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# Conservation of disclination strength in two-dimensional lattice models of liquid crystalline textures

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# Conservation of disclination strength in two-dimensional lattice models of liquid crystalline textures

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The disclination strength defined on the boundary of textures generated by recently proposed simple modelling methods appears to be the sum of the strengths of primitive disclinations inside the boundary. In this paper, a rationalization is provided for these observations in two dimensions using an analytical expression for the conservation law for wedge type disclinations.



## 1. Introduction

In liquid crystal systems, a variety of fascinating texture patterns are observed when viewed under crossed polars [1]. The observed texture depends on boundary conditions, container shape, the dimension of the system, external fields, and mesophase type [1–3]. The textures are often attributed to disclinations, that is, singular points, lines, or walls in a director field [3]. Interactions and types of disclinations have been studied in terms of their topology and energy [2–4]. Experimentally, the fusion of two disclinations is often observed, resulting in their annihilation or the creation of a new disclination, with the total disclination strength conserved [5]. Theoretically, the conservation law of disclination strength has been proven for some cases [3, 6, 7]. For a system with wedge type disclinations, the conservation law might be expected to hold since all disclination lines are regarded as parallel to each other [3].

In the previous study of the texture patterns generated by a lattice model [8], we obtained wedge type disclination patterns for fixed boundary conditions which encourage a disclination in the centre of the system. In the patterns where larger disclination strengths were imposed on the boundary, several primitive disclinations of $\pm 1/2$ strength were observed instead of a single disclination, and the sum of the strengths of these primitive disclinations appeared to be equal to the disclination strength characterizing the boundary. A similar observation seems to hold for the patterns obtained by Bedford *et al.* [9]. In this paper, it is shown that the disclination strength is conserved for the two-dimensional system which satisfies the Frank equation [10] for a fixed boundary condition. Also, it is shown that the conservation holds for more general cases.

## 2. Conservation law of disclination strength

We consider a two-dimensional director field **n** in the $xy$-plane. The orientation of a director at $(x, y)$ is specified by an angle $\phi(x,y)$ relative to the $x$ axis, which satisfies

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0, \tag{1}$$

derivable from the continuum theory [10]. The solution, which can include a disclination, is given [10] as

$$\phi = S\varphi + \phi_0 \text{ with } \varphi = \arctan\frac{y}{x}, \tag{2}$$

where $S$ is the disclination strength and $\phi_0$ is a constant. The solution for the system on which the boundary condition $\phi_\gamma$ is imposed may be expressed by the linear combination of the primitive solutions of equation (2):

$$\phi(x, y) = \sum_{i=1}^{m} S_i\varphi_i(x, y) + \phi_0(x, y) \text{ with } \varphi_i(x, y) = \arctan\frac{y - y_i}{x - x_i}, \tag{3}$$

where $(x_i, y_i)$ indicates the location of the primitive disclinations with the strength $S_i$. $\phi_0(x, y)$ is a function which does not comprise singularities inside the boundary and satisfies $\nabla^2\phi_0 = 0$. The problem is to determine the values of $(x_i, y_i)$, $S_i$, $\phi_0$, and $m$, the number of primitive disclinations, so as to satisfy the condition that $\phi = \phi_\gamma$ on the boundary. Apart from the problem of determining these parameters, it is shown that the sum of the strengths of primitive disclinations is equal to the disclination strength $S_\gamma$ characterizing the boundary condition . Taking the gradient of $\phi$ in equation (3) and integrating it along the boundary $\gamma$, we obtain

$$\begin{aligned} S_\gamma &\equiv \frac{1}{2\pi}\oint_\gamma \nabla\phi \cdot d\mathbf{s} \\ &= \sum_{i=1}^{m} S_i \frac{1}{2\pi}\oint_\gamma \nabla\varphi_i \cdot d\mathbf{s} + \frac{1}{2\pi}\oint_\gamma \nabla\phi_0 \cdot d\mathbf{s} \\ &= \sum_{i=1}^{m} S_i, \end{aligned} \tag{4}$$

where the direction of the contour integral is taken positive, that is, the integration is performed along $\gamma$, looking at the system on the left side. The second term in the second line of equation (4) vanishes because $\phi_0$ does not include singularities inside $\gamma$.

