq E_h(u^0) \leq C\,|\log h|\,; \quad (28)$$
2. away from the filament Γ^0, the approximate energies stay bounded
$$E_h(u^0, \phi_\sigma(0)) \leq C(\sigma), \quad (29)$$
where $\phi_\sigma(0)$ denotes the smoothly truncated squared distance function to Γ_0 defined in (32). Here σ is some positive number depending only on the curves $\Gamma_t, t \in [0,T]$ but not on h.

2.2 Remarks about the main result

Here we give some further remarks about our main convergence result.

(1) Similar to the Ginzburg-Landau approximation in the case of vortex in $\mathbb{R}^2$, for smooth initial conditions Γ_0 close to a straight line parallel to the x_3−axis, one can easily construct initial data u^0 satisfying Definition 2.5. Specifically, let $\Gamma_0 \subset \mathbb{R}^3$ be a curve given in the form of

$$\Gamma_0 = \{(\gamma(x_3), x_3)\colon x_3 \in [0,1)\},$$

where $\gamma\colon [0,1) \to \mathbb{R}^2$ is a smooth 1-periodic function. Then

$$u^0(x) := \pm\frac{(x'-\gamma(x_3))^\perp}{|x'-\gamma(x_3)|} \quad \text{for } x = (x', x_3) \in \mathbb{R}^3 \setminus \Gamma_0 \quad (30)$$

is well-prepared (locally around the filament Γ_0). The precise computation is shown in Appendix 5.2. Another equivalent choice is to simply use the radial vector in the normal plane of the curve, i.e., (30) without the rotation $\perp$.

(2) The bulk of the paper is presented in the easiest case of periodic boundary conditions. We only assume this to omit technical difficulties which would pollute the proof. The interested reader is referred to the discussions in Section 4 considering boundary conditions and Appendix 5.3 considering the whole space.

Our proof does not use the fact that we work in three dimensions. In fact the proof applies word by word for any codimension-two mean curvature flow. Then the vector field u is defined on (subsets of) $\mathbb{R}^d$ with values in $\mathbb{S}^1$ and the energy E_h takes the exact same form. However, we prefer to keep the language simple and restrict ourselves to the physically most relevant case of a filament in $\mathbb{R}^3$.

(3) The term vorticity set refers to the support of the limit of the measures corresponding to the rescaled thresholding energies. To be precise, we define the measure μ_h as

$$\mu_h(t) = \frac{1}{|\log h|\, h} \left(1 - u^h(x,t) \cdot G_h * u^h(x,t)\right) dx.$$

Then the vorticity set is given by $\mathrm{supp}(\mu(t))$ where $\mu(t) = \lim_h \mu_h(t)$. The analogous concept also exists for the Ginzburg-Landau dynamics (5) in which the measure is defined as

$$\mu_\varepsilon(t) = \frac{1}{|\log \varepsilon|} \left(\frac{1}{2} |\nabla u_\varepsilon(x,t)|^2 + \frac{1}{4\varepsilon^2}(1 - |u_\varepsilon(x,t)|^2)^2 \right) dx$$

For the case of filament motion, Lin [36, Theorem 4.1] showed that the limit $\mu(t) = \lim_{\varepsilon\to 0} \mu_\varepsilon(t)$ satisfies $c_1 \mathcal{H}^1 \lfloor \Gamma_t \le \mu(t) \le c_2 \mathcal{H}^1 \lfloor \Gamma_t$ for some constants c_1 and c_2. This is consistent with the fact that the limit of $u_\varepsilon(\cdot, t)$ still winds around Γ_t with winding number one. Our current result only states that the limit $\mu(t) = \lim_{h\to 0} \mu_h(t)$ satisfies $\mu(t) \le c_2 \mathcal{H}^1 \lfloor \Gamma_t$. However, we expect a lower bound to be feasible if one can show that the thresholding energy is bounded from below by $c|\log h|$ for typical functions u with a nontrivial winding number around a curve. We leave this latter statement to a future project.

(4) Note that the limit description is given by two dynamical equations. One is for the vorticity set Γ_t which evolves by MCF. The other is the evolution of u away from Γ_t. It is given by the harmonic heat flow on $\mathbb{S}^1$. Precisely, u satisfies

$$\partial_t u = \Delta u + |\nabla u|^2 u \tag{31}$$

which is the (L^2-)gradient flow for the Dirichlet energy $\dfrac{1}{2} \displaystyle\int |\nabla u|^2 \, dx$ for $\mathbb{S}^1$-valued function u. Another maybe more transparent description can also be given. Away from Γ_t, if we write $u(x,t)$ (locally) as $e^{i\theta(x,t)}$ for some phase function θ, then (31) is equivalent to

$$\partial_t \theta = \Delta \theta.$$

(5) The result stated in (20) gives that u^h converges weakly to u in H^1. We believe this can be improved to be strong convergence in H^1. Such a statement is proved for the Ginzburg-Landau dynamics (5) [36, Section 5]. The usual strategy in establishing this is to show that small energy implies that $|u|$ is close to one, and then higher order regularity is proved by means of some blow-up argument. It will be interesting to have similar statement for the thresholding scheme. Furthermore, it is also of practical importance to have a convergence rate. We defer these issues to future works.

Throughout the paper we will make use of the following notation. By C and $C(\sigma)$ we denote generic constants independent of the time-step size h, where $C(\sigma)$ may depend on the parameter σ. The dependence on σ is not important in this paper. In particular we may allow $C(\sigma)$ tend to zero or infinity as $\sigma \to 0$. However, the asymptotics in terms of h is crucial in our analysis and will be spelled out explicitly. We write $A \lesssim B$ if there exists a generic constant $C < \infty$ such that $A \le C\, B$. If a quantity A stays bounded by B as $h \to 0$, we write $A = O(B)$. The same applies for $A = o(B)$, which means $\frac{A}{B} \to 0$ as $h \to 0$. In particular, we will use $O(1)$ and $o(1)$ referring to constants which are bounded and convergent to 0 as $h \to 0$. For simplicity, we often omit the notation $h \to 0$. Furthermore, to describe asymptotics at the heuristic level, we often use the symbol $\approx$ which will always be followed by rigorous explanations. By $\int dx$ we denote the integral $\int_{\mathbb{T}^3} dx$, while $\int dz$ denotes the integral $\int_{\mathbb{R}^3} dz$.

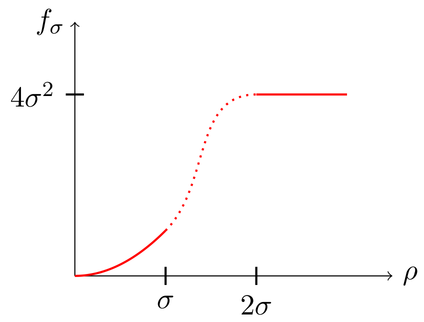

Figure 2: The smooth cut-off of the profile $\rho \mapsto \rho^2$.

2.3 Main propositions and lemmas

We assume the existence of a smooth mean curvature flow Γ_t (13)-(14) and will exploit the properties of the squared distance function to Γ_t to construct a localization function. Precisely, for $\sigma > 0$, we consider the function $\phi = \phi_\sigma(x,t)$ which at any time t is (a truncated version of) the squared distance to the curve Γ_t defined as

$$\phi(x,t) = \phi_\sigma(x,t) := \frac{1}{2} f_\sigma(d(x,\Gamma_t)), \tag{32}$$

where $d(x,\Gamma) := \inf\{|x-y| \colon y \in \Gamma\}$ is the distance function to the set Γ and $f_\sigma \colon (0,\infty) \to (0,\infty)$ is a smooth monotone non-decreasing function such that

$$f_\sigma(\rho) = \begin{cases} \rho^2 & \text{if } \rho < \sigma \\ 4\sigma^2 & \text{if } \rho > 2\sigma, \end{cases} \tag{33}$$

cf. Fig. 2. By [5, Lemma 3.7], the gradient of ϕ solves the heat equation

$$\partial_t \nabla \phi - \Delta \nabla \phi = 0 \quad \text{on } \Gamma_t. \tag{34}$$

The eigenvalues of the Hessian $\nabla^2 \phi$ are well-controlled [5, Theorem 3.2]. In particular, near Γ_t, the Hessian has two eigenvalues equal to one and the third strictly less than one. (For a general codimension-2 surface in $\mathbb{R}^d$, the Hessian has two eigenvalues equal to one and the remaining $d-2$ eigenvalues are strictly less than one.) From these, we deduce that for small $\sigma > 0$, the following holds:

$$\nabla^2 \phi \leq Id \quad \text{on } \{(x,t) \colon d(x,\Gamma_t) < \sigma\}, \text{ i.e., } \xi \cdot \nabla^2 \phi \, \xi \leq |\xi|^2 \text{ for any } \xi \in \mathbb{R}^3. \tag{35}$$

Furthermore, we have

$$\partial_t \phi = 0, \quad \text{and} \quad \Delta \phi = 2 \quad \text{on } \Gamma_t. \tag{36}$$

Now applying Taylor expansion to $\partial_t \phi - \Delta \phi$, we obtain by (36) and (34) that

$$\partial_t \phi - \Delta \phi \leq -2 + \frac{C(\sigma)}{2} d^2(x,\Gamma_t) = -2 + C(\sigma)\phi \quad \text{in } \{(x,t) \colon d(x,\Gamma_t) < \sigma\}. \tag{37}$$

We point out here that the use of the squared distance function is not coincidental as it was used to characterize mean curvature flow in the sense that Γ_t evolves by mean curvature flow *if and only if* ϕ solves (34) [5, Lemma 3.7].

We are very much inspired by the following localized version of the energy-dissipation relation (6) for the Ginzburg-Landau dynamics (5) derived in [36, p. 421-422]. A direct computation followed by an application of (36) and (37) shows

$$
\begin{aligned}
&\frac{d}{dt}\int \phi_\sigma \left(\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon}W(u_\varepsilon)\right) dx \\
&\quad = -\int \phi_\sigma |\partial_t u_\varepsilon|^2 + \sum_{i,j} \partial_i\partial_j\phi\, \partial_i u\, \partial_j u + (\partial_t - \Delta\phi)\left(\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon}W(u_\varepsilon)\right) dx \\
&\quad \leq -\int \phi_\sigma |\partial_t u_\varepsilon|^2 dx + C(\sigma)\int \phi_\sigma \left(\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon}W(u_\varepsilon)\right) dx.
\end{aligned}
\tag{38}
$$

Then a Gronwall argument gives that the (localized) Ginzburg-Landau energy stays bounded away from the filament. Note that in the above, equations (35) and (37) are used in a subtle but crucial way,

$$
\begin{aligned}
&\sum_{i,j} \partial_i\partial_j\phi\, \partial_i u\, \partial_j u + (\partial_t - \Delta\phi)\left(\frac{1}{2}|\nabla u_\varepsilon|^2\right) \\
&\leq |\nabla u_\varepsilon|^2 + (-2 + C(\sigma)\phi)\left(\frac{1}{2}|\nabla u_\varepsilon|^2\right) \leq C(\sigma)\frac{\phi}{2}|\nabla u_\varepsilon|^2.
\end{aligned}
$$

Curiously, our monotonicity formula (Lemma 2.8) is in a sense an analogue of this property and will also be used in a crucial step.

To mimic the previous computation, the localized thresholding energies (23) play a pivotal role in our analysis. The following proposition is the key ingredient in our proof of Theorem 2.2. Essentially, it provides a localized energy-dissipation inequality very much like the time integrated version of (38).

Proposition 2.6 (Energy inequality). *Let Γ_t (for $0 \leq t \leq T$), ϕ, and u^h be given in* (13)-(14), (32)*, and* (17)*. Then as $h \to 0$, we have*

$$
E_h(u^h(T), \phi_\sigma(T)) + \int_0^T \int \phi_\sigma \left|G_{h/2} * \partial_t^h u^h\right|^2 dx\, dt \leq C(\sigma) E_h(u^0, \phi_\sigma(0)) + o(1). \tag{39}
$$

Its proof relies on several results which we present next.

The following basic facts about the energy E_h are stated for more general localization function.

Lemma 2.7. *Let $u\colon \mathbb{T}^3 \to \mathbb{S}^1$ be a unit vector field and $\psi\colon \mathbb{T}^3 \to \mathbb{R}$ a bounded function.*

(i) The approximate energy E_h can be written as the following weighted integral of finite differences:

$$
E_h(u, \psi) = \frac{1}{2}\int \psi(x) \int G(z) \left|\frac{u(x) - u(x - \sqrt{h}z)}{\sqrt{h}}\right|^2 dz\, dx. \tag{40}
$$

Furthermore, the energies E_h approximate the Dirichlet energy in the sense that

$$
\lim_{h \downarrow 0} E_h(u, \psi) = \int \psi |\nabla u|^2 dx \quad \text{for unit vector fields } u \in W^{1,2}. \tag{41}
$$

(ii) If $\psi \geq 0$, then the energy satisfies the following approximate monotonicity formula,

$$
E_{N^2h}(u, \psi) \leq E_h(u, \psi) + C\|\nabla\psi\|_\infty \sqrt{N^2h}\, E_h(u), \quad \text{for } N \in \mathbb{N}. \tag{42}
$$

(iii) If $\psi \geq 0$, then the Dirichlet energy of u is controlled by the energy:

$$\int \psi \left|\nabla G_{h/2} * u\right|^2 dx \lesssim E_h(u, \psi). \tag{43}$$

We note the additional property that in fact the energies E_h Γ-converge to the Dirichlet energy. This is because by (ii), the the pointwise convergence in (i) is almost monotone.

The following lemma sharpens the monotonicity statement of (42) in the case of $\phi \equiv 1$. It has an interesting implication, namely a "sharp" version of the comparison between the approximate energy E_h of u and the Dirichlet energy of its convolution $G_{h/2} * u$ in Lemma 2.7 (iii). As mentioned earlier, this sharp inequality will play a crucial role in our analysis.

Lemma 2.8 (Monotonicity)**.** *The approximate energies E_h are monotone in h, i.e., for any fixed measurable $u\colon \mathbb{T}^3 \to \mathbb{S}^1$, we have*

$$\frac{d}{dh} E_h(u) \leq 0. \tag{44}$$

Furthermore, we have the sharp inequality

$$\int |\nabla G_{h/2} * u|^2 \, dx \leq E_h(u). \tag{45}$$

The following lemma gives a bound $O(\frac{1}{h}|\log h|)$ for the squared L^2-norm of the discrete time derivative of the approximate solutions. Note that the bound diverges as $h \to 0$. We believe this bound is far from optimal but it is sufficient for our purposes.

