Motion of Singularities in the Heat Flow of Harmonic Maps into a Sphere

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Abstract. Numerical experiments are used to determine the motion of singularities in the heat flow of harmonic maps into a unit sphere. These singularities are closely related to point defects in a nematic liquid crystals. The motion of singularities is affected by initial positions and interaction between singularities and boundary conditions. In particular, it is shown that the motion of singularities is the same as the motion of point defects in nematic liquid crystals under Neumann boundary conditions. For Dirichlet boundary conditions, the results do not properly reflect the crystal defect motion due to the shortcoming of the model.

AMS subject classifications: 65M99, 65S05
Key words: Heat flow of harmonic maps, singularity, boundary effect, interaction.

1. Introduction

The properties of liquid crystals have been widely studied by physicists, chemists, material scientists, mathematicians and so on. The results of these investigations are successfully applied in technology, including the display development and manufacturing. A simplified version of the general Ericksen-Leslie system [12, 18] for modeling the hydrodynamic flow of nematic liquid crystal materials has the form

\[ \begin{align*}
\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla P &= -\lambda \nabla \cdot \left( \nabla \mathbf{d} \odot \nabla \mathbf{d} - \frac{1}{2} |\nabla \mathbf{d}|^2 \mathbf{I}_n \right), \\
\nabla \cdot \mathbf{u} &= 0, \\
\mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} &= \gamma \left( \Delta \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d} \right),
\end{align*} \tag{1.1} \]

where \( \mathbf{u} : \Omega \times (0,T) \rightarrow \mathbb{R}^n \) is the velocity field of the underlying incompressible fluid, \( P : \Omega \times (0,T) \rightarrow \mathbb{R} \) is the pressure function, \( \mathbf{d} : \Omega \times (0,T) \rightarrow S^2 := \{ \mathbf{v} \in \mathbb{R}^3 : |\mathbf{v}| = 1 \} \)

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the averaged orientation of the nematic liquid crystal molecules. The positive constants \( \mu, \lambda \) and \( \gamma \) denote fluid viscosity, competition between kinetic energy and potential energy, and macroscopic elastic relaxation time for the molecular orientation field, respectively. From the viewpoint of mathematics, the Ericksen-Leslie equations are coupled by Navier-Stokes and harmonic heat flow equations. Such coupled systems have been studied in Refs. [4, 19, 28–30] by a penalty function method. Besides, the Doi-Onsager model, which simplifies the states of liquid crystal particles was considered in [20, 21]. If \( u = 0 \) and \( \gamma = 1 \), the third equation in (1.1) reduces to the heat flow of harmonic maps into a sphere — viz.

\[
d_t = \Delta d + |\nabla d|^2 d, \\
|d| = 1.
\]  

(1.2)

If \( u = 0 \), the Eq. (1.2) represents the orientation field of nematic liquid crystal molecules and geometrical methods have been successfully used to study this situation. Weinan and Wang [11] considered an implicit unconditionally stable first-order projection scheme. For two-dimensional equations, Struwe [25] and Chang [2] proved the existence of unique global weak solutions with at most finitely many singular points. Chang et al. [3] and Huang et al. [15] constructed examples of finite-time singularities for two- and three-dimensional equations, respectively. Other examples of finite-time singularities for three-dimensional equations have been presented by Coron and Ghidaglia [9] and also by Chen and Ding [5]. The existence of global partially regular weak solutions in higher dimensions is shown by Chen and Struwe [6] and by Chen and Lin [7].

In mathematical sense, defects in nematic liquid crystals can be considered as singularities. They attracted a substantial attention in the recent years. Here, we assume the validity of the continuum theory — i.e. the direction of liquid crystals is supposed to be continuous with respect to the spatial variables. Nevertheless, black filaments are often found in liquid crystal displays. It was noted by Friedel [13] in the beginning of twenties of the last century that this phenomenon is caused by discontinuities in the arrangement of liquid crystal molecules so that there is no well-defined direction. Such a state is called dislocation. We note that there are only two types of stable defects in crystals — viz. disclination lines and point defects. The dislocation can be characterised by the strength \( S \) represented either by half-integer or integer value and \( S \in \mathbb{Z} \) for point defects [17].