There are a number of possible ways to determine the set of parameters, $(x_i, y_i)$, $S_i$, $\phi_0$, and $m$. These include the modelling methods proposed by Bedford *et al.* [9], and by us [8], which are equivalent to solving equation (1) numerically for a fixed boundary condition [8]. The modelling shows that multiple solutions are possible for a given boundary condition, each representing a configuration at one of the local energy minima. This implies that various sets of parameters might be allowed for a given boundary condition $\phi_\gamma$, but $S_i$ satisfies the conservation condition expressed by equation (4).

The above discussion assumes that $\phi$ satisfies equation (1), that is, the system is in a local energy minimum. As is shown below, the conservation holds even for systems which deviate from a local minimum. This applies to the case where the simulation of Bedford *et al.* [9] is terminated before the system reaches an energy minimum, or to the case of Monte Carlo simulations where configurations with higher energy are allowed.

Let us consider a director field $\phi(x, y)$, which this time does not necessarily satisfy equation (1), defined in the region $\Omega$ encircled by the boundary $\gamma$. On $\gamma$ is imposed a boundary condition which is characterized by the disclination strength $S_\gamma$ defined, in a way similar to equation (4), by

$$S_\gamma = \frac{1}{2\pi}\oint_{(\gamma)} \nabla\phi \cdot d\mathbf{s}, \tag{5}$$

where the direction of $\gamma$ is taken positive. Let us suppose that $\Omega$ contains some disclination points, for example, $P_1$ and $P_2$ as shown in figure 1. Enclosing $P_1$ and $P_2$ by circuits $\gamma_1$ and $\gamma_2$, we define a region $\Omega_q$ surrounded by the circuit $\gamma_q$ starting from $A$ going through $BC\gamma_1DEFG\gamma_2HI$ and returning to $A$. The disclination strength of the circuit $\gamma_q$ is then expressed by

$$\begin{aligned} S_{\gamma_q} &= \frac{1}{2\pi}\oint_{(\gamma_q)} \nabla\phi \cdot d\mathbf{s} \\ &= \frac{1}{2\pi}\left\{\int_A^B + \int_B^C + \oint_{(\gamma_1)} + \int_D^E + \int_E^F + \int_F^G + \oint_{(\gamma_2)} + \int_H^I + \int_I^A\right\}\nabla\phi \cdot d\mathbf{s}. \end{aligned} \tag{6}$$

Due to the cancellation of integrals on $BC$ and $DE$ and those on $FG$ and $IH$, $S_{\gamma_q}$ is simplified as

$$S_{\gamma_q} = \frac{1}{2\pi}\left\{\oint_{(\gamma)} + \oint_{(\gamma_1)} + \oint_{(\gamma_2)}\right\}\nabla\phi \cdot d\mathbf{s}. \tag{7}$$

On the other hand, using the two-dimensional Gauss theorem, the contour integral on $\gamma_q$ in equation (6) is transformed to the surface integral over $\Omega_q$, which vanishes because $\nabla\phi$ is regular in $\Omega_q$. Consequently, $S_{\gamma_q}=0$, and equation (7) becomes

$$\frac{1}{2\pi}\oint_{(\gamma)} \nabla\phi \cdot d\mathbf{s} = \frac{1}{2\pi}\oint_{(-\gamma_1)} \nabla\phi \cdot d\mathbf{s} + \frac{1}{2\pi}\oint_{(-\gamma_2)} \nabla\phi \cdot d\mathbf{s}, \tag{8}$$

which reads

$$S_\gamma = S_{\gamma_1} + S_{\gamma_2}. \tag{9}$$

The above consideration is readily extended to the case of $n$ disclination points

$$S_\gamma = \sum_{i=1}^{n} S_{\gamma_i}. \tag{10}$$

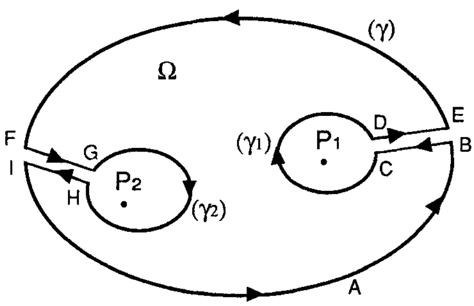


Figure 1. Two-dimensional region $\Omega$ enclosed by $\gamma$ where two primitive disclinations $P_1$ and $P_2$ are assumed.