Lemma 2.9. *Let u^h be defined in* (17)*. Then it satisfies the following a priori estimate.*

$$\int_0^T \int \left|\partial_t^h u^h\right|^2 dx\, dt \lesssim \left(1 + \frac{T}{h}\right) E_h(u^0). \tag{46}$$

On the other hand, using the energy dissipation (25), we automatically have the following "better" estimate if the backward in time finite difference is smoothed out by convolving on the length scale $\sqrt{h}$:

$$\int_0^T \int \left|G_{h/2} * \partial_t^h u^h\right|^2 dx\, dt \leq E_h(u^0). \tag{47}$$

Both (46) and (47) will be used in our proof.

Recall that we will recover *two* equations to describe the limit of u^h as $h \longrightarrow 0$. The first is the motion law of the vorticity set which in the limit is a curve moving by its curvature. The second is the equation for the phase function which lives away from the vorticity set and in the limit solves a diffusion equation. To this end, we consider *inner* and *outer variations* of u^n leading to *two* of Euler-Lagrange equations for the minimization problem (24).

- The inner variation u_s of $u\colon \mathbb{T}^3 \to S^1$ is given by the variation of domain along a smooth vector field ξ:

$$u_s(x) = u\big(x - s\xi(x)\big), \quad \text{so that} \quad \partial_s u_s\big|_{s=0} = -\xi \cdot \nabla u. \tag{48}$$

- The outer variation $\tilde{u}_s$ of u in direction of a smooth vector field φ is given by

$$\tilde{u}_s := \frac{u + s\varphi}{|u + s\varphi|}, \quad \text{so that} \quad \partial_s \tilde{u}_s\big|_{s=0} = (Id - u \otimes u)\, \varphi. \tag{49}$$

Using the above, we have the following statements.

Lemma 2.10 (Euler-Lagrange equations)**.** *Let u^h be the piecewise constant in time interpolation* (17)*. Then it satisfies the following two statements.*

(i) For any smooth vector field $\xi\colon \mathbb{T}^3\times[0,T]\to\mathbb{R}^3$ we have

$$2\iint G_{h/2}*\partial_t^h u^h\cdot(\xi\cdot\nabla)\,G_{h/2}*u^h\,dx\,dt \tag{50}$$
$$=\frac{1}{h}\iint(\nabla\cdot\xi)\,(1-u^h\cdot G_h*u^h)\,dx\,dt-2\sum_{i,j}\iint\partial_i\xi_j\,\partial_iG_{h/2}*u^h\cdot\partial_jG_{h/2}*u^h\,dx\,dt+o(1).$$

(ii) For any smooth function $\zeta\colon\mathbb{T}^3\times[0,T]\to\mathbb{R}$, we have

$$\iint(u_j^h\partial_t^{-h}G_h*u_i^h-u_i^h\partial_t^{-h}G_h*u_j^h)\zeta+(u_j^h\nabla G_h*u_i^h-u_i^h\nabla G_h*u_j^h)\cdot\nabla\zeta\,dx\,dt=o(1). \tag{51}$$

Now we get to the proofs for all the statements and the main result.

3 Proofs of the lemmas and the main result

We first state some basic facts about the heat kernel which will be used frequently. Recall the notation for the heat kernel on $\mathbb{R}^d$:

$$G_h(z):=\frac{1}{(4\pi h)^{d/2}}\exp\Big(-\frac{|z|^2}{4h}\Big)\quad z\in\mathbb{R}^d,\quad h>0.$$

The following semi-group and factorization properties hold for G:

$$\begin{aligned}&G_{s+t}=G_s*G_t && \text{for } s,t>0,\\ &G_h(z)=G_h^1(z_1)\,G_h^{d-1}(z') && \text{for } z=(z_1,z'),\quad z_1\in\mathbb{R},\quad z'\in\mathbb{R}^{d-1}\end{aligned} \tag{52}$$

where G^1 and G^{d-1} are the one- and $(d-1)$-dimensional Gaussian kernels respectively. We also have the following statements about G_h:

$$0\le G_h(z)\lesssim\frac{1}{h^{d/2}},\quad \int_{\mathbb{R}^d}G_h(z)\,dz=1,\quad \int_{\mathbb{R}^d}\frac{|z|^2}{h}G_h(z)\,dz=2, \tag{53}$$

$$\nabla G_h(z)=-\frac{z}{2h}G_h(z),\quad |\nabla G_h(z)|\lesssim\frac{1}{\sqrt{h}}G_{2h}(z), \tag{54}$$

$$\nabla^2G_h(z)=\left(\frac{z}{2h}\otimes\frac{z}{2h}-\frac{1}{2h}Id\right)G_h(z). \tag{55}$$

Due to the symmetry of the heat kernel, $G_h(x-z)=G_h(z-x)$, the convolution with G_h is self-adjoint in the L^2-sense:

$$\langle f,\,G_h*g\rangle_{L^2}=\int f(x)(G_h*g)(x)\,dx=\int(G_h*f)(x)g(x)\,dx=\langle G_h*f,\,g\rangle_{L^2}\,. \tag{56}$$

Finally, we have the following expansion of the commutator (27) between G_h* and multiplication by a test function ψ. For later convenience, it is stated for $G_{h/2}$.

Lemma 3.1. *For $\psi:\mathbb{T}^3\longrightarrow\mathbb{R}$ and $V:\mathbb{T}^3\longrightarrow\mathbb{R}^d$, it holds that*

$$\left(\frac{1}{h}\left[G_{h/2}*,\psi\right]V\right)(x)=\nabla\psi(x)\cdot\big(\nabla G_{h/2}*V\big)(x)+O\big(\|\nabla^2\psi\|_\infty\frac{|z|^2}{h}G_{h/2}*|V|\big). \tag{57}$$

It will be seen that the first term of (57) dominates the second. Hence we will often write the commutator asymptotically as

$$\frac{1}{h}\left[G_{h/2}*,\psi\right]V\approx(\nabla\psi\cdot\nabla)\,G_{h/2}*V\quad\text{or}\quad\left[G_{h/2}*,\psi\right]V\approx h\nabla\psi\cdot\left(\nabla G_{h/2}*V\right). \tag{58}$$

Proof. Expanding $\psi(x-z)-\psi(x)=-z\cdot\nabla\psi(x)+O(|z|^2\|\nabla\psi\|_\infty)$, we obtain

$$\begin{aligned}
&\frac{1}{h}\left[G_{h/2}*,\psi\right]V\\
&=\frac{1}{h}\int G_{h/2}(z)\left(\psi(x-z)-\psi(x)\right)V(x-z)\,dz\\
&=\frac{1}{h}\int G_{h/2}(z)\left(-z\cdot\nabla\psi(x)+O(|z|^2\|\nabla\psi\|_\infty)\right)V(x-z)\,dz\\
&=\nabla\psi(x)\int\frac{-z}{h}G_{h/2}(z)V(x-z)\,dz+O\left(\int G_{h/2}(z)\frac{|z|^2}{h}\left\|\nabla^2\psi\right\|_\infty|V(x-z)|\,dz\right)\\
&=\nabla\psi(x)\cdot(\nabla G_{h/2}*V)(x)+O\left(\left\|\nabla^2\psi\right\|_\infty\left(\frac{|z|^2}{h}G_{h/2}(z)\right)*|V|\right),
\end{aligned}$$

which is precisely the statement of the lemma. □

3.1 Proof of the lemmas

We first give the proof of Lemma 2.4 illustrating the minimizing movements interpretation of the thresholding scheme.

Proof of Lemma 2.4. We will only prove the localized version (26) as the global minimization property (24) follows by choosing $\psi\equiv 1$. The energy-dissipation estimate (25) follows by successively comparing the functional values for (24) evaluated at u^n and u^{n-1}.

We first note that the combination of convolution and thresholding $u^n:=\frac{G_h*u^{n-1}}{|G_h*u^{n-1}|}$ is equivalent to maximizing $(u\cdot G_h*u^{n-1})(x)$ *pointwise at each* x among all $u\colon\mathbb{T}^3\to\mathbb{R}^2$ with $|u|\le 1$. (This simply follows from the fact that for each $a\neq 0\in\mathbb{R}^2$, $\hat a=\frac{a}{|a|}$ is the unique maximizer of $a\cdot b$ among $|b|\le 1$.) Therefore, for any non-negative function $\psi\ge 0$, u^n minimizes the linear functional

$$-\frac{2}{h}\int\psi\,u\cdot G_h*u^{n-1}\,dx.$$

Using

$$\begin{aligned}
-2u\cdot G_h*u^{n-1}=&-u\cdot G_h*u+(u-u^{n-1})\cdot G_h*(u-u^{n-1})\\
&-u^{n-1}\cdot G_h*u^{n-1}+u^{n-1}\cdot G_h*u-u\cdot G_h*u^{n-1},
\end{aligned}$$

we see that u^n effectively minimizes the following functional

$$\begin{aligned}
\frac{1}{h}\int\psi(1-u\cdot G_h*u)+\frac{1}{h}\int\psi(u-u^{n-1})\cdot G_h*(u-u^{n-1})&\\
+\frac{1}{h}\int\psi(u^{n-1}\cdot G_h*u-u\cdot G_h*u^{n-1}).&
\end{aligned}$$

Note that by (56), we can write the last term of the above as

$$\frac{1}{h}\int u\cdot G_h*(\psi u^{n-1})-u\cdot\psi G_h*u^{n-1})=\frac{1}{h}\int u\cdot[G_h*,\psi]u^{n-1}.$$

Subtracting the irrelevant term $\frac{1}{h}\int u^{n-1}[G_h*,\psi]u^{n-1}$ to the minimization gives exactly expression (26).

Finally, note that with $\psi \equiv 1 > 0$ and tracing back our steps we see that thresholding is indeed *equivalent* to solving the global minimization problem (24). □

Now we continue to the proofs of the other technical lemmas.

Proof of Lemma 2.7. Statement (i)(40) follows from a direct computation. Indeed, due to the normalization $\int G(z)\,dz = 1$, we have

$$E_h(u,\phi) = \frac{1}{2h}\int \psi(x)\int G(z)\,2\left(1-u(x)\cdot u(x-\sqrt{h}z)\right)dx\,dz.$$

Then (40) follows from the identity $2(1-u\cdot v) = |u-v|^2$ valid for any pair of unit vectors u and v.

For (i)(41), note that for $u\in W^{1,2}$, the finite differences $\frac{u(x)-u(x-\sqrt{h}z)}{\sqrt{h}}$ in the representation (40) of E_h converge to the directional derivative $(z\cdot\nabla)\,u(x)$ pointwise almost everywhere. Thus we obtain by Fatou's lemma

$$\frac{1}{2}\int\psi(x)\int G(z)\,|(z\cdot\nabla)\,u(x)|^2\,dz\,dx \le \liminf_{h\to 0} E_h(u,\psi). \tag{59}$$

(Alternatively, it is also straightforward to see that the finite differences converge weakly in $L^2(G(z)dz\,dx)$, which clearly implies (59).) Next we compute the inner integral explicitly:

$$\begin{aligned}\int G(z)\,|(z\cdot\nabla)u(x)|^2\,dz &= \sum_{i=1}^d |\partial_{x_i}u(x)|^2\int G(z)z_i^2\,dz\\ &= \sum_{i=1}^d |\partial_{x_i}u(x)|^2\iint G^1(z_1)G^{d-1}(z')z_1^2\,dz_1\,dz' = 2\,|\nabla u(x)|^2,\end{aligned}$$

where we have used the symmetry and factorization property of the kernel (52). Therefore, we obtain

$$\int\psi(x)\,|\nabla u(x)|^2\,dx \le \liminf_{h\to 0} E_h(u,\psi)\quad\text{for all non-negative test functions }\psi. \tag{60}$$

Therefore, by linearity in ψ, it suffices to prove the statement with $\psi\equiv 1$. Note that this will imply the *strong* convergence of the difference quotients in $L^2(G(z)dz\,dx)$.

An application of the fundamental theorem of calculus and the translation invariance of $\int\,dx$ yield

$$\begin{aligned}E_h(u) &= \frac{1}{2}\iint G(z)\int_0^1\int_0^1 (z\cdot\nabla)\,u(x+s\sqrt{h}z)\cdot(z\cdot\nabla)\,u(x+t\sqrt{h}z)\,ds\,dt\,dz\,dx\\ &= \frac{1}{2}\iint G(z)\,(z\cdot\nabla)\,u(x)\otimes z\colon\int_0^1\int_0^1\nabla u(x+(t-s)\sqrt{h}z)\,ds\,dt\,dz\,dx.\end{aligned}$$

Since $(z\cdot\nabla)\,u(x)\otimes z\in L^2(G(z)dz\,dx)$ and furthermore

$$\int_0^1\int_0^1\nabla u(x+(t-s)\sqrt{h}z)\,ds\,dt \rightharpoonup \nabla u(x)\quad\text{in }L^2(G(z)dz\,dx),$$

we obtain

$$\lim_{h\to 0}E_h(u) = \frac{1}{2}\iint G(z)\,|(z\cdot\nabla)\,u(x)|^2\,dz\,dx.$$

Therefore we do have

$$\lim_{h\to 0} E_h(u) = \int |\nabla u|^2\, dx,$$

and by linearity and the lower-semicontinuity we obtain (41).

(ii) follows from (i) and Jensen's inequality. Indeed, we may rewrite E_{N^2h} as

$$E_{N^2h}(u,\psi) \overset{(i)}{=} \frac{1}{2}\iint G(z)\,\psi(x)\Big|\frac{1}{N}\sum_{n=1}^{N}\frac{u(x-(n-1)\sqrt{h}z)-u(x-n\sqrt{h}z)}{\sqrt{h}}\Big|^2 dz\,dx,$$

and by Jensen's inequality the integrand can be estimated:

$$\begin{aligned}\Big|\frac{1}{N}\sum_{n=1}^{N}&\frac{u(x-(n-1)\sqrt{h}z)-u(x-n\sqrt{h}z)}{\sqrt{h}}\Big|^2\\ &\leq \frac{1}{N}\sum_{n=1}^{N}\Big|\frac{u(x-(n-1)\sqrt{h}z)-u(x-n\sqrt{h}z)}{\sqrt{h}}\Big|^2.\end{aligned}$$

By the translation invariance of $\int dx$ in the case of $\psi\equiv 1$ we obtain the monotonicity

$$E_{N^2h}(u) \leq E_h(u). \tag{61}$$

For non-constant $\psi\geq 0$, we obtain

$$\begin{aligned}E_{N^2h}(u,\psi) &\leq \frac{1}{2}\iint G(z)\left(\frac{1}{N}\sum_{n=1}^{N}\psi\big(x+(n-1)\sqrt{h}z\big)\right)\Big|\frac{u(x)-u(x-\sqrt{h}z)}{\sqrt{h}}\Big|^2 dx\,dz\\ &\leq \frac{1}{2}\iint G(z)\left(\psi(x)+\|\nabla\psi\|_\infty N\sqrt{h}|z|\right)\Big|\frac{u(x)-u(x-\sqrt{h}z)}{\sqrt{h}}\Big|^2 dx\,dz.\end{aligned}$$

Using $G(z)|z|\lesssim G_4(z)$ and the monotonicity (61) for the error-term we obtain (42).