Repnik et al. [24] studied the interaction between defects and the annihilation of point defects in nematic liquid crystals. Svetec and Slavinec [26] considered the annihilation of hedgehog-antihedgehog defects in confined nematic liquid crystals and demonstrated the collision and merging of defects. Bogi et al. [1] studied the anchoring influence of two parallel \( +1/2 \) and \( -1/2 \) disclination lines on the annihilation dynamics in nematic liquid crystals. Dierking et al. [10] discovered that a backflow effect induced by elastic constants and anisotropy leads to the defect overlap and velocity asymmetry in the annihilation of umbilic defects of strength \( S = \pm 1 \). This is confined to Hele-Shaw cells with homeotropic boundary conditions. Besides, Tóth et al. [27] demonstrated that backflow, which is the coupling between the order parameter and the velocity fields, has a significant effect on the motion of defects in nematic liquid crystals. Moreover, the topological strength of defects
affects the velocity of the motion. As numerical experiments in [16] show, the defects of opposite signs attract and repel each other at small and large distances, respectively.

Ponti [23] identified two surface discontinuities in a nematic liquid crystals. Our computations also show the presence of surface discontinuities. Nehring and Saupe [22] analysed elastic free energy density involving the second-order derivative of the direction. This term influences the surface-like elastic constant $k_{13}$ [14] and causes a surface discontinuity, as reported by various authors.

In this work we discuss the evolution of singularities in the initial vector field for three-dimensional equations under Neumann and anchoring Dirichlet boundary conditions. The relations between $d$ and the directions of nematic liquid crystal molecules show that the motion of the singularities of the Eq. (1.2) can reflect the motion of defects in a nematic liquid crystals. In the Eq. (1.2), $d$ is distinguished by head and tail, while the direction of the nematic liquid crystal molecules is not — e.g. $(1, 0, 0) \leftrightarrow (-1, 0, 0)$. As numerical results show, for Neumann boundary conditions the motion of singularities can well simulate these point defects. For Dirichlet boundary conditions this is not true because of the shortcomings of the Ericksen-Leslie model.

Our numerical experiments involve three types of singularities denoted as I, II, and III. The singularities of types I and II have strength $S = +1$. The vector field where the singularities of type I (type II) are located, is similar to the direction field of the electric field formed by allocating a positive (negative) unit charge at the singularity position. The type III singularities have strength $S = -1$. They can be generated by two unit electric charges of the same sign and are located exactly at their midpoints. The vector field has at least two perpendicular axes and the singularity of type III can be induced by two positive unit charges on one axis or two negative unit charges on the other. For convenience, we call them positive- and negative-charge axis, respectively. Fig. 1 shows the singularities of all types in the two-dimensional unit square. Under Dirichlet boundary conditions, the motion of type I singularities differs from that of type II and the motion of type III singularities is affected by the relationship between its positive- or negative-charge axis and the anchoring direction. In nematic liquid crystals, there is no difference between singularities of type I and II or between positive- and negative-charge axes.

![Figure 1: Three types of singularities in two-dimensional unit square. The dots represent the singularities. (a), (b) and (c) show singularities of types I, II and III, respectively. In (c), positive- and negative-charge axes of the singularity are, respectively, horizontal and vertical axes through it.](image_url)
The remainder of this paper is organised as follows. In Section 2, we describe a numerical method for the harmonic heat flow equation with Dirichlet and Neumann boundary conditions. Section 3 contains the results of numerical experiments and a qualitative analysis of singularity movements. The motion laws and the variation of the singularity are summarised in Section 4.

2. A Numerical Method

We consider an initial boundary value problem for the first equation in (1.2) — viz.

\[ d_t = \Delta d + |\nabla d|^2 d \quad \text{in} \quad \Omega \times (0, T), \]
\[ d(x, 0) = d^0(x), \quad x \in \Omega, \quad \tau \]

where \(d^0(x)\) is a three-dimensional unit vector field. The Dirichlet boundary condition is

\[ d|_{\partial \Omega} = b, \quad t \in [0, T) \]

with a three-dimensional unit vector \(b\). We set \(\Omega = [0, 1]^3\) and divide each director into \(N\) equal parts so that the grid step size is \(h = 1/N\). For convenience, we write \((i, j, k)\) for the grid point \((x_i, y_j, z_k)\) and \(\tau\) for the time step.