For (iii), we first observe that by $\int \nabla G_h(z)\,dz = 0$ and Cauchy-Schwarz we have

$$\begin{aligned}\int \psi\left|\nabla G_{h/2}*u\right|^2 dx &= \int\psi\left|\int \nabla G_{h/2}(z)\,(u(x)-u(x-z))\,dz\right|^2 dx \\ &\leq \int\psi\left(\int\left|\nabla G_{h/2}(z)\right|dz\right)\left(\int\left|\nabla G_{h/2}(z)\right||u(x)-u(x-z)|^2\,dz\right)dx.\end{aligned} \tag{62}$$

Using the integral estimate $\int\left|\nabla G_{h/2}(z)\right|dz\lesssim\frac{1}{\sqrt{h}}$ for the first inner integral and the pointwise estimate $\left|\nabla G_{h/2}(z)\right|\lesssim\frac{1}{\sqrt{h}}G_h(z)$ for the second one, we obtain

$$\int\psi\left|\nabla G_{h/2}*u\right|^2 dx \lesssim E_h(u,\psi).$$ □

Proof of Lemma 2.8. In order to verify the monotonicity of the energy let us compute E_h in Fourier space, i.e., in terms of the Fourier coefficients $\hat{u}(k)$ of u. Indeed, since $|u|\equiv 1$ and by Plancharel we have

$$E_h(u) = \frac{1}{h}\int u\cdot(u-G_h*u)\,dx = \frac{1}{h}\sum_{k\in\mathbb{Z}^3}\bar{\hat{u}}(k)\cdot\left(\hat{u}-\widehat{G_h*u}\right)(k) = \frac{1}{h}\sum_{k\in\mathbb{Z}^3}\big(1-\widehat{G}_h(k)\big)|\hat{u}(k)|^2,$$

where the Fourier coefficients (note that G_h is not periodic) of the kernel G_h are given by

$$\widehat{G}_h(k) = \int_{\mathbb{R}^3} G_h(z)\,e^{-2\pi i\,k\cdot z}dz = \exp\Big(-4\pi^2 h|k|^2\Big).$$

Therefore, we may simply compute the derivative of E_h:

$$\frac{d}{dh}E_h(u) = \sum_{k\in\mathbb{Z}^3} \frac{\partial}{\partial h}\left[\frac{1}{h}\left(1-\widehat{G}_h(k)\right)\right]|\hat{u}(k)|^2.$$

Since

$$\frac{\partial}{\partial h}\left[\frac{1}{h}\left(1-\widehat{G}_h\right)\right] = -\frac{1}{h^2}\left(1-\widehat{G}_h\right) - \frac{1}{h}\partial_h\widehat{G}_h = -\frac{1}{h^2}\left(1+h\partial_h\widehat{G}_h-\widehat{G}_h\right),$$

it is enough to check whether

$$\left(1+h\partial_h\widehat{G}_h-\widehat{G}_h\right) \geq 0. \tag{63}$$

To do so, we write $s := \left(\frac{2\pi}{\Lambda}\right)^2 h|k|^2$. Then the above holds due to the fact that $e^s \geq 1+s$ for all $s \geq 0$. This concludes the argument for (44).

Computing the derivative in (44) in physical space, i.e., in terms of u instead of $\hat{u}$, we obtain

$$\frac{dE_h}{dh} = \int \partial_h\left[\frac{1}{h}\left(1-u\cdot G_h * u\right)\right]dx.$$

Since G_h is the fundamental solution of the heat equation, cf. (16), we compute

$$\partial_h\left[\frac{1}{h}\left(1-u\cdot G_h * u\right)\right] = -\frac{1}{h^2}\left(1-u\cdot G_h * u\right) - \frac{1}{h}u\cdot\Delta G_h * u.$$

Therefore, using the semi-group property of G and the anti-symmetry of its gradient ∇G we obtain

$$-\frac{1}{h}E_h(u) - \frac{1}{h}\int u\cdot\Delta G_h * u\,dx = -\frac{1}{h}E_h(u) + \frac{1}{h}\int|\nabla G_{h/2} * u|^2 dx,$$

which is precisely (45).

□

Remark 3.2. An alternative approach to the proof above is to use directly the energy dissipation relation of the energy $\frac{1}{2}\int|v|^2\,dx$ for the heat equation. Combined with $|u| = 1$ we obtain

$$E_h(u) = \frac{2}{h}\int_0^{h/2}\int|\nabla G_t * u|^2\,dx\,dt. \tag{64}$$

This means that the thresholding energy E_h is nothing but an average of (twice the) Dirichlet energies along the heat flow. By the energy dissipation relation of the Dirichlet energy for the heat equation we obtain in particular

$$\int\left|\nabla G_{h/2} * u\right|^2 dx \leq E_h(u) \leq \int|\nabla u|^2\,dx.$$

Note that in our case, the second inequality is empty because our state variable u is not in $W^{1,2}$. In view of (64), the reverse inequality of (43), namely an estimate of $E_h(u)$ in terms of the Dirichlet energy of $G_{h/2} * u$, seems not obvious. However, there are two simple cases. If $u \in W^{2,2}$, such an estimate is available. The second easy example is the vector field u^0 defined in (30). It is easy to check that such an estimate is available as well for u^0.

Proof of Lemma 2.9. Using the triangle and Young's inequalities, we have for any two vector fields u, v

$$|u-v|^2 \lesssim |G_h * (u-v)|^2 + |G_h * u - u|^2 + |G_h * v - v|^2.$$

If additionally $|u| \equiv 1$, we have

$$|G_h * u - u|^2 = 2(1 - u \cdot G_h * u) - (1 - G_h * u \cdot G_h * u).$$

Therefore when applying this to $u = u^n$ and $v = u^{n-1}$, the symmetry of the kernel G_h implies

$$\int_0^T \int \left|\partial_t^h u^h\right|^2 dx\, dt \lesssim \int_0^T \int \left|G_h * \partial_t^h u^h\right|^2 dx\, dt + 2 \sum_{n=0}^N \left(E_h(u^n) - E_{2h}(u^n)\right),$$

which by the energy-dissipation estimate (25) yields the claim. □

Next we turn to the derivation of the two Euler-Lagrange equations for u.

Proof of Lemma 2.10(i). We first prove (50), the Euler-Lagrange equation coming from *inner* variations u_s defined in (48). From the minimality (24), we obtain

$$\frac{d}{ds}\Big|_{s=0} \left(E_h(u_s^n) + \frac{1}{h} \int \left(u_s^n - u^{n-1}\right) \cdot G_h * \left(u_s^n - u^{n-1}\right) dx \right) = 0. \tag{65}$$

We begin by computing the first variation $\frac{d}{ds} E_h(u_s^n)$ of the energy E_h, which will give us the right-hand side of (50). We work on a fixed time slice and drop the superscript n for a cleaner notation. Note that

$$\frac{d}{ds}\Big|_{s=0} E_h(u_s) = \frac{1}{h} \int u \cdot G_h * (\xi \cdot \nabla u) + \xi \cdot \nabla u \cdot G_h * u\, dx.$$

Since $\xi \cdot \nabla u = \nabla \cdot (\xi\, u) - (\nabla \cdot \xi)\, u$ and by the symmetry property (56) of $G_h *$, we obtain

$$\frac{d}{ds}\Big|_{s=0} E_h(u_s) = \frac{1}{h} \int u \,[\nabla G_h *, \xi \cdot]\, u\, dx - \frac{2}{h} \int (\nabla \cdot \xi)\, u \cdot G_h * u\, dx.$$

Now we claim that

$$\begin{aligned} &\frac{1}{h} \int u \,[\nabla G_h *, \xi \cdot]\, u\, dx \\ &\quad = 2 \int \nabla \xi \colon u \nabla^2 G_h * u\, dx + \frac{1}{h} \int (\nabla \cdot \xi)\, u \cdot G_h * u\, dx + O\left(\left\|\nabla^2 \xi\right\|_\infty \sqrt{h} E_h(u) \right). \end{aligned} \tag{66}$$

This is intuitively correct, since we expect

$$[\nabla G_h *, \xi \cdot]\, u \approx \nabla \xi \colon (-z \otimes \nabla G_h(z)) * u$$

so that we formally have

$$\frac{1}{h} \int u \,[\nabla G_h *, \xi \cdot]\, u\, dx \approx \int \nabla \xi \colon u\, (-\frac{z}{h} \otimes \nabla G_h(z)) * u\, dx.$$

Note that the kernel on the right may be rewritten as $-\frac{z}{h} \otimes \nabla G_h = \frac{1}{h} G_h\, Id + 2 \nabla^2 G_h$, which concludes the formal reasoning for (66).

Granted (66), we have

$$\frac{d}{ds}\Big|_{s=0} E_h(u_s) = 2 \int \nabla \xi \colon u \nabla^2 G_h * u\, dx - \frac{1}{h} \int (\nabla \cdot \xi)\, u \cdot G_h * u\, dx + o(1) \tag{67}$$

which is essentially the right hand side of (50), modulo an integration by parts.

In order to make (66) rigorous, we rewrite the integral on its left-hand side as

$$\frac{1}{h}\int u\,[\nabla G_h *, \xi\cdot]\,u\,dx = \frac{1}{2h}\iint \nabla G_h(z)\cdot(\xi(x)-\xi(x-z))\,(-2u(x)\cdot u(x-z))\,dz\,dx$$

Since $|u(x)|^2,\ |u(x-z)|^2 \equiv 1$ so that $2-2u(x)u(x-z) = |u(x)-u(x-z)|^2$ and

$$\iint \nabla G_h(z)\cdot(\xi(x)-\xi(x-z))\ dz\,dx = 0,$$

we have

$$\begin{aligned}
&\frac{1}{h}\int u\,[\nabla G_h *, \xi\cdot]\,u\,dx \\
=\ &\frac{1}{2h}\iint \nabla G_h(z)\cdot(\xi(x)-\xi(x-z))\,|u(x)-u(x-z)|^2\,dz\,dx \\
=\ &\frac{1}{2h}\iint \nabla G_h(z)\cdot\big(z\cdot\nabla\xi(x) + O(\left\|\nabla^2\xi\right\|_\infty |z|^2)\big)\,|u(x)-u(x-z)|^2\,dz\,dx.
\end{aligned}$$

The above integral splits into two contributions:

1. The one coming from the first-order term $z\cdot\nabla\xi(x)$ simplifies to

   $$\frac{1}{2h}\iint \nabla\xi\colon z\otimes\nabla G_h(z)(-2u(x)\cdot u(x-z))\,dz\,dx,$$

   because here again the terms including $|u(x)|^2\equiv 1$ or $|u(x-z)|^2\equiv 1$ vanish identically. As in the conclusion of the above formal argument, we obtain the leading-order term in the expansion (66).

2. The second-order term $O(|z|^2)$ in the expansion of the test vector field ξ is negligible as $h\to 0$. Indeed, since

   $$\left|\frac{|z|^2}{h}\nabla G\right| \lesssim \left|\frac{|z|^3}{h^2}G_h\right| \lesssim \frac{1}{\sqrt{h}}G_{2h},$$

   we have

   $$\begin{aligned}
   &\frac{1}{h}\iint |z|^2|\nabla G_h(z)|\,|u(x)-u(x-z)|^2\,dz\,dx \\
   \lesssim\ &\frac{1}{\sqrt{h}}\iint G_{2h}(z)\,|u(x)-u(x-z)|^2\,dz\,dx \overset{(40)}{\sim} \sqrt{h}E_{2h}(u) \overset{(44)}{\leq} \sqrt{h}E_h(u).
   \end{aligned}$$

This concludes the rigorous justification of (66).

Going from (67) to the symmetrized form on the right-hand side of (50) requires another manipulation which we provide now. To this end, we rewrite

$$2\int \nabla\xi : u\nabla^2 G_h * u\,dx = 2\int \nabla\xi\colon G_{h/2}*u\,\nabla^2 G_{h/2}*u\,dx + 2\int \left[G_{h/2}*, \nabla\xi\right] u\,\nabla^2 G_{h/2}*u\,dx, \quad (68)$$

where we have used the symmetry and semi-group properties (52) of the kernel. The leading-order term is the first right-hand side term, which after integration by parts equals

$$-2\sum_{i,j}\int \partial_i\xi_j\partial_i G_{h/2}*u\,\partial_j G_{h/2}*u\,dx - 2\int \Delta\xi\cdot G_{h/2}*u\,\nabla G_{h/2}*u\,dx.$$

Here, the first term is the desired term in the Euler-Lagrange equation (50); the second one is of lower order: since by $G_{h/2} * u\,\nabla G_{h/2} * u = \nabla(\frac{1}{2}|G_{h/2} * u|^2)$, we have

$$-2\int \Delta\xi \cdot G_{h/2} * u\,\nabla G_{h/2} * u\,dx = 2\int \Delta(\nabla\cdot\xi)\frac{1}{2}\left|G_{h/2} * u\right|^2 dx,$$

which by $\int \Delta(\nabla\cdot\xi)\,dx = 0$ is equal to

$$-\int \Delta(\nabla\cdot\xi)\left(1 - \left|G_{h/2} * u\right|^2\right) dx.$$

Therefore, the first right-hand side term of (68) and the right-hand side of the Euler-Lagrange equation (50) indeed agree to leading order:

$$\left|-2\int \Delta\xi \cdot G_{h/2} * u\,\nabla G_{h/2} * u\,dx\right| \lesssim \left\|\nabla^3\xi\right\|_\infty \int \left(1 - \left|G_{h/2} * u\right|^2\right) dx = \left\|\nabla^3\xi\right\|_\infty hE_h(u) = o(1),$$

where we have used the symmetry and semi-group properties (52) of the kernel once more.

Now we turn to the second right-hand side term of (68). By the commutator estimate (57), we obtain

$$\begin{aligned}\int \left[G_{h/2}*, \nabla\xi\right] u\,\nabla^2 G_{h/2} * u\,dx =& h\sum_{i,j,k}\int \partial_i\partial_j\xi_k \colon \nabla_i G_{h/2} * u\,\partial_j\partial_k G_{h/2} * u\,dx\\ &+ O\Big(\|\nabla^3\xi\|_\infty h\int \left|\nabla^2 G_{h/2} * u\right| dx\Big).\end{aligned}$$

Note that the second right-hand side term vanishes as $h \to 0$. Indeed, using Jensen's inequality, we have

$$\|\nabla^3\xi\|_\infty h\int \left|\nabla^2 G_{h/2} * u\right| dx \lesssim \|\nabla^3\xi\|_\infty\sqrt{h}\left(h\int \left|\nabla^2 G_{h/2} * u\right|^2 dx\right)^{\frac{1}{2}}.$$

Exploiting $\int \nabla^2 G_{h/2}\,dz = 0$ and repeating the argument (62) with $\sqrt{h}\nabla^2 G_{h/2}$ instead of $\nabla G_{h/2}$, we obtain

$$\|\nabla^3\xi\|_\infty\sqrt{h}\sqrt{E_h(u)} = o(1).$$

By symmetry of the second derivatives of ξ, and integrating by parts, we obtain

$$h\sum_{i,j,k}\int \partial_i\partial_j\xi_k\partial G_{h/2} * u\,\partial_j\partial_k G_{h/2} * u\,dx = -\frac{h}{2}\sum_{i,j,k}\int \partial_i\partial_j(\nabla\cdot\xi)\partial_i G_{h/2} * u\,\partial_j G_{h/2} * u\,dx,$$

which is controlled by

$$\|\nabla^3\xi\|_\infty h\int \left|\nabla G_{h/2} * u\right|^2 dx \overset{(43)}{\lesssim} \|\nabla^3\xi\|_\infty hE_h(u) = o(1).$$

Next we turn to the first variation of the metric term:

$$\frac{d}{ds}\Big|_{s=0}\frac{1}{h}\int \left(u_s^n - u^{n-1}\right)\cdot G_h * \left(u_s^n - u^{n-1}\right) dx = -2\int \frac{u^n - u^{n-1}}{h}\cdot G_h * (\xi\cdot\nabla u^n)\,dx.$$

Using the semigroup property (52) of G_t, the self-adjointness (56) of $G*$, and the relation $\xi\cdot\nabla u = \nabla\cdot(\xi\,u) - (\nabla\cdot\xi)\,u$, we obtain

$$\begin{aligned}&-2\int \frac{u^n - u^{n-1}}{h}\cdot G_h * (\xi\cdot\nabla u^n)\,dx\\ &\qquad = -2\int G_{h/2} * \left(\frac{u^n - u^{n-1}}{h}\right)\cdot(\xi\cdot\nabla)\,G_{h/2} * u^n\,dx + \mathrm{Err} \qquad (69)\end{aligned}$$

where

$$\mathrm{Err} = -2 \int G_{h/2} * \left(\frac{u^n - u^{n-1}}{h} \right) \cdot \left(\left[\nabla G_{h/2} *, \xi \cdot \right] u^n - G_{h/2} * \left((\nabla \cdot \xi)\, u^n \right) \right) dx. \tag{70}$$

Note that, after integration in time, (69) is precisely the left hand side of (50) if we can indeed show that, the time integral of Err converges to zero as $h \to 0$.

We now show that this is indeed the case. Omitting the superscript n for a moment and setting again $u^z := u(\cdot + z)$ we may rewrite the commutator

$$\left[\nabla G_{h/2} *, \xi \cdot \right] u = \int \nabla G_{h/2}(z) \cdot \left(\xi^{-z} - \xi \right) \left(u^{-z} - u \right) dz + u \, G_{h/2} * (\nabla \cdot \xi).$$

Estimating $|\xi^{-z} - \xi| \le \|\nabla \xi\|_\infty |z|$ and collecting the two terms involving the divergence of the test vector field ξ we obtain

$$\left[\nabla G_{h/2} *, \xi \cdot \right] u - G_{h/2} * \left((\nabla \cdot \xi)\, u \right) = - \left[G_{h/2} *, (\nabla \cdot \xi) \right] u + O\Big(\|\nabla \xi\| \int \frac{|z|^2}{h} G_{h/2}(z) |u^{-z} - u| dz \Big).$$

Note that $\frac{|z|^2}{h} G_{h/2}(z) \lesssim G_h(z)$. Now we estimate the commutator on the right-hand side:

$$\left| \left[G_{h/2} *, (\nabla \cdot \xi) \right] u \right| \le \|\nabla^2 \xi\| \left(|z| \, G_{h/2}(z) \right) * |u| \lesssim \|\nabla^2 \xi\| \sqrt{h}.$$

Therefore by Cauchy-Schwarz, we have the following estimate for the time integral of Err,

$$\int \mathrm{Err}(t)\, dt \lesssim \left(\|\nabla \xi\|_\infty + \|\nabla^2 \xi\|_\infty \right) \times \\ \left(\iint \left| G_{h/2} * \partial_t^h u^h \right|^2 dx\, dt \right)^{\frac{1}{2}} \left(\iint \Big(h + \int G_h(z) \left| u^h(x-z) - u^h(x) \right|^2 dz \Big) dx\, dt \right)^{\frac{1}{2}}.$$

Using the representation (40) of the energy and the energy-dissipation estimate (25), we see that the error term is bounded by

$$C \left(\|\nabla \xi\|_\infty + \|\nabla^2 \xi\|_\infty \right) \left(E_h(u^0) \right)^{\frac{1}{2}} \left(hT(1 + E_h(u^0) \right)^{\frac{1}{2}} \overset{(28)}{=} O(\sqrt{h} \log h).$$

Together with (66), this concludes the proof of (50). □

Proof of Lemma 2.10(ii). First we prove the slightly different version

$$\left(Id - u^h \otimes u^h \right) \left(G_h * \partial_t^{-h} u^h - \Delta_h u^h \right) = 0, \tag{71}$$

where Δ_h is an approximation of the Laplacian, given by the following average of second differences:

$$\Delta_h u(x) := \int G(z) \frac{u(x + \sqrt{h} z) - 2u(x) + u(x - \sqrt{h} z)}{2h} \, dz.$$

Note that indeed $\lim_{h \to 0} \Delta_h u = \Delta u$ for $u \in W^{2,2}$ and thus (71) is the analogue of the classical equation

$$(Id - u \otimes u)(\partial_t u - \Delta u) = 0. \tag{72}$$

In order to derive (71), we start from the minimality (24), which yields (65) with u_s^n replaced by $\tilde{u}_s^n$. We use the representation (40) of the energy to compute the first variation $\frac{d}{ds} E_h(\tilde{u}_s^n)$, again drop the superscript n, and use the short-hand notation $u^z := u(\cdot + z)$ in the following computation:

$$\frac{d}{ds}\Big|_{s=0} E_h(\tilde{u}_s) = \frac{1}{h} \int G_h(z) \int (u - u^{-z}) \cdot \left((Id - u \otimes u)\varphi - (Id - u^{-z} \otimes u^{-z}) \varphi^{-z} \right) dx\, dz,$$

which because of the translation invariance of $\int dx$ is equal to

$$\frac{1}{h}\int G_h(z)\int \big[(u-u^{-z})-(u^z-u)\big]\cdot(Id-u\otimes u)\varphi dx\,dz = -2\int \Delta_h u\cdot(Id-u\otimes u)\varphi\,dx.$$

The first variation of the metric term is

$$\frac{d}{ds}\Big|_{s=0}\frac{1}{h}\int\left(\tilde u^n_s-u^{n-1}\right)\cdot G_h*\left(\tilde u^n_s-u^{n-1}\right)dx = 2\int G_h*\left(\frac{u^n-u^{n-1}}{h}\right)\cdot(Id-u^n\otimes u^n)\varphi\,dx.$$

This yields the "classical" version (71) of the second Euler-Lagrange equation (51).

To obtain the "weak" form (51) of the Euler-Lagrange equation (71), we proceed as in the well-known case of harmonic map heat flow [15]. We briefly recall this idea described in Evans' book [21, §5.1.1]. We follow this more general approach because it is a natural way to derive the equations for u (or the phase) away from the filament, and furthermore because it directly generalizes to higher dimensions, which we will exploit in §4.3.

The idea is to take the wedge-product of (71) and u which leads to cancellations of nonlinear terms involving derivatives. More precisely, testing the i^{th} component of (71) with the j^{th} component u_j times a test function ζ and subtracting the the same quantity with exchanged roles for i and j one obtains that a solution to (72) solves

$$\iint (u_j\partial_t u_i-u_i\partial_t u_j)\,\zeta-(u_j\Delta u_i-u_i\Delta u_j)\,\zeta\,dx\,dt=0$$

and when integrating by parts in the last term, the terms $\nabla u_i\cdot\nabla u_j\,\zeta$ cancel and we obtain

$$\iint (u_j\partial_t u_i-u_i\partial_t u_j)\,\zeta+(u_j\nabla u_i-u_i\nabla u_j)\cdot\nabla\zeta\,dx\,dt=0 \tag{73}$$

for all test functions ζ. Note that this formulation has the advantage of being compact in $W^{2,2}$.

In our case of (71), we follow the same idea. Let us omit the superscript h again for this computation. We obtain in the first step that our solution $u=u^h$ of (71) satisfies

$$\iint \left(u_j\partial_t^h G_h*u_i-u_i\partial_t^h G_h*u_j\right)\zeta-(u_j\Delta_h u_i-u_i\Delta_h u_j)\,\zeta\,dx\,dt=0,$$

where Δ_h denotes the above mentioned approximation of the Laplacian and ∂_t^{-h} the difference quotient backwards in time. The integration by parts gets replaced by the following discrete version. Writing again $u^z:=u(\,\cdot\,+z)$ we have

$$\begin{aligned}&\int (u_j\Delta_h u_i-u_i\Delta_h u_j)\,\zeta\,dx\\ &\quad=\frac{1}{2h}\int G_h(z)\int u_j[(u_i^z-u_i)-(u_i-u_i^{-z})]\zeta-u_i[(u_j^z-u_j)-(u_j-u_j^{-z})]\zeta\,dx\,dz,\end{aligned}$$

which by the translation invariance of $\int dx$ is equal to

$$\begin{aligned}&\frac{1}{2h}\int G_h(z)\int u_j(u_i^z-u_i)\zeta-u_j^z(u_i^z-u_i)\zeta^z-u_i(u_j^z-u_j)\zeta+u_i^z(u_j^z-u_j)\zeta^z\,dx\,dz\\ &\quad=\frac{1}{2h}\int G_h(z)\int (u_i^z-u_i)(u_j\zeta-u_j^z\zeta^z)-(u_j^z-u_j)(u_i\zeta-u_i^z\zeta^z)\,dx\,dz.\end{aligned}$$

Writing $u_i\zeta-u_i^z\zeta^z=-u_i(\zeta^z-\zeta)-(u_i^z-u_i)\zeta^z$ (and the same for u_j instead of u_i), the terms involving the correction $(u_i^z-u_i)\zeta^z$ cancel and we obtain

$$\int (u_j\Delta_h u_i-u_i\Delta_h u_j)\,\zeta\,dx=-\frac{1}{2h}\int G_h(z)\int (u_i^z-u_i)u_j(\zeta^z-\zeta)-(u_j^z-u_j)u_i(\zeta^z-\zeta)\,dx\,dz.$$

Now we may replace the finite difference $\zeta^z - \zeta$ by the gradient, i.e., we expand $\zeta(x+z)-\zeta(x) = z \cdot \nabla\zeta(x) + O(|z|^2)$. Since $\nabla G(z) = -\frac{z}{2}G(z)$ is antisymmetric, this yields the first-order term

$$-\int (u_i \nabla G_h * u_j - u_j \nabla G_h * u_i) \cdot \nabla \zeta \, dx.$$

The second-order term is controlled by

$$\int \left(\frac{|z|}{\sqrt{h}}\right)^2 G_h(z) \int |u^z - u| \, dx \, dz.$$

Using Jensen's inequality and the relation $\left(\frac{|z|}{\sqrt{h}}\right)^2 G_h(z) \lesssim G_{2h}(z)$ we obtain the bound

$$\left(\int G_{2h}(z) \int |u^z - u|^2 \, dx \, dz\right)^{\frac{1}{2}} \sim (h E_{2h}(u))^{\frac{1}{2}} \overset{(44)}{\leq} (h E_h(u))^{\frac{1}{2}}.$$

By the energy-dissipation inequality (25), this is of order $(h|\log h|)^{\frac{1}{2}} \to 0$, which concludes the proof of (51). $\square$

3.2 Proof of the localized energy dissipation Proposition 2.6

We fix $\sigma > 0$ sufficiently small such that (35) holds for all $t \in [0,T]$. This is possible since by assumption the flow Γ_t is smooth. We set $\phi = \phi_\sigma$ and let w.l.o.g. $T = Nh$ for some $N \in \mathbb{N}$. As in [36], our aim is to derive a Gronwall-type inequality for the localized energies $E_h(u^h, \phi)$. For $n \in \mathbb{N}$, comparing u^n to its predecessor u^{n-1} in the localized minimizing movements interpretation (26) of Lemma 2.4 with our specific test function $\phi^n := \phi(nh) \geq 0$ we obtain

$$\begin{aligned}\frac{1}{h}\left(E_h(u^n,\phi^n) - E_h(u^{n-1},\phi^{n-1})\right) \overset{(26)}{\leq} & -\int \phi^n \frac{u^n - u^{n-1}}{h} \cdot G_h * \left(\frac{u^n - u^{n-1}}{h}\right) dx \\ & - \int \frac{u^n - u^{n-1}}{h} \cdot \frac{1}{h}\left[G_h *, \phi^n\right] u^{n-1} \, dx \\ & + E_h\big(u^{n-1}, \frac{\phi^n - \phi^{n-1}}{h}\big).\end{aligned}$$

We now sum over n from 1 to N and multiply by the time-step size h, to obtain

$$E_h(u^h(T), \phi(T)) - E_h(u^h(0), \phi(0)) \leq I_1 + I_2 + I_3 \tag{74}$$

where

$$I_1 = -h \sum_{n=1}^N \int \phi^n \frac{u^n - u^{n-1}}{h} \cdot G_h * \left(\frac{u^n - u^{n-1}}{h}\right) dx, \tag{75}$$

$$I_2 = -h \sum_{n=1}^N \int \frac{u^n - u^{n-1}}{h} \cdot \frac{1}{h}\left[G_h *, \phi^n\right] u^{n-1} \, dx, \tag{76}$$

$$I_3 = h \sum_{n=1}^N E_h\big(u^{n-1}, \frac{\phi^n - \phi^{n-1}}{h}\big). \tag{77}$$

Next we manipulate these three integrals separately.