The implicit central difference scheme for the first equation in (2.1) has the form

\[ \frac{d_{i,j,k}^{n+1} - d_{i,j,k}^n}{\tau} = \Delta d_{i,j,k}^{n+1} + |\nabla d_{i,j,k}^n|^2 d_{i,j,k}^{n+1}, \quad l = 1, 2, 3, \]

(2.2)

where \(i, j, k \in [1, N-1]\) and we write \(d_{i,j,k}^{n,l}\) for \(d^l(ih, jh, kh; n\tau)\). It follows that

\[ \Delta d_{i,j,k}^{n+1} = \frac{1}{h^2} \left( \delta_x^2 d_{i,j,k}^{n+1} + \delta_y^2 d_{i,j,k}^{n+1} + \delta_z^2 d_{i,j,k}^{n+1} \right), \]

where

\[ \delta_x^2 d_{i,j,k}^{n+1} = d_{i+1,j,k}^{n+1} - 2d_{i,j,k}^{n+1} + d_{i-1,j,k}^{n+1}, \]

\[ |\nabla d_{i,j,k}^n|^2 = \frac{\sum_{l=1}^{3} \left( |\delta_x d_{i,j,k}^n| + |\delta_y d_{i,j,k}^n| + |\delta_z d_{i,j,k}^n| \right)^2}{3} \]

\[ = \frac{1}{h^2} \sum_{l=1}^{3} \left( (d_{i+1,j,k}^{n,l} - d_{i,j,k}^{n,l})^2 + (d_{i,j,k+1}^{n,l} - d_{i,j,k}^{n,l})^2 + (d_{i,j,k-1}^{n,l} - d_{i,j,k}^{n,l})^2 \right). \]

Substituting these representations into the Eq. (2.2) and setting \(a = \tau/h^2\), we arrive at the system of linear equations

\[ -a \left( d_{i+1,j,k}^{n+1} + d_{i-1,j,k}^{n+1} + d_{i,j+1,k}^{n+1} + d_{i,j-1,k}^{n+1} + d_{i,j,k+1}^{n+1} + d_{i,j,k-1}^{n+1} \right) + (6a + 1)d_{i,j,k}^{n+1} \]
\[ = \frac{a}{4} \sum_{l=1}^{3} \left( (d_{i+1,j,k}^{n,l} - d_{i,j,k}^{n,l})^2 + (d_{i,j,k+1}^{n,l} - d_{i,j,k}^{n,l})^2 + (d_{i,j,k-1}^{n,l} - d_{i,j,k}^{n,l})^2 \right) + d_{i,j,k}^{n+1}. \]

(2.3)
The local truncation error of the scheme (2.3) is $O(\tau + h^2)$. The coefficient matrix in (2.3) is symmetric positive definite with all eigenvalues greater than 1. Therefore, the scheme is unconditionally stable and the solution of (2.1) can be determined by PCG method.

The computations run as follows:

**Step 1.** Solve the system of linear equations (2.3) by PCG method thus obtaining $d^{n+1}$.

**Step 2.** Normalise $d^{n+1}$ according to constrain $|d| = 1$ — i.e. replace $d^{n+1}$ by $d^{n+1}/|d^{n+1}|$.

Consider now the Neumann boundary condition

$$\frac{\partial d}{\partial n} = 0, \quad d \in \partial \Omega \times [0, T).$$

By adding a virtual grid on the boundary, we obtain

- $d_{-1,j,k} = d_{1,j,k}$,
- $d_{N+1,j,k} = d_{N-1,j,k}$,
- $d_{i,-1,k} = d_{i,1,k}$,
- $d_{i,N+1,k} = d_{i,N-1,k}$,
- $d_{i,j,-1} = d_{i,j,1}$,
- $d_{i,j,N+1} = d_{i,j,N-1}$.

Proceeding analogously to the Dirichlet boundary conditions case, we obtain a system of linear equations similar to (2.3). It can be handled by the same methods.