Analysis of I_3. This is the easiest term. Since $\phi^n - \phi^{n-1} = \int_{(n-1)h}^{nh} \partial_t \phi \, dt$, the interpolation $u^h(t)$ is piecewise constant in time, and the energy E_h is linear in the second argument, we may rewrite I_3 as

$$h \sum_{n=1}^N E_h\Big(u^{n-1}, \frac{\phi^n - \phi^{n-1}}{h}\Big) = \int_0^T E_h(u^h(t), \partial_t \phi) \, dt. \tag{78}$$

The above form will be combined with other terms in the conclusion section.

Analysis of I_1. We claim that this term is almost negative. Indeed, putting $V := \frac{u^n - u^{n-1}}{h}$ and $\phi := \phi^n$, we may rewrite each summand of I_1 as

$$-\int \phi V \cdot G_h * V dx = -\int \phi \left|G_{h/2} * V\right|^2 dx - \int G_{h/2} * V \cdot \left[G_{h/2}*, \phi\right] V\, dx. \tag{79}$$

It is thus enough to estimate the time-integral of the second right-hand side integral of (79) which will be shown to be an error term. Using (57), we expand the commutator as

$$\left[G_{h/2}*, \phi\right] V = \left(\nabla\phi \cdot \nabla G_{h/2} * V + O\big(\|\nabla^2\phi\|_\infty \frac{|z|^2}{h} G_{h/2} * |V|\big)\right) h.$$

Hence the the contribution of the second right-hand side integral in (79) to I_1 can be decomposed into two terms. The first-order term is

$$\begin{aligned}
& h\sum_{n=1}^N \left| h\int (G_{h/2} * \partial_t^h u^h) \nabla\phi^n \cdot \nabla\Big(G_{h/2} * \partial_t^h u^h\Big) dx\right| \\
= \quad & h\sum_{n=1}^N \left|\frac{h}{2}\int \nabla\phi^n \cdot \nabla\Big(|G_{h/2} * \partial_t^h u^h|^2\Big) dx\right| = h\sum_{n=1}^N \left|\frac{h}{2}\int \triangle\phi^n \Big(|G_{h/2} * \partial_t^h u^h|^2\Big) dx\right| \\
\lesssim \quad & \left\|\nabla^2\phi\right\|_\infty h^2 \sum_{n=1}^N \left|\int |G_{h/2} * \partial_t^h u^h|^2 dx\right| \lesssim \left\|\nabla^2\phi\right\|_\infty h \int_0^T \int \left|G_{h/2} * \partial_t^h u^h\right|^2 dx\, dt,
\end{aligned}$$

while the second-order term to I_1 is estimated by $\|\nabla^2\phi\|_\infty \le C(\sigma)$ times the following expression,

$$\begin{aligned}
& h^2 \sum_{n=1}^N \int \left|G_{h/2} * \partial_t^h u^h\right| \left|\left(\frac{|z|^2}{h} G_{h/2}\right) * |\partial_t^h u^h|\right| dx \\
&= h \iint \left|G_{h/2} * \partial_t^h u^h\right| \left|\left(\frac{|z|^2}{h} G_{h/2}\right) * |\partial_t^h u^h|\right| dx\, dt \\
&\le h \left(\iint |G_{h/2} * \partial_t^h u^h|^2 dx\, dt\right)^{\frac12} \left(\iint \left(\left(\frac{|z|^2}{h} G_{h/2}\right) * |\partial_t^h u^h|\right)^2 dx\, dt\right)^{\frac12}.
\end{aligned}$$

Since $\frac{|z|^2}{h} G_{h/2} \lesssim G_h$ and by the L^2-contraction property of the heat kernel, the second right-hand side integral in I_1 can be estimated by

$$\iint \left(\left(\frac{|z|^2}{h} G_{h/2}\right) * |\partial_t^h u^h|\right)^2 dx\, dt \lesssim \iint |\partial_t^h u^h|^2 dx\, dt.$$

Combining the two estimates for the first- and second-order terms with the energy-dissipation estimate (25) and the estimate (46) on the time derivative of u, the contribution of the second right-hand side integral of (79) to (74) is controlled by

$$\begin{aligned}
& \left|\int_0^T \int G_{h/2} * \partial_t^h u^h \cdot \left[G_{h/2}*, \phi\right] \partial_t^h u^h\, dx\, dt\right| \\
& \le C(\sigma) \left(h E_h(u^0) + h\left(E_h(u^0)\right)^{\frac12} \left(\left(1 + \frac{T}{h}\right) E_h(u^0)\right)^{\frac12}\right) \overset{(28)}{\le} C(\sigma)(1+T)\sqrt{h}|\log h| \to 0
\end{aligned}$$

so that the second term of (79) is negligible as $h \to 0$. To conclude, we have

$$I_1 = -h\sum_{n=1}^N \int \phi \left|G_{h/2} * \left(\frac{u^n - u^{n-1}}{h}\right)\right|^2 dx + o(1). \tag{80}$$

Analysis of I_2. This is the leading-order and most difficult term in (74). We first give a short formal argument as a motivation. Expanding the commutator as in (57), or heuristically as in (58), we obtain the leading-order term as

$$-\iint \partial_t^h u^h \cdot \frac{1}{h}\left[G_h *, \phi\right] u^h \, dx \, dt \approx -2 \iint \partial_t^h u^h \cdot (\nabla\phi \cdot \nabla)\, G_h * u^h \, dx \, dt, \tag{81}$$

which is roughly the left-hand side of the Euler-Lagrange equation (50) with $\xi = \nabla\phi$.

In order to make the above rigorous, we make use of some cancellations, in particular the fact that the vectors $\partial_t^h u^h$ and u^h are almost orthogonal.

First, we observe that because of the antisymmetry $\int V[G_h*, \phi]V \, dx = 0$ of the commutator, we may write this integral as

$$I_2 = -h \sum_{n=1}^{N} \int \frac{u^n - u^{n-1}}{h} \cdot \frac{1}{h}\left[G_h *, \phi^n\right] \Big(\frac{u^n + u^{n-1}}{2}\Big) \, dx.$$

There are two cancellations in this integral we will take advantage of:

- To first order, the commutator behaves like $\nabla\phi \cdot \nabla G_h * \big(\frac{u^n+u^{n-1}}{2}\big)$, which improves the order of the kernel from $\frac{1}{h}$ with the commutator to $\frac{1}{\sqrt{h}}$ for the kernel of the leading-order term.
- The two vectors $\frac{u^n-u^{n-1}}{h}$, $\frac{u^n+u^{n-1}}{2}$ are orthogonal, and this is still approximately true after the convolution with the heat kernel.

Now we fix n and write for simplicity $u := u^n$, $v := u^{n-1}$ and $\phi := \phi^n$. Then we rewrite each summand in I_2 in the following more symmetric fashion:

$$\begin{aligned} &\int \frac{u-v}{h} \cdot \frac{1}{h}\left[G_h *, \phi\right] \Big(\frac{u+v}{2}\Big) dx \\ &= \int G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot \frac{1}{h}\left[G_{h/2} *, \phi\right] \Big(\frac{u+v}{2}\Big) - \frac{1}{h}\left[G_{h/2} *, \phi\right] \Big(\frac{u-v}{h}\Big) \cdot G_{h/2} * \Big(\frac{u+v}{2}\Big) \, dx. \end{aligned} \tag{82}$$

Second, we will dissect carefully the commutators appearing above. The computation is more elaborate than the simple first order asymptotics (57). For any vector field w and any smooth test function ϕ, we expand the commutator now as

$$\begin{aligned} \left[G_{h/2} *, \phi\right] w &= \int G_{h/2}(z) \left(\phi(\,\cdot\, - z) - \phi(\,\cdot\,)\right) w(\,\cdot\, - z) \, dz \\ &= \Big(\Big(-\partial_i\phi z_i + \frac{1}{2}\partial_{ij}\phi z_i z_j - \frac{1}{6}\partial_{ijk}\phi z_i z_j z_k\Big) G_{h/2}\Big) * w + O\Big(|z|^4 G_{h/2} * |w|\Big), \end{aligned}$$

where we have summed over repeated indice. Using the identities

$$\begin{aligned} -z_i G_{h/2} = h\partial_i G_{h/2}, \quad z_i z_j G_{h/2} = h^2 \partial_i\partial_j G_{h/2} - h\delta_{ij} G_{h/2}, \\ -z_i z_j z_k G_{h/2} = h^3 \partial_i\partial_j\partial_k G_{h/2} - h\big(\delta_{ij} z_k + \delta_{ik} z_j + \delta_{jk} z_i\big) G_{h/2}, \end{aligned}$$

and the equality of mixed partials, we obtain

$$\begin{aligned} &\frac{1}{h}\left[G_{h/2} *, \, \phi\right] w \\ &= \, (\nabla\phi \cdot \nabla)\, G_{h/2} * w + \frac{h}{2}\nabla^2\phi \colon \nabla^2 G_{h/2} * w - \frac{1}{2}\Delta\phi \, G_{h/2} * w \\ &\quad + \frac{h^2}{6}\sum_{i,j,k} \partial_i\partial_j\partial_k\phi \, \partial_i\partial_j\partial_k G_{h/2} * w - \frac{h}{2}\left(\nabla\Delta\phi \cdot \nabla\right) G_{h/2} * w + O\Big(\frac{|z|^4}{h} G_{h/2} * |w|\Big). \end{aligned} \tag{83}$$

In order to concentrate on the key issue, we will first write down the dominating terms and show the negligibility of the error terms afterwards. Using the above expansion of the commutator for the difference quotient $w = \frac{u-v}{h}$ or the average $w = \frac{u+v}{2}$, respectively, we have, up to leading order,

$$
\begin{aligned}
&\text{Term (82)}\\
&\approx \int G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot (\nabla\phi\cdot\nabla)\, G_{h/2} * \Big(\frac{u+v}{2}\Big) - (\nabla\phi\cdot\nabla)\, G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot G_{h/2} * \Big(\frac{u+v}{2}\Big)\, dx \qquad (84)\\
&=2 \int G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot (\nabla\phi\cdot\nabla)\, G_{h/2} * \Big(\frac{u+v}{2}\Big) dx + \int \Delta\phi\, G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot G_{h/2} * \Big(\frac{u+v}{2}\Big)\, dx \qquad (85)\\
&\approx 2 \int G_{h/2} * \Big(\frac{u-v}{h}\Big) \cdot (\nabla\phi\cdot\nabla)\, G_{h/2} * \Big(\frac{u+v}{2}\Big)\, dx. \qquad (86)
\end{aligned}
$$

Hence,

$$
\begin{aligned}
I_2 \approx & -2h \sum_{n=1}^{N} \int G_{h/2} * \Big(\frac{u^n - u^{n-1}}{h}\Big) \cdot (\nabla\phi^n\cdot\nabla)\, G_{h/2} * \Big(\frac{u^n + u^{n-1}}{2}\Big) dx\\
\approx & -2 \iint G_{h/2} * \partial_t^{-h} u^h \cdot (\nabla\phi\cdot\nabla)\, G_{h/2} * u^h\, dx\, dt \qquad (\text{since } u^n \approx u^{n-1}). \qquad (87)
\end{aligned}
$$

which is precisely the left-hand side of the Euler-Lagrange equation (50) with $\xi = \nabla\phi$. Hence we expect to have

$$
I_2 = -\frac{1}{h} \iint \Delta\phi\, (1 - u^h \cdot G_h * u^h)\, dx\, dt + 2 \sum_{i,j} \iint \partial_i\partial_j\phi\, \partial_i G_{h/2} * u^h \cdot \partial_j G_{h/2} * u^h\, dx\, dt + o(1). \qquad (88)
$$

Note that writing I_2 as (87) is essentially the same as what we first noted in (81), modulo the splitting of G_h* into two separate $G_{h/2}$, but now all the intermediate approximations and errors arising from (82) to (84)–(87) are spelled out carefully.

Conclusion. With the above analysis of I_1, I_2, and I_3, in particular, combining expressions (80), (88), and (78), we obtain,

$$
\begin{aligned}
E_h(u^h(T), \phi(T)) \le & E_h(u^0, \phi(0)) - \int_0^T \int \phi \big| G_{h/2} * \partial_t^h u^h \big|^2 dx\, dt\\
& + 2 \int_0^T \sum_{i,j} \int \partial_i\partial_j\phi\ \partial_i G_{h/2} * u^h \cdot \partial_j G_{h/2} * u^h\, dx\, dt \qquad (89)\\
& + \int_0^T \frac{1}{h} \int (\partial_t\phi - \Delta\phi) \big(1 - u^h \cdot G_h * u^h\big)\, dx\, dt + o(1).
\end{aligned}
$$

Recall that the missing argument that the error is indeed $o(1)$ as $h \to 0$ will be given shortly.

Now we decompose the last two right-hand side integrals into their near- and far-field contributions corresponding to respectively the regions

$$
A_\sigma := \{(x,t)\colon d(x,\Gamma_t) < \sigma\} \quad \text{and} \quad A_\sigma^c := \{(x,t)\colon d(x,\Gamma_t) \ge \sigma\}.
$$

In the far-field region A_σ^c, we have $\phi \ge \frac{1}{2}\sigma^2$ and therefore $|\partial_t\phi - \Delta\phi|, |\partial_i\partial_j\phi| \le C(\sigma)\, \phi$. This implies that we may estimate the far-field contribution to the right-hand side of (89) by

$$
\begin{aligned}
& 2 \iint_{A_\sigma^c} \partial_i\partial_j\phi\ \partial_i G_{h/2} * u^h \cdot \partial_j G_{h/2} * u^h\, dx\, dt + \frac{1}{h} \iint_{A_\sigma^c} (\partial_t\phi - \Delta\phi) \big(1 - u^h \cdot G_h * u^h\big)\, dx\, dt\\
& \overset{(43)}{\le} C(\sigma) \frac{1}{h} \iint \phi \big(1 - u^h \cdot G_h * u^h\big)\, dx\, dt.
\end{aligned}
$$

Next we turn to the more interesting near-field contribution. In order to control the last two right-hand side integrals of (89) over region A_σ, we use the expansion of the heat operator (37) and the estimate on the Hessian (35) to obtain

$$
\begin{aligned}
&2\iint_{A_\sigma} \partial_i\partial_j\phi\, \partial_i G_{h/2} * u^h \cdot \partial_j G_{h/2} * u^h \,dx\,dt + \frac{1}{h}\iint_{A_\sigma} (\partial_t\phi - \Delta\phi)\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \\
&\quad\le 2\iint_{A_\sigma} \left|\nabla G_{h/2} * u^h\right|^2 dx\,dt + \frac{1}{h}\iint_{A_\sigma} (-2 + C\phi)\left(1 - u^h\cdot G_h * u^h\right) dx\,dt.
\end{aligned}
$$

Note that ϕ "cuts out" the vorticity set Γ_t and therefore we expect $E_h(u^h,\phi)$ to stay finite as $h\to 0$. However, there are two competing diverging terms, namely the Dirichlet energy $2\int\left|\nabla G_{h/2} * u^h\right|^2 dx$ and the thresholding energy $-2E_h(u^h)$. Miraculously, the monotonicity (44) of the energy in the time step size, or more exactly its equivalent statement (45) (in Lemma 2.8) provides precisely the correct relationship between the two quantities.

With the above observation, we now compute:

$$
\begin{aligned}
&E_h(u^h(T),\phi(T)) \\
\le& E_h(u^0,\phi(0)) - \int_0^T\int \phi\left|G_{h/2} * \partial_t^h u^h\right|^2 dx\,dt + \frac{C(\sigma)}{h}\int_0^T\int \phi\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \\
&+ 2\iint_{A_\sigma} \left|\nabla G_{h/2} * u^h\right|^2 dx\,dt + \frac{1}{h}\iint_{A_\sigma} (-2 + C\phi)\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \\
\le& E_h(u^0,\phi(0)) - \int_0^T\int \phi\left|G_{h/2} * \partial_t^h u^h\right|^2 dx\,dt + \frac{C(\sigma)}{h}\int_0^T\int \phi\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \\
&+ 2\iint_{A_\sigma} \left|\nabla G_{h/2} * u^h\right|^2 dx\,dt - 2\iint_{A_\sigma} \frac{1}{h}\left(1 - u^h\cdot G_h * u^h\right) dx\,dt. \qquad (90)
\end{aligned}
$$

We can bound the line (90) from above by

$$
\begin{aligned}
&2\iint \left|\nabla G_{h/2} * u^h\right|^2 dx\,dt - 2\iint_{A_\sigma} \frac{1}{h}\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \\
\le& 2\int_0^T E_h(u^h)\,dt - 2\iint_{A_\sigma} \frac{1}{h}\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \quad \text{(by (45))} \\
\le& 2\iint_{A_\sigma^c} \frac{1}{h}\left(1 - u^h\cdot G_h * u^h\right) dx\,dt \le \frac{C(\sigma)}{h}\iint \phi\left(1 - u^h\cdot G_h * u^h\right) dx\,dt. \qquad (91)
\end{aligned}
$$

The above finally gives

$$
E_h(u^h(T),\phi(T)) \le E_h(u^0,\phi(0)) - \int_0^T\int \phi\left|G_{h/2} * \partial_t^h u^h\right|^2 dx\,dt + C(\sigma)\int_0^T E_h(u^h,\phi)\,dt + o(1).
$$

A standard Gronwall-argument yields (39). □

Analysis of the error terms. Now we estimate the errors coming from (84)–(87).

Error in (87). This error is due to replacing u^{n-1} by u^n and is bounded by

$$
\begin{aligned}
&\left|h\iint \left(G_{h/2} * (\partial_t^{-h} u^h)\right)\nabla\phi\cdot\nabla\left(G_{h/2} * \partial_t^{-h} u^h\right) dx\,dt\right| \\
=& \left|h\iint \nabla\phi\cdot\nabla\left(\left|G_{h/2} * \partial_t^{-h} u^h\right|^2\right) dx\,dt\right| \\
\lesssim& \|\nabla^2\phi\|_\infty h\iint \left|G_{h/2} * \partial_t^{-h} u^h\right|^2 dx\,dt \overset{(25)}{=} O(h|\log h|) \to 0 \quad \text{as} \quad h\to 0.
\end{aligned}
$$

Error in (86). This is caused by omiting the second term in (85) which involves the Laplacian of ϕ, $\Delta\phi$. We will show that after integration in time, this term is negligible. For this, we use the identity $(a-b)\cdot(a+b) = |a|^2 - |b|^2$ to see that

$$
\begin{aligned}
& h\sum_{n=1}^{N}\int \Delta\phi^n\, G_{h/2} * \Big(\frac{u^n - u^{n-1}}{h}\Big)\cdot G_{h/2} * \Big(\frac{u^n + u^{n-1}}{2}\Big)dx \qquad (92)\\
&= h\sum_{n=1}^{N}\int \Delta\phi^n \frac{1}{2}\left(\frac{1}{h}\left(1 - \left|G_{h/2} * u^{n-1}\right|^2\right) - \frac{1}{h}\left(1 - \left|G_{h/2} * u^{n}\right|^2\right)\right) dx\\
&\leq h\sum_{n=1}^{N}\|\partial_t \nabla^2\phi\|_\infty \frac{h}{2}\int \frac{1}{h}\left(1 - \left|G_{h/2} * u^{n}\right|^2\right) dx\\
&\quad + \|\nabla^2\phi\|_\infty \frac{h}{2}\int \frac{1}{h}\left(1 - \left|G_{h/2} * u^{N}\right|^2\right) + \frac{1}{h}\left(1 - \left|G_{h/2} * u^{0}\right|^2\right) dx.
\end{aligned}
$$

Note that we used that the terms $1 - |G_{h/2} * u|^2$ are non-negative. By the symmetry of G, we have

$$
\int \frac{1}{h}\big(1 - |G_{h/2} * u|^2\big)dx = E_h(u)
$$

and hence, using the energy-dissipation estimate (25), we obtain the bound

$$
Th\|\partial_t\nabla^2\phi\|_\infty E_h(u^0) + \|\nabla^2\phi\|_\infty h E_h(u^0) \lesssim \left(\|\partial_t\nabla^2\phi\|_\infty + \|\nabla^2\phi\|_\infty\right)(1+T)h|\log h|,
$$

which vanishes in the limit $h \to 0$.

Error in (84). The error in this line comes from omitting the higher-order terms in the expansion of the commutators (83). To this end, we integrate by parts all derivatives which are on the time-derivative $G_{h/2} * \big(\frac{u-v}{h}\big)$. The resulting terms are of the form

$$
\int h\, P(\nabla)\nabla^2\phi\; Q(\nabla)G_{h/2} * \Big(\frac{u+v}{2}\Big)\cdot G_{h/2} * \Big(\frac{u-v}{h}\Big)dx, \qquad (93)
$$

where the linear differential operators $P(\nabla)$, $Q(\nabla)$ are both of order ≤ 2. For the terms for which there is no derivative falling onto $G_{h/2} * \left(\frac{u+v}{2}\right)$, we proceed as in the lines following (92). Therefore, we may assume that the polynomial Q is either homogeneous of order 1, or 2. In these cases we estimate by Cauchy-Schwarz after integration in time:

$$
\begin{aligned}
& h\sum_{n=1}^{N}\int h\, P(\nabla)\nabla^2\phi^n\; Q(\nabla)G_{h/2} * \Big(\frac{u^n + u^{n-1}}{2}\Big)\cdot G_{h/2} * \Big(\frac{u^n - u^{n-1}}{h}\Big)dx\\
&\lesssim h\|P(\nabla)\nabla^2\phi\|_\infty \left(h\sum_{n=0}^{N}\int \left|Q(\nabla)G_{h/2} * u^n\right|^2 dx\right)^{\frac{1}{2}} \left(h\sum_{n=1}^{N}\int \left|G_{h/2} * \Big(\frac{u^n - u^{n-1}}{h}\Big)\right|^2 dx\right)^{\frac{1}{2}}.
\end{aligned}
$$

By the energy-dissipation estimate, the last right-hand side term is estimated by $E_h(u^0)$ while the first right-hand side integral can be manipulated as follows. By our assumption on Q we have $\int Q(\nabla)G_{h/2}(z)\,dz = 0$ and therefore by Jensen's inequality

$$
\begin{aligned}
\int \left|Q(\nabla)G_{h/2} * u\right|^2 dx &= \int \left|\int Q(\nabla)G_{h/2}(z)\,(u(x-z) - u(x))\,dz\right|^2 dx\\
&\lesssim \int \left|Q(\nabla)G_{h/2}(z)\right| dz \int \left|Q(\nabla)G_{h/2}(z)\right| |u(x-z) - u(x)|^2\, dz\, dx.
\end{aligned}
$$

Since Q is of degree ≤ 2, we have the integral estimate $\int \left|Q(\nabla)G_{h/2}\right| dz \lesssim \frac{1}{h}$ and the pointwise estimate $\left|Q(\nabla)G_{h/2}(z)\right| \lesssim \frac{1}{h}G_h(z)$. Thus

$$\int \left|Q(\nabla)G_{h/2} * u\right|^2 dx \lesssim \frac{1}{h}E_h(u). \tag{94}$$

Plugging in this estimate and using the energy-dissipation estimate (25) once more, we obtain the bound

$$h\|P(\nabla)\nabla^2\phi\|_\infty \left(T\frac{1}{h}E_h(u^0)\right)^{\frac{1}{2}} \left(E_h(u^0)\right)^{\frac{1}{2}} \overset{(28)}{\lesssim} \sqrt{h}\|P(\nabla)\nabla^2\phi\|_\infty(1+T)\left|\log h\right|,$$

which as before vanishes as $h \to 0$.

The third-order term works in the same fashion—only that the differential operators P and Q add up to order 3 instead of 2. This weakens the estimate (94) by an order of $\frac{1}{h}$. But we have one more power of h in the prefactor so that we obtain (93) with the prefactor h^2 instead of h.

Finally, we estimate the error coming from the fourth-order term in the expansion of the commutator by

$$\begin{aligned}
&h\sum_{n=1}^N \int \left(\frac{|z|^4}{h}G_{h/2}\right) * \left|\frac{u^n - u^{n-1}}{h}\right| + \left|G_{h/2} * \left(\frac{u^n - u^{n-1}}{h}\right)\right| \int \frac{|z|^4}{h}G_{h/2}(z)\,dz\,dx \\
&\lesssim h\iint \left|\partial_t^h u^h\right| dx\,dt \lesssim hT^{\frac{1}{2}}\left(\iint \left|\partial_t^h u^h\right|^2 dx\,dt\right)^{\frac{1}{2}} \overset{(46)}{\lesssim} \sqrt{h}(1+T)E_h(u^0) \to 0.
\end{aligned}$$

With the above, we have thus taken care of all the error terms, concluding the proof of Proposition (2.6).

3.3 Proof of the main result Theorem 2.2

Step 1: Compactness.

From our localized energy-dissipation inequality of Proposition 2.6, the relation between Dirichlet and thresholding energy of Lemma 2.7, and the estimate on the initial data (28) we obtain for any fixed $\sigma > 0$

$$\sup_{t\in(0,T)} \int \phi_\sigma \left|\nabla G_{h/2} * u^h\right|^2 dx + \int_0^T \int \phi_\sigma \left|G_{h/2} * \partial_t^h u^h\right|^2 dx\,dt \leq C(\sigma) + o(1). \tag{95}$$

Therefore, we may extract a subsequence which converges weakly to a map $u \in H^1_{\mathrm{loc}}(\mathbb{T}^3 \setminus \Gamma)$ in the sense that

$$\begin{aligned}
G_{h/2} * u^h &\to u && \text{in } L^2, \\
\nabla G_{h/2} * u^h &\rightharpoonup \nabla u && \text{in } L^2_{\mathrm{loc}}((\mathbb{T}^3 \times (0,T)) \setminus \Gamma), \quad \text{and} \\
\partial_t^h G_{h/2} * u^h &\rightharpoonup \partial_t u && \text{in } L^2_{\mathrm{loc}}((\mathbb{T}^3 \times (0,T)) \setminus \Gamma).
\end{aligned} \tag{96}$$

The convergence (96) upgrades to the L^2-convergence of u^h since by Jensen's inequality and $G_{h/2} \lesssim G_h$ we have

$$\begin{aligned}
\int |u - G_{h/2} * u|^2 dx &= \int \left|\int G_{h/2}(z)(u(x) - u(x-z))\,dz\right|^2 dx \\
&\lesssim \int\int G_{h/2}(z)\left|u(x) - u(x-z)\right|^2 dz\,dx \lesssim hE_h(u^h,\zeta) \lesssim h|\log h| \to 0.
\end{aligned}$$

Step 2: Convergence of the vorticity set.

Using again Proposition 2.6 we obtain the convergence of the vorticity set.

Step 3: Convergence of u^h away from the vorticity set.

By (19)–(21) we may pass to the limit in the weak form of the Euler-Lagrange equation (51) whenever the test function ζ localizes away from Γ.

4 Other variants of thresholding

In this section, we discuss variants of thresholding which are motivated by the minimizing movements interpretation.

4.1 Extensions to Neumann and Dirichlet boundary conditions

For convenience and a cleaner presentation, up to now we have restricted ourselves to the simplest case of periodic boundary conditions. However, when working on a bounded domain $\Omega \subset \mathbb{R}^d$, it is more natural to consider Neumann or Dirichlet boundary conditions corresponding to $\frac{\partial u}{\partial n}\big|_{\partial\Omega} = 0$ or $u\big|_{\partial\Omega} = \bar{u}$ for the state variable u. Here $\bar{u}$ is some prescribed function on $\partial\Omega$. We will show that it is very easy to incorporate these boundary conditions while keeping the same heat kernel G_h for the whole space. Hence numerical efficiency and the appealing simplicity of the scheme can be maintained. The main idea is to extend u appropriately from Ω to $\mathbb{R}^d$.

Let $\Omega \subset \mathbb{R}^3$ be a smooth bounded domain. In order to solve the equation with Neumann boundary conditions on $\partial\Omega$, we first rewrite the minimization problem (24) in the following equivalent symmetrized form

$$\min \Bigg\{ \frac{1}{h} \int_{\mathbb{R}^3} \int_{\mathbb{T}^3} G_h(x-y)\,(1 - u(x)\cdot u(y))\,dx\,dy \\ + \frac{1}{h} \int_{\mathbb{R}^3} \int_{\mathbb{T}^3} G_h(x-y)\left(u - u^{n-1}\right)(x)\cdot\left(u - u^{n-1}\right)(y)\,dx\,dy \Bigg\},$$

Note that the outer integral $\int_{\mathbb{R}^3} dy$ in (24) can be replaced by $\int_{\mathbb{T}^3} dy$ without changing the integral drastically as the kernel $G_h(x-y)$ decays exponentially in $|x-y|$. Therefore a natural generalization of this minimization problem to the bounded domain Ω with Neumann boundary conditions is

$$\min \Bigg\{ \frac{1}{h} \int_{\Omega} \int_{\Omega} G_h(x-y)\,(1 - u(x)\cdot u(y))\,dx\,dy \\ + \frac{1}{h} \int_{\Omega} \int_{\Omega} G_h(x-y)\left(u - u^{n-1}\right)(x)\cdot\left(u - u^{n-1}\right)(y)\,dx\,dy \Bigg\}, \quad (97)$$

where the minimum runs over all vector fields $u\colon \Omega \to \mathbb{R}^2$ with $|u| \le 1$ a.e. in Ω.