### 3. Numerical Results

In this section, we use some experiments to identify the laws of singularity motions for two boundary conditions and calculate the heat flow of the harmonic map equation in the domain $[0, 1]^3$. Choosing time step $\tau = 0.01$ and grid step $h = 1/N$ with $N = 95$, we select initial values with singularities located outside of the grid points. Our numerical experiments can be divided into two parts: one for the Neumann and another for the anchoring Dirichlet boundary conditions. In each situation the motions of single and multiple singularities are calculated. The motions of singularities are analysed by their configurations and positions and a number of conclusions about singularity motions is drawn from the data obtained. To illustrate the characteristics and position of a singularity, we display the projection of $d$ and the distribution of $|\nabla d|$ on the nearest to the singularity grid plane.

Recall that according to [8], the energy of $d$ is defined by

$$E(d) = \frac{1}{2} \int_{\Omega} |\nabla d|^2 dx.$$

#### 3.1. Neumann boundary condition

We consider the motion of singularities under the Neumann boundary condition, starting with the stability and motion of a single singularity when its initial position is changed. After that the interaction of two moving singularities is analysed and then the cumulative influence of the initial positions and interactions are taken into account.
3.1.1. Single singularity at calculation area center

A positive unit charge at \((x_0, y_0, z_0)\) creates an electric field whose direction field has the form

\[
\frac{(x - x_0, y - y_0, z - z_0)}{\sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2}}.
\]

To derive a singularity of type I or II at \((0.5, 0.5, 0.5)\), we, respectively, allocate a positive or negative unit charge there. Allocating two positive unit charges at \((-0.2, 0.5, 0.5)\) and \((1.2, 0.5, 0.5)\) leads to a type III singularity at the point \((0.5, 0.5, 0.5)\) in the direction field of their electric fields. We select these three direction fields as the initial values. Then there is only a single singularity at the center of the calculation area present. As is shown in Fig. 2, the vector fields with the singularities of type I or II do not substantially vary over time. However, the vector fields with the type III singularities change and eventually become stable. Their transformation process can be considered as the case where two positive charges generating the singularity are well-separated from each other. The numerical results demonstrate that all singularities located at the center of calculation area are stable.

![Figure 2: Projections of d at the plane \(z = 0.5035\). The blue and yellow vectors represent the vector fields at times \(t = 0\) and \(t = 10\), respectively, and the singularity in the center is stable.](image)

3.1.2. Single singularity outside of calculation area center

In this section, the initial values are obtained by the same method as before, but the initial positions of singularities do not coincide with the point \((0.5, 0.5, 0.5)\). The singularity is now unstable, moves toward the nearest boundary and eventually disappears there, while the direction field converges to the same direction.

1. The movement of type I singularities for various initial positions is shown in Fig. 3 and the energy evolution in Fig. 5. According to Fig. 3(b) and 3(c), the singularities of type I move to every boundary at the same speed under the same margin distance. If the opposite to this initial value is selected, the singularity of type I transforms into the singularity of type II. The examples also show that the type II singularities migrate similar to the singularities of type I.
2. The movement of type III singularities for various initial positions is shown in Fig. 4 and the energy evolution in Fig. 5. The examples show that the singularities move faster in the directions parallel to \( y \) or \( x \) axes. In general, the type III singularities move faster in the direction parallel to their negative-charge axes than to the directions parallel to the positive-charge ones.

(a) \( s_0 = (0.4, 0.5, 0.5) \)
(b) \( s_0 = (0.4, 0.4, 0.5) \)
(c) \( s_0 = (0.4, 0.4, 0.4) \)

Figure 3: Motions of a type I singularity with various initial positions. In (a), (b) and (c), the movement directions of the singularity are \(-(1, 0, 0)\), \(-(1, 1, 0)\) and \(-(1, 1, 1)\), respectively.

(a) \( s_0 = (0.4, 0.5, 0.5) \)
(b) \( s_0 = (0.4, 0.4, 0.5) \)
(c) \( s_0 = (0.4, 0.4, 0.4) \)

Figure 4: Motions of a type III singularity with various initial positions.

(a)
(b)

Figure 5: Evolution of energy. Left: type I and right: type III.
3.1.3. Multiple singularities

1. Two singularities of type II and type I.
   At the initial time we have a singularity of type II at \((0.3, 0.5, 0.5)\) and another one of type I at \((0.7, 0.5, 0.5)\). They repel each other and subsequently disappear at the boundary — cf. Fig. 6(a).