This may be interpreted as extending u by zero off Ω. Note that $u = 0$ has equal distance to all points on the sphere $\mathbb{S}^1$ and therefore does not prefer any of these values. Another way to interpret the minimization problem (97) is that there is no interaction with points outside the domain Ω and since no boundary conditions are enforced in the minimization procedure, it is reasonable to expect the minimizer to attain natural boundary conditions, i.e., Neumann boundary conditions.

Note that for any unit vector field $u\colon \Omega \to \mathbb{S}^1$, the first term in (97) can also be written as a weighted average of finite differences,

$$E_{\Omega,h}(u) := \frac{1}{h} \int_{\Omega} \int_{\Omega} G_h(x-y)\,(1 - u(x)\cdot u(y))\,dx\,dy = \frac{1}{2} \int_{\Omega} \int_{\Omega} G_h(x-y) \left| \frac{u(x) - u(y)}{\sqrt{h}} \right|^2 dx\,dy. \quad (98)$$

Hence similar to Lemma 2.7, it can be shown to converge to the Dirichlet energy $\int_\Omega |\nabla u|^2$.

We can now follow the proof of Lemma 2.4 line by line with u and u^{n-1} replaced by χu and χu^{n-1}, respectively, where $\chi = \mathbf{1}_\Omega$. It holds again that (97) is equivalent to the minimization problem

$$\min\left\{-\frac{2}{h}\int \chi u\cdot G_h*(\chi u)\,dx,\ \ u:\Omega\to\mathbb{R}^2,\ \ |u|\le 1\right\}.$$

The solution can then be read off as

$$u^n = \frac{v^n}{|v^n|},\quad \text{where } v^n = G_h*(\chi u^{n-1}). \tag{99}$$

Therefore, we propose the following algorithm.

Algorithm 4.1. (Neumann boundary conditions) *Let the initial condition and time-step size be $u^0\colon \Omega\setminus\Gamma_0\to\mathbb{R}^2$ and $h>0$. Given the configuration u^{n-1} at time $t=(n-1)h$, the configuration u^n at time $t=nh$ is constructed by the following two operations:*

1. *Diffusion $v^n := G_h*(\mathbf{1}_\Omega u^{n-1})$;*
2. *Thresholding/Projection onto $\mathbb{S}^1$: $u^n := \dfrac{v^n}{|v^n|}$ in Ω.*

In the above, Γ_0 is some initial (smooth) curve in Ω. Again we require that u^0 is well-prepared according to Definition 2.5.

Next we consider Dirichlet boundary conditions given by a $W^{1,2}_{\mathrm{loc}}$ function $\bar u$ on $\mathbb{R}^3\setminus\Omega$ with $|\bar u|=1$ a.e.. We start from (99) and make the following ansatz

$$u^n := \frac{v^n}{|v^n|},\quad \text{where } v^n = G_h*(\chi u^{n-1}+(1-\chi)\bar u), \tag{100}$$

i.e., we essentially set u to be $\bar u$ outside Ω. The corresponding minimization problem is then

$$\min\Big\{E_{\Omega,h}(u)+\frac{1}{h}\int_\Omega\int_\Omega G_h(x-y)\left(u-u^{n-1}\right)(x)\cdot\left(u-u^{n-1}\right)(y)\,dx\,dy \\ +\frac{2}{h}\int_\Omega\int_{\mathbb{R}^3\setminus\Omega} G_h(x-y)\,(1-u(x)\cdot\bar u(y))\,dy\,dx\Big\}. \tag{101}$$

The fact that the last term can be interpreted as a penalization can be seen at its asymptotic behavior: Given $u,\bar u\colon\Omega\to\mathbb{R}^2$ and suppose $\Omega\subset\mathbb{R}^3$ is a smooth bounded domain. Then

$$\lim_{h\to 0}\frac{1}{\sqrt h}\int_\Omega\int_{\mathbb{R}^3\setminus\Omega} G_h(x-y)\,(1-u(x)\cdot\bar u(y))\,dy\,dx = \sigma\int_{\partial\Omega}2\,(1-u\cdot\bar u)\qquad\left(\sigma=\frac{1}{\sqrt\pi}\right).$$

These asymptotics are not surprising in light of [20, Lemma A.3] and [32, Lemma 2.8]. Indeed, it is shown there that the measures $\frac{1}{\sqrt h}(1-\chi)\,G_h*\chi\,dx$ converge to $\sigma\,|\nabla\chi|$ with surface tension σ, so that for any pair of vector fields $u,\bar u$, the leading-order term of the left-hand side is of the form

$$\frac{1}{\sqrt h}\int 2(1-u\cdot\bar u)(1-\chi)G_h*\chi\,dx\ \text{ which converges to }\ \sigma\int 2(1-u\cdot\bar u)\,|\nabla\chi|\ \text{ as } h\to 0.$$

It is important to point out the difference in the scaling factor in front of the integral in (101). In particular, if the boundary data are well-prepared, i.e., $|\bar u|=1$ on $\partial\Omega$, then as $h\downarrow 0$, the third term in (101) behaves like

$$\frac{2\sigma}{\sqrt h}\int_{\partial\Omega}(1-u\cdot\bar u) = \frac{\sigma}{\sqrt h}\int_{\partial\Omega}|u-\bar u|^2,$$

so that this term is indeed a form of penalization forcing u to assume the boundary values $u = \bar{u}$ on $\partial\Omega$.

Based on the above, we now state the corresponding algorithm for the evolution with Dirichlet boundary conditions.

Algorithm 4.2. (Dirichlet boundary conditions) *Let the initial and boundary conditions, and the time-step size be $u^0 : \Omega\backslash\Gamma_0 \to \mathbb{R}^2$ and $\bar{u} : \mathbb{R}^3\backslash\Omega \to \mathbb{R}^2$, and $h > 0$. Given the configuration u^{n-1} at time $t = (n-1)h$, the configuration u^n at time $t = nh$ is constructed the following two operations:*

1. *Diffusion of the by $\bar{u}$ extended vector field: $v^n := G_h * (\mathbf{1}_\Omega u^{n-1} + \mathbf{1}_{\mathbb{R}^3\backslash\Omega}\bar{u})$;*
2. *Thresholding/Projection onto $\mathbb{S}^1$: $u^n := \dfrac{v^n}{|v^n|}$ in Ω.*

4.2 Vortex motion with pinning

When studying vortices (points) in $\mathbb{R}^2$, the Ginzburg-Landau approximation as well as the thresholding scheme discussed above are trivial on the time scale under consideration in the sense that the vortices do not move. The easiest way to obtain non-trivial motion goes by the name "pinning" which originates from a chemical potential $a(x) \geq a_0 > 0$. Lin [36] proved the convergence as $\varepsilon \to 0$ of solutions to the equation

$$\partial_t u_\varepsilon = \frac{1}{a(x)} \nabla \cdot (a(x) \nabla u_\varepsilon) - \frac{1}{\varepsilon^2} \nabla_u W(u_\varepsilon), \tag{102}$$

where $W(u) = \frac{1}{4}(|u|^2 - 1)^2$. The above is the gradient flow of the following weighted energy

$$\int a(x) \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} W(u) \right) dx \tag{103}$$

$$\frac{d}{dt} \int a(x) \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} W(u) \right) dx = - \int a(x) |\partial_t u|^2. \tag{104}$$

The motion law for the vortices in the limit $\varepsilon \to 0$ is then the ordinary differential equation

$$\dot{X} = - \frac{\nabla a(X)}{a(X)} \ \Big(= - \nabla \log a(X) \Big),$$

which is again a gradient flow.

The fact that $a(x)$ arises in both the energy (103) and the dissipation law (104) gives a hint that thresholding can be generalized to this setting as well. Indeed, as in the codimension one case, when extending thresholding to networks with arbitrary surface tensions, the "natural" mobilities (in the sense of the scheme) are inversely proportional to the surface tensions [20].

Now the straight-forward generalization of the minimizing movements interpretation (24) of thresholding to the vortex motion case is

$$\frac{1}{h} \int a(x) \left(1 - u \cdot G_h * u\right) dx + \frac{1}{h} \int a(x) \left(u - u^{n-1}\right) \cdot G_h * \left(u - u^{n-1}\right) dx. \tag{105}$$

Tracing back our steps in the argument for (24), we see that u^n minimizes the linear functional

$$-\frac{1}{h} \int u \cdot \left(a\, G_h * u^{n-1} + G_h * (a\, u^{n-1}) \right) \, dx$$

among all vector fields $u : \mathbb{R}^2 \to \mathbb{R}^2$ with $|u| \leq 1$ a.e. Therefore we obtain the following variant of thresholding for vortex motion.

Algorithm 4.3. (Vortex motion) *Let* $\{X_1^0, \dots, X_M^0\} \subset ([0,\Lambda)^2)^M$ *be the initial locations of vortices. Let further the initial data and time-step size be* $u^0 \colon [0,\Lambda)^2 \setminus \{X_1^0, \dots, X_M^0\} \to \mathbb{R}^2$ *and* $h > 0$*. Given the configuration* u^{n-1} *at time* $t = (n-1)h$*, the configuration* u^n *at time* $t = nh$ *is constructed by the following two operations:*

1. *Approximate convection-diffusion process:* $v^n := G_h * (a\, u^{n-1}) + a\, G_h * u^{n-1}$*;*

2. *Thresholding/Projection onto* $\mathbb{S}^1$*:* $u^n := \dfrac{v^n}{|v^n|}$.

Note that v^n may be written as

$$v^n = 2a\, G_h * u^{n-1} + [G_h *, a]u^{n-1} \approx 2a\, G_h * u^{n-1} + 2h\nabla a \cdot \nabla G_h * u^{n-1},$$

so that another, yet a priori not energy dissipative, scheme can be obtained by replacing the first step of Algorithm 4.3 by

$$v^n := a\, G_h * u^{n-1} + h\nabla a \cdot \nabla G_h * u^{n-1}.$$

We mention in passing that the dynamical law (102) can be changed to the following "convection-diffusion-reaction" form

$$\partial_t u_\varepsilon = \Delta u_\varepsilon + V(x) \cdot \nabla u_\varepsilon - \frac{1}{\varepsilon^2} \nabla_u W(u_\varepsilon) \tag{106}$$

where V is some arbitrary (smooth) vector field. Even though there is no "global" variational interpretation for (106) unless $V = \frac{\nabla a}{a}$ for some function a, the overall minimizing movements strategy and proof of convergence will still work as *locally* at each point x_0, V can always be approximated as a gradient of some function. More specifically, we simply take $f(x) = \langle V(x_0), (x - x_0)\rangle$ and $a(x) = e^{f(x)}$ for x near x_0. Then

$$\left| V(x) - \frac{\nabla a(x)}{a(x)} \right| = |V(x) - \nabla f(x)| = |V(x) - V(x_0)| = O(|x - x_0|).$$

For a thresholding scheme to take into account the convection term in (106) we perform an extra step in between the diffusion and thresholding steps in which we deform the ambient domain along the flow generated by the vector field V. As long as V has sufficient smoothness, this step will at most modify the thresholding energy by a prefactor of $1 + O(h)$. Hence the overall energy will still remain bounded in finite time.

4.3 Harmonic map heat flow in higher dimensions

The methods used in Section 2 give a simple proof of convergence for the following time-splitting method for the harmonic map heat flow

$$\partial_t u - \Delta u = |\nabla u|^2 u \tag{107}$$

with $u \colon \mathbb{T}^d \to \mathbb{S}^{N-1}$ with initial conditions in H^1.

Algorithm 4.4. (Harmonic heat flow) *Let the initial condition and time-step size be* $u^0 \colon \mathbb{T}^d \to \mathbb{S}^{N-1}$ *and* $h > 0$*. Given the configuration* u^{n-1} *at time* $t = (n-1)h$*, the configuration* u^n *at time* $t = nh$ *is constructed by the following two operations:*

1. *Diffusion: convolve* u^{n-1} *with the heat kernel, i.e., put* $v^n := G_h * u^{n-1}$*;*

2. *Thresholding/Projection onto* $\mathbb{S}^{N-1}$*: set* $u^n := \frac{v^n}{|v^n|}$.

Proposition 4.5. *Given initial data $u^0 \in H^1([0,\Lambda)^d, \mathbb{R}^N)$ with $|u^0| = 1$ a.e., the (piecewise constant interpolations of the) approximate solutions u^h are pre-compact, i.e., there exists a subsequence $h \downarrow 0$ and a map $u \in H^1([0,\Lambda)^d \times (0,T), \mathbb{R}^N)$ with $|u| \le 1$ a.e. such that*

$$\begin{aligned} u^h &\to u && \text{in } L^2([0,\Lambda)^d \times (0,T)), && (108)\\ \nabla G_h * u^h &\rightharpoonup \nabla u && \text{in } L^2([0,\Lambda)^d \times (0,T)) \quad \text{and} && (109)\\ \partial_t^h \big(G_h * u^h\big) &\rightharpoonup \partial_t u && \text{in } L^2([0,\Lambda)^d \times (0,T)). && (110) \end{aligned}$$

Furthermore, u solves the harmonic map heat flow equation (107).

Proof. Note that the minimizing movements interpretation did not use that fact that the range of u is only two-dimensional. In fact the proof applies line by line in this framework as well. In particular, we have the a priori estimate (25); with the important difference that now

$$E_h(u^0) \le \int \left|\nabla u^0\right|^2 \quad \text{is uniformly bounded as } h \downarrow 0.$$

This allows us to prove the compactness statement of the theorem.

The convergences (109)–(110) allow us to pass to the limit in the Euler-Lagrange equation (51), which establishes the equivalent weak form (73) of (107). □

5 Appendix

5.1 Asymptotic expansion of thresholding scheme for filament

In this section, following [45], we briefly describe the main steps in the asymptotic expansion of the thresholding scheme demonstrating the appearance of filament curvature motion. Similar asymptotics for the Ginzburg-Landau dynamics (5) is derived in [42].