2. Two singularities of type III and type I.
   At the initial time there is a singularity of type III at \((0.2, 0.5, 0.5)\) and another one of type I at \((0.8, 0.5, 0.5)\). These singularities attract each other and subsequently annihilate via collision — cf. Fig. 6(b).

3. Three singularities of type I and type III.
   Case 1. At the initial time there are two singularities of type I at \((0.3, 0.5, 0.5)\) and \((0.7, 0.5, 0.5)\) and one singularity of type III at \((0.5, 0.5, 0.5)\). The motions of the singularities and the energy evolution are displayed in Fig. 7. Two side singularities of type I move at the same speed toward the singularity of type III in the middle and subsequently collide. After collision, only one singularity of type I remains.
This singularity is located at the center of the computation area and is stable according to the results in Section 3.1.1. Therefore, the corresponding energy converges over time to a non-zero value. This differs from the other cases, where all singularities disappear and the energy converges to zero.

Case 2. At the initial time there are two singularities of type I at (0.2, 0.5, 0.5) and (0.6, 0.5, 0.5) and one singularity of type III at (0.4, 0.5, 0.5). The side singularities of type I move toward type III singularity in the middle and the right one moves faster than the left one — cf. Fig. 8. The two singularities on the right side collide and annihilate. Afterwards, the remaining left singularity moves to the boundary $x = 0$ and disappears. The energy evolution is shown in Fig. 7.

Case 3. At the initial time there are two singularities of type I at (0.3, 0.5, 0.4) and (0.7, 0.5, 0.4) and one singularity of type III at (0.5, 0.5, 0.4). The side singularities of type I move at the same speed toward the singularity of type III in the middle — cf. Fig. 9. Then they collide and only the singularity of type I remains. After the collision, the remaining singularity moves to the boundary $z = 0$ and disappears. The energy evolution is shown in Fig. 7.

Figure 7: Motion of the three singularities in Case 1 (top) and the evolution of energy for the three cases (bottom).
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4. Three singularities of type II and type III.

Choosing the initial values opposite to the initial values of the previous three cases in item (3), we obtain two singularities of type II and one singularity of type III. Examples show that the movements of these singularities are the same as in Case 3.
The results above show that the initial positions have an important influence on the movements of singularities. If at the initial time the singularity is located at the center of the calculation area, then it is stable. Otherwise, it moves to a boundary and disappears. Moreover, singularities interact with each other. Let us summarise our findings.

1. Singularities are inclined toward moving to the nearest boundary. A single singularity is stable if it is located within the same distance to each boundary, otherwise it moves to a boundary and disappear.

2. Being located at the same distance to the boundary, the singularities of type I or type II move to each boundary at the same speed. The type III singularities move faster in the direction parallel to their negative-charge axes than in the direction parallel to the positive-charge ones.

3. Two singularities will repel each other if their strengths are of the same sign. Otherwise, they attract each other.

4. The motion of singularities is equivalent if their initial vector fields differ only in sign.

3.2. Dirichlet boundary condition

We now impose the anchoring Dirichlet boundary condition assuming that on the boundary the direction field is constant. The anchoring direction of the boundary is denoted by \( \mathbf{b} \). It is a three-dimensional unit vector. The anchoring direction has an important influence on the motion of singularities, producing the so-called boundary anchoring effect. This boundary anchoring effect is studied by following the movements of single singularities. The movements of multiple singularities is used to analyse the interaction and the boundary anchoring effect influence on the movements of singularities. Experimental results show that for the singularities of different type, the anchoring effects of the boundary differ in terms of direction. In contrast to the Neumann boundary condition, if the initial vector fields are distinguished only by opposite signs, the motion of their singularities are not equivalent.

3.2.1. Motion of a single singularity

We suppose that there is only one singularity of the initial direction field, which is located at the center of the computation area. In contrast to the Neumann boundary conditions, now the singularities always unstable. The movement of the singularity depends only on its type and the anchoring direction of the boundary. The singularity always moves to one of the boundaries and eventually disappears there. All cases converge to a steady state and the direction field takes a constant value in the end.

1. Singularities of type I.

Chose \( \mathbf{d}^0 = (x - 0.5, y - 0.5, z - 0.5) \) and normalise it so that the initial value is \( \mathbf{d}^0 / |\mathbf{d}^0| \). There is only one singularity of type I in the domain \([0, 1]^3\) located at the
point \((0.5, 0.5, 0.5)\) and the variables \(x, y\) and \(z\) in the initial value are equivalent. The numerical results for the anchoring direction \(b\) parallel to the \(x\)-axis are displayed in Fig. 10. The singularity disappears at some instant in time between \(t = 1.3\) and \(t = 1.35\). Finally, everywhere except the boundary the vector field \(d\) is constant — viz. \((-b)\). For arbitrary anchoring direction, the movement direction of the singularity is the same as the anchoring direction.

![Figure 10](image1.png)

**Figure 10:** Motions of a type I singularity under two anchoring boundary conditions.

2. Singularity of type II.

Choose \(d^0 = -(x - 0.5, y - 0.5, z - 0.5)\) and normalise it so that the initial value is \(d^0/|d^0|\). The sign of this initial value is opposite sign to corresponding sign in the previous situation. There is only one singularity of type II in the domain \([0,1]^3\) at \((0.5, 0.5, 0.5)\). The numerical results for the anchoring direction \(b\) parallel to the \(x\)-axis are displayed in Fig. 11. The singularity disappears at some instant in time between \(t = 1.3\) and \(t = 1.35\). Finally, everywhere except the boundary the vector field \(d\) is constant — viz. \((-b)\). For arbitrary anchoring direction, the movement direction of the singularity is opposite to the anchoring direction.

![Figure 11](image2.png)

**Figure 11:** Motions of a type II singularity under two anchoring boundary conditions.
3. Singularity of type III.

Considering

\[ g = \frac{(x + 0.2, y - 0.5, z - 0.5)}{(x + 0.2)^{2} + (y - 0.5)^{2} + (z - 0.5)^{2}}, \]

\[ f = \frac{(x - 1.2, y - 0.5, z - 0.5)}{(x - 0.2)^{2} + (y - 0.5)^{2} + (z - 0.5)^{2}}. \]

we choose \( d^{0} = g + f \) and normalise it so that the initial value is \( d^{0}/|d^{0}| \). There is only one singularity of type III in the domain \([0, 1]^{3}\) at \((0.5, 0.5, 0.5)\). Since the initial values are symmetric with respect to \( y \) and \( z \), we can consider only the cases where the anchoring direction of the boundary is parallel to \( x \)-axis and \( z \)-axis. For the given singularity, the \( x \)-axis and \( z \)-axis are parallel to the positive-charge and negative-charge axes, respectively. The numerical results are displayed in Fig. 12.

If the anchoring direction \( b \) of the boundary, is parallel to the \( x \)-axis or \( z \)-axis, the singularity moves in the direction \(-b\) and \( b\), respectively. Finally, everywhere except the boundary \( d = -b \). If \( b = (1, 0, 0) \), the singularity disappears after \( t = 1.8 \) and if \( b = (0, 0, 1) \) it disappears prior to \( t = 1.2 \).

![Image](image_url)

**Figure 12:** Motions of a type III singularity under two anchoring boundary conditions.

The results above can be now summarised as follows:

1. For single singularity the anchoring effect of the boundary forces the singularity to move in the direction \( b \) or \(-b\) if the vector \( b \) is parallel to its negative or positive charge axis. Any axis passing through the singularity of type I or II can be regarded as its negative or positive axis.

2. Before disappearing, the singularities of type I and II move at the same speed in every direction. The singularity of type III moves faster in the direction parallel to its negative-charge axis than in the direction parallel to its positive-charge one, consistent with the second conclusion for Neumann boundary condition.
3.2.2. Motions of multiple singularities

Let us consider the situation with multiple singularities in the initial vector field. The interaction between singularities will now also affects their movements in addition to the anchoring effect of the boundary. According to previous considerations, the singularities will either repel or attract each other depending on their strengths signs. The experiments below show that the type of singularities and the distance between them also influence the interaction. In the diagrams below, black and blue vectors are used in order to represent the interaction between the singularities and the anchoring effect of the boundary.