As we are only dealing with the initial conditions Γ_0, u^0, let us omit the index 0 in the following. Denoting $x = (x_1, x_2, x_3) = (x', x_3) \in \mathbb{R}^3$, we work in the geometry that the filament can be written as a graph over the x_3-axis. Precisely, let the initial curve Γ be given by

$$\Gamma = \{(\gamma_1(x_3), \gamma_2(x_3), x_3) : x_3 \in \mathbb{R}\}, \quad \text{for some smooth functions } \gamma_1 \text{ and } \gamma_2.$$

Identifying $x' = (x_1, x_2) = x_1 + ix_2$ and $\gamma = (\gamma_1, \gamma_2) = \gamma_1 + i\gamma_2$, we use the following as the initial condition for the state variable $v = v(x,t)$:

$$u(x) = \frac{x' - \gamma(x_3)}{|x' - \gamma(x_3)|}.$$

Then the solution at time $t > 0$ of the linear heat equation starting from u is given by

$$v(x,t) = \frac{1}{(4\pi t)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \exp\left(-\frac{|z-x|^2}{4t}\right) \frac{z' - \gamma(z_3)}{|z' - \gamma(z_3)|}\, dz \quad \text{where} \quad z = (z', z_3), \ \ t > 0. \tag{111}$$

We now consider the *outer* and *inner* expansions of the above integration.

(I) Outer expansion: $|x' - \gamma(x_3)| \gg \sqrt{t}$. For the outer expansion we introduce the length scale ε, the relative coordinate y and the two complex numbers ζ and η given by

$$\varepsilon := \sqrt{t}, \quad y := \frac{z - x}{\varepsilon}, \quad \zeta := x' - \gamma(x_3), \quad \eta := \varepsilon y' + \gamma(x_3) - \gamma(x_3 + \varepsilon y_3).$$

We observe the following two asymptotics: First, since the parametrization γ is smooth

$$\eta = \varepsilon(y' - \partial_{x_3}\gamma(y_3)\, y_3) + O(\varepsilon^2 y_3^2). \tag{112}$$

Second, for any two complex numbers η and ζ with $|\eta| \ll |\zeta|$ it holds

$$\frac{\zeta+\eta}{|\zeta+\eta|} = \frac{\zeta}{|\zeta|} + \left(\frac{\eta}{|\zeta|} - \frac{\zeta}{|\zeta|}\mathrm{Re}\left(\frac{\eta}{\zeta}\right)\right) + O\Big(\Big|\frac{\eta}{\zeta}\Big|^2\Big).$$

Hence the integral (111) can be written as

$$v(x,t) = \frac{\zeta}{|\zeta|} + \frac{1}{(4\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{-\frac{|y|^2}{4}}\Big[\frac{\eta}{|\zeta|} - \frac{\zeta}{|\zeta|}\mathrm{Re}\left(\frac{\eta}{\zeta}\right)\Big]\,dy + \frac{1}{(4\pi)^{\frac{3}{2}}}\int_{\mathbb{R}^3} e^{-\frac{|y|^2}{4}} O\Big(\Big|\frac{\eta}{\zeta}\Big|^2\Big)\,dy.$$

Note that the first term of the above expansion is simply $u(x)$. The second, linear in η, is in fact almost an expectation of a Gaussian variable, cf. (112). So its leading order term vanishes while the contribution form the second order term is $O(\varepsilon^2)$. Hence we conclude that

$$v(x,t) = u(x) + O(t), \quad \text{leading to} \quad \frac{v(x,t)}{|v(x,t)|} = \exp\big(i(\theta + O(t))\big) \tag{113}$$

where θ is the initial phase variable for $u(x)$.

(II) Inner expansion: $|x' - \gamma(x_3)| \lesssim \sqrt{t}$**.** Introducing a constant $\delta \ll 1$ and the new spatial and temporal variables $\eta = \frac{x'-\gamma(x_3)}{\delta}$ and $\tau = \frac{t}{\delta^2}$, we expand $v(x,t)$ as

$$v(x,t) = Ae^{iS} = (A_0 + \delta A_1 + \cdots)e^{i(S_0+\delta S_1+\cdots)}. \tag{114}$$

Substituting the above into the heat equation $\partial_t v = \Delta v$, we obtain

$$\partial_\tau S - \Delta S + 2\frac{\nabla A}{A}\cdot\nabla S + \delta(\kappa\mathbf{N} - \dot{\Gamma}_t)\cdot\nabla S \;=\; O(\delta^2), \tag{115}$$

$$\partial_\tau A - \Delta A + \delta(\kappa\mathbf{N} - \dot{\Gamma}_t)\cdot\nabla A + |\nabla S|^2 A \;=\; O(\delta^2). \tag{116}$$

The initial conditions for S and A are θ and 1, respectively.

For the $O(1)$ terms in (114) we have

$$\partial_\tau S_0 - \Delta S_0 + 2\frac{\nabla A_0}{A_0}\cdot\nabla S_0 = 0, \quad \text{and} \quad \partial_\tau A_0 - \Delta A_0 + |\nabla S_0|^2 A_0 = 0.$$

The solutions are respectively, $S_0(\eta,\tau) = \theta$ and $A_0(\eta,\tau) = A\left(\frac{\eta^2}{\tau}\right)$ where the function $A : \mathbb{R}_+ \to \mathbb{R}_+$ has the following asymptotic behavior:

$$A(z) \approx \begin{cases} z^{\frac{1}{2}}(c_0 + c_1 z + \cdots), & \text{for } z \ll 1,\\ e^{-\frac{1}{z}}(1 + c_2 z^{-2} + \cdots), & \text{for } z \gg 1. \end{cases}$$

Incorporating the $O(\delta)$ term in (114) and making the ansatz that S converges to a steady state S_∞ as $\eta \to \infty$, we obtain

$$-\Delta S_\infty + \delta(\kappa\mathbf{N} - \dot{\Gamma}_t)\cdot\nabla S_\infty = O(\delta^2). \tag{117}$$

The solution to this equation is given by

$$S_\infty = \eta\int_0^\theta \Big[G_\eta(\eta,\varphi) + \delta(\kappa\mathbf{N} - \dot{\Gamma}_t)\cdot(\cos\varphi, \sin\varphi)G(\eta,\varphi)\Big]\,d\varphi, \tag{118}$$

where

$$G(\eta,\theta) = -\exp\left\{\frac{\delta}{2}(\kappa\mathbf{N} - \dot{\Gamma}_t)\cdot(\eta\cos\theta, \eta\sin\theta)\right\} K_0\left(\frac{\delta\eta|\kappa\mathbf{N} - \dot{\Gamma}_t|}{2}\right), \tag{119}$$

with $K_0(x) = -\log\dfrac{x}{2} + \text{const}$ for $x \ll 1$ being the zeroth-order modified Bessel function.

Substituting (119) into (118), we obtain

$$S_\infty = \theta - \frac{3}{2} r \Big\langle \kappa \mathbf{N} - \dot{\Gamma}_t, \big(\sin\theta, 1-\cos\theta\big)\Big\rangle K_0\Big(\frac{r|\kappa\mathbf{N} - \dot{\Gamma}_t|}{2}\Big) + O(r|\kappa\mathbf{N} - \dot{\Gamma}_t|), \tag{120}$$

where $r = |x' - \gamma(x_3)|$.

Now comparing (120) with (113) from the outer expansion, we conclude that

$$|\kappa\mathbf{N} - \dot{\Gamma}_t| K_0\Big(\frac{|\kappa\mathbf{N} - \dot{\Gamma}_t|}{2}\Big) + O(|\kappa\mathbf{N} - \dot{\Gamma}_t|) = O(t),$$

so that

$$\dot{\Gamma}_t - \kappa\mathbf{N} = O\left(\frac{t}{|\log t|}\right) = o(t).$$

Hence the thresholding scheme is consistent for $t \ll 1$.

Switching back to the notation h for the time step size, we note here that the one-step and accumulative errors are respectively, $O\Big(\frac{h}{|\log h|}\Big)$ and $O\Big(\frac{1}{|\log h|}\Big)$. We defer to future work in making the above asymptotic analysis, in particular the error estimates, rigorous.

5.2 Construction of initial conditions

We derive the appropriate bounds for the ansatz (30) for the initial conditions to show they are well-prepared according to Definition 2.5 . As we will only deal with the initial conditions Γ_0 and u^0, we may as well omit the index 0 in this section. Let $\Gamma \subset \mathbb{R}^3$ be a curve given by

$$\Gamma = \{(\gamma(x_3), x_3) \colon x_3 \in [0,1)\},$$

where $\gamma = (\gamma_1, \gamma_2) \colon [0,1) \to \mathbb{R}^2$ is a smooth periodic vector field. We define

$$u(x) := \frac{x' - \gamma(x_3)}{|x' - \gamma(x_3)|} \quad \text{for } x = (x', x_3) \in \mathbb{R}^3 \setminus \Gamma. \tag{121}$$

By Lemma 2.7 the energy of u can be written as an average of squared finite differences. More precisely, using (40) with $\psi = \mathbf{1}_\Omega$, we can write the energy in any bounded open set $\Omega \subset [0,\Lambda) \times \mathbb{R}^2$ as

$$E_h(u, \mathbf{1}_\Omega) = \frac{1}{2} \int_{\mathbb{R}^3} G(z) \int_\Omega \left| \frac{u(x) - u(x - \sqrt{h} z)}{\sqrt{h}} \right|^2 dx\, dz.$$

Now we split the domain of integration in x into a near-field region, which is the $\sqrt{h}$-neighborhood of the filament $A_h := \{x \in \Omega \colon d(x, \Gamma_0) < \sqrt{h}\}$, and its complement, the far-field region. Using $|u| = 1$, the integral over the near-field region is estimated by

$$\frac{1}{2} \int_{\mathbb{R}^3} G(z) \int_{A_h} \left| \frac{u(x) - u(x - \sqrt{h} z)}{\sqrt{h}} \right|^2 dx\, dz \le \frac{1}{2} \int_{\mathbb{R}^3} G(z) \int_{A_h} \frac{4}{h} dx\, dz \le \frac{2}{h} |A_h|.$$

Since the tubular neighborhood A_h of the smooth curve Γ_0 has Lebesgue measure $|A_h| \le Ch\mathscr{H}^1(\Gamma_0)$ for sufficiently small h, the right-hand side is uniformly bounded as $h \downarrow 0$.

The leading-order term of the energy is the integral over the far-field region, which has precisely the asymptotic behavior (28). Indeed, the trivial inequality $\left|\frac{p}{|p|} - \frac{q}{|q|}\right| \le 2\frac{|p-q|}{|p|}$ (which is valid for any two non-zero vectors p, q) applied to $p = x' - \gamma(x_3)$ and $q = x' - \sqrt{h} z' - \gamma(x_3 - \sqrt{h} z_3)$ implies

$$\left| \frac{u(x) - u(x - \sqrt{h} z)}{\sqrt{h}} \right|^2 \le 4 \frac{|\sqrt{h} z'|^2 + |\gamma(x_3) - \gamma(x_3 - \sqrt{h} z_3)|^2}{h|x' - \gamma(x_3)|^2} \le 4 \frac{(1 + \|\partial_{x_3}\gamma\|_\infty^2)|z|^2}{|x' - \gamma(x_3)|^2}$$

for all $z \in \mathbb{R}^3$. Therefore, the integral over the far-field region is estimated by

$$\begin{aligned}
&\frac{1}{2}\int_{\mathbb{R}^3} G(z) \int_{\Omega\setminus A_h} \left|\frac{u(x)-u(x-\sqrt{h}z)}{\sqrt{h}}\right|^2 dx\,dz \\
&\leq 2(1+\|\partial_{x_3}\gamma\|_\infty^2)\left(\int_{\mathbb{R}^3}|z|^2 G(z)\,dz\right)\int_{\Omega\setminus A_h}\frac{1}{|x'-\gamma(x_3)|^2}dx.
\end{aligned}$$

The prefactor as well ass the Gaussian integral are clearly bounded. If $R<\infty$ is sufficiently large such that $\Omega \subset B_R$ then the last integral can be estimated by

$$\begin{aligned}
\int_{\Omega\setminus A_h}\frac{1}{|x'-\gamma(x_3)|^2}dx \leq \int_0^1\int_{\{\sqrt{h}<|x'|<2R\}}\frac{1}{|x'|^2}dx'\,dx_3 = 2\pi\int_{\sqrt{h}}^{2R}\frac{1}{r^2}r\,dr \\
= 2\pi(\log(2R)-\log(\sqrt{h})) = C(R)(1+|\log h|).
\end{aligned}$$

This finishes the proof of the upper bound

$$E_h(u,\mathbf{1}_\Omega)\leq C|\log h|.$$

The matching lower bound

$$E_h(u,\mathbf{1}_\Omega)\geq c|\log h|$$

can be obtained by a reverse variant of the basic inequality $\left|\frac{p}{|p|}-\frac{q}{|q|}\right|\leq 2\frac{|p-q|}{|p|}$ above, namely $\left|\frac{p}{|p|}-\frac{q}{|q|}\right|\geq\frac{1}{|p|}\big(|p-q|-\big||p|-|q|\big|\big)$. Furthermore, the uniform bound on the energy away from the filament (29) follows from the derivation of the upper bound above.

When working with several filaments, as for example a periodic pattern of almost parallel filaments, again with periodic boundary conditions in the x_3-direction, the vector fields (121) around each filament with the appropriate choices of the sign may be easily glued together. We also want to stress that this construction is not restricted to dimension 3, but applies in general codimension-2 surface Γ in $\mathbb{R}^d$.

5.3 Cut-off at infinity

When adapting our proof to the whole space $\mathbb{R}^3$ one has to be careful, as the squared gradient as well as our energy densities are not integrable at infinity. Note for example that the gradient of the unit vector field $u(x)=\frac{x}{|x|}$ decays with rate $\frac{1}{|x|}$, which is not in $L^2(\mathbb{R}^2)$. By slicing it is clear that the behavior for the initial conditions discussed in Appendix 121 is divergent as well. This can be cured by choosing an appropriate cut-off at infinity. More precisely, the function $\phi_\sigma(x,t)$ given in (32) which we used to localize around the mean curvature flow Γ_t can then be replaced by $\phi_\sigma(x,t)\psi_R(|x|)$, where $\psi_R=\psi_R(r)$ is a smooth monotone non-increasing function with $\psi_R(r)=1$ for $0\leq r\leq R$ and $\psi(r)=\exp(-r)$ for $r\geq 2R$ such that $|\frac{d^k}{dr^k}\psi_R|\leq C_k\psi_R$ for all $k\in\mathbb{N}$.

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