Let
\[ p = \frac{(x - 0.3, y - 0.5, z - 0.5)}{(x - 0.3)^2 + (y - 0.5)^2 + (z - 0.5)^2}, \]
\[ q = \frac{(x - 0.7, y - 0.5, z - 0.5)}{(x - 0.7)^2 + (y - 0.5)^2 + (z - 0.5)^2}. \]

1. One singularity of type II and one of type I.

Set \( d^0 = -p + q \) and normalise it so that the initial value is \( d^0 / |d^0| \). In the domain \([0, 1]^3\) there is one singularity of type II at \((0.3, 0.5, 0.5)\) and one singularity of type I at \((0.7, 0.5, 0.5)\). They both are located on the axis \( y = 0.5, z = 0.5 \) which is the positive-charge axis for the singularity of type III, and the force diagrams for these singularities with various anchoring boundary conditions are presented in Table 1.

| b = (1,0,0) | b = -(1,0,0) | b = (1,0,0) |
|------------|-------------|------------|
| ![Diagram 1] | ![Diagram 2] | ![Diagram 3] |

Their strengths are of the same sign, so that their interaction is repulsive as indicated by the black vectors. The directions of the anchoring effect for two singularities are opposite, as indicated by the blue vectors. The movements of these singularities under various anchoring boundary conditions are shown in Fig. 13. The singularities are far away from each other. Combining the force diagram and the repulsion of the singularities under the anchoring direction \( b = -(1,0,0) \), we conclude that the interaction between the singularities is stronger than the anchoring effect of the boundary.

2. One singularity of type III and one of type I.

Let \( d^0 = ((x - 0.5)^2 + (y - 0.5)^2 + (z - 0.5)^2 - 0.09, y - 0.5, z - 0.5) \). Then, the initial value is \( d^0 / |d^0| \). In the domain \([0, 1]^3\) there is one singularity of type III at \((0.2, 0.5, 0.5)\) and one singularity of type I at \((0.8, 0.5, 0.5)\). They are located on the axis \( y = 0.5, z = 0.5 \) which is the positive-charge axis for the singularity of type III,
whose negative-charge plane is the plane $x = 0.2$ — i.e. any axis through a singularity in this plane is a negative-charge axis for this singularity. The force diagrams for these singularities with various anchoring boundary conditions are presented in Table 1. Their strengths are of opposite signs, so that the corresponding interaction is attractive. The motions of these singularities under various anchoring boundary conditions are shown in Fig. 14. In our numerical experiments, the singularities approach to or move away from each other.

For $b = (1, 0, 0)$ the interaction between singularities of type III and type I is weaker than the anchoring effect of the boundary. Moreover, at a time instant the singularities in 1 are located at the points $(0.2, 0.5, 0.5)$ and $(0.8, 0.5, 0.5)$. According to the force diagram, for $b = -(1, 0, 0)$ the interaction between the singularities of type II and I is stronger than the anchoring effect of the boundary. Therefore, the interaction between the singularities of type III and I located at the same distance is weaker than that of singularities of type II and I.

Furthermore, according to the movement of three singularities in Case 1, the attraction between the singularities of type III and I is stronger than the exclusion of two singularities of type I. Hence, the interaction between singularities diminishes as the distance between them grows.
Motion of Singularities in the Heat Flow of Harmonic Maps into a Sphere

Let \( d_0 = p + q \). Then, the initial value is \( d_0/|d_0| \). In the domain \([0, 1]^3\) there are two singularities of type I at \((0.3, 0.5, 0.5)\) and \((0.7, 0.5, 0.5)\) and one singularity of type III at \((0.5, 0.5, 0.5)\). They all are located on the positive-charge axis \( y = 0.5, z = 0.5 \) of the singularity of type III. The negative-charge plane of this singularity is \( x = 0.5 \). The force diagrams of the singularities under various anchoring boundary conditions are presented in Table 2.

3. Two singularities of type III and one of type I.

The middle singularity attracts side singularities depending on their strengths and distance between singularities and this attraction is stronger than their repulsion. Simultaneously, the side singularities attract the middle one with the same magnitude but in opposite directions, so that the resultant force is zero. The anchoring effects on the singularities are again shown by blue vectors. The motions of these singularities

![Figure 14: Distribution of \( |\nabla d| \) when there are two singularities of type III and type I. The singularities will either repel each other and disappear at the boundary or attract and subsequently collide to disappear. (a) and (b) show that the singularities always move along the axis \( y = 0.5, z = 0.5 \) when \( b \) is parallel to it. (c) shows that the singularities move slightly off the axis \( y = 0.5, z = 0.5 \) when \( b \) is vertical to it.](image-url)
for various anchoring boundary conditions are shown in Fig. 15. If \( \mathbf{b} = (0, 0, 1) \), the singularities collide, thus producing one singularity of type I — cf. Fig. 16(a). This singularity moves to the nearest boundary and disappears. According to the singularity movements, the interaction between the singularities is stronger than the anchoring effect.

4. Two singularities of type III and one of type II.

Let \( \mathbf{d}^0 = -\mathbf{p} - \mathbf{q} \). Then the initial value is \( \mathbf{d}^0 / |\mathbf{d}^0| \). In the domain \([0, 1]^3\) there are two singularities of type II at \((0.3, 0.5, 0.5)\) and \((0.7, 0.5, 0.5)\) and one singularity of type III at \((0.5, 0.5, 0.5)\). They all are located on the negative-charge axis \( y = 0.5, z = 0.5 \) for the singularity of type III. The positive charge plane for this singularity is \( x = 0.5 \). The force diagrams for these singularities under various anchoring boundary conditions are presented in Table 2. The initial direction field \( \mathbf{d}^0 \) differs from the previous one only by the opposite sign. The force diagram and numerical results are similar to the previous case (3) with opposite anchoring directions. The motions of these singularities under various anchoring boundary conditions are shown in Fig. 17. If \( \mathbf{b} = (0, 0, 1) \), the singularities collide, thus producing one singularity of type II — cf. Fig. 16(b). This singularity moves to the nearest boundary and disappears. The interaction between the singularities is stronger than the anchoring effect.
4. Conclusions

The singularities of the Eq. (1.2) are closely related to point defects in nematic liquid crystals. Therefore, the direction of nematic liquid crystal molecules can be described by the Eq. (1.2) if \( u = 0 \). In addition, the term \( d \) in the Eq. (1.2) is distinguished by head and tail, whereas the direction of nematic liquid crystal molecules is not. In nematic liquid crystals, there is no difference between the singularities of type I and II, neither between positive- and negative-charge axes for singularities of type III. For Neumann boundary conditions, the
movements of singularities are the same even if the initial values have opposite signs but the same magnitude. In this case, the motion of point defects can be properly simulated by the motion of singularities. For Dirichlet boundary condition, the movement of singularities of types I and II differs. Besides, the movement of the singularities of type III is related to their positive- and negative-charge axes and to anchoring directions. For the same anchoring boundary conditions, d inside the computational domain will almost converge to the same direction, although the motion of singularities may be not equivalent. Under Dirichlet boundary condition, the value of d on the boundary may be discontinuous in the final stable state. In certain situations, the direction on the boundary is almost opposite to the direction in the inner area in the end. However, for the nematic liquid crystals, they are considered as the same directions.

Singularities are inclined to move toward the closest boundary. Therefore, the initial position of the singularity has a substantial influence on its stability. For the same distance, a singularity of type I or II moves at the same speed in every direction. In contrast, the singularity of type III moves faster in the direction of its negative-charge-axis and slower in the positive-charge-axis direction. For Neumann boundary conditions and in the absence of external effects, a single singularity is stable if only if it is located at the center of the computational area. Its position and shape remain the same over time. Otherwise, singularities will disappear at the boundary or are annihilated via collision. This is caused by many factors, including movement trends, interactions between various singularities and the anchoring effect of the boundary.

Two singularities always interact with each other. If their strengths have the same sign, they repel each other. Otherwise, they attract each other. The magnitude of the interaction is related to the distance between the singularities and their types: the farther away they are from each other, the weaker their interaction is. For singularities located at the same distance, the interaction between the ones of type I and II is stronger than that between those of type I (or II) and III.

Under the Neumann boundary condition, the motion of the singularities is affected by initial positions and their interaction. Under the Dirichlet boundary condition, the motion of the singularity is also affected by the anchoring effect of the boundary. The anchoring effect of the boundary forces singularities to move in the direction determined by their type. A singularity experiences an anchoring effect of the same or opposite direction of the boundary if b is parallel to its negative- or positive-charge axes, respectively. Thus the anchoring effect on a singularity of type I (II) has always the same or opposite direction of the boundary.

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