The sign of the disclination strength $S_{\gamma_i}$ coincides with that of the conventional disclination strength as long as the direction of $\gamma_i$ is taken positive. Note that the only condition in deriving equation (10) is that $\phi$ is continuous everywhere except at disclination points.

## 3. Conservation of disclination strength in lattice models

Here, we show some examples of the conservation of disclination strength observed in two-dimensional lattice models. First, we consider the solution of the continuum theory, equation (2), in discrete form. Second, patterns generated by a matrix method [8] are reviewed. Finally, the patterns obtained by recent simulation methods [9, 11] under various conditions are analysed. In every case, the strength and location of a primitive disclination is detected by calculating the strength along a circuit connecting four lattice sites which form a square.

### 3.1. *Continuum theory solutions*

In figure 2 are displayed the solution of the continuum theory, equation (2), for $S = 3/2$ and $-2$ in a discrete form. Primitive disclinations of strength $\pm 1/2$ are found around the core region of the system. But these are not true disclinations because equation (2) should have only one disclination with strength of $S$ ($= 3/2$ or $-2$ in this case) located at the centre of the system. These primitive disclinations are



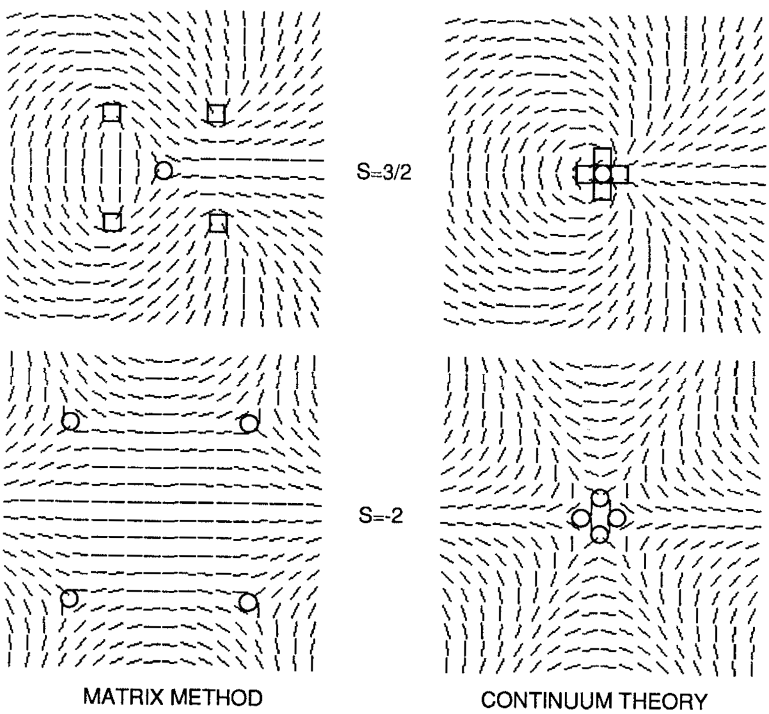


Figure 2. Texture patterns [8] obtained by the continuum theory (right) and by the matrix method (left) with fixed boundary conditions of $S = 3/2$ (top) and $S = -2$ (bottom). Circles and squares indicate primitive disclinations of strength of $-1/2$ and $1/2$, respectively.

attributed to an artifact due to insufficiently discrete sampling of the continuum field, and they will remain even with a finer division; the finer the division, the closer these primitive disclinations approach to the centre of the core. In the infinitely fine limit, these primitive disclination points collapse exactly to a single disclination point with strength $S$. Hence, a disclination with larger $S$ might be regarded as being composed of some primitive disclinations.

The disclination strengths along the boundaries are evidently 3/2 and $-2$, respectively. The sum of the strengths of the apparent primitive disclinations coincides with the $S$ value of the boundary. This observation holds for other $S$ values up to $\pm 7/2$ in the present study, except $S=1$ and 3 where the strength of some primitive disclinations is undetermined because $|\nabla\phi| = \pi/2$ for adjacent lattice sites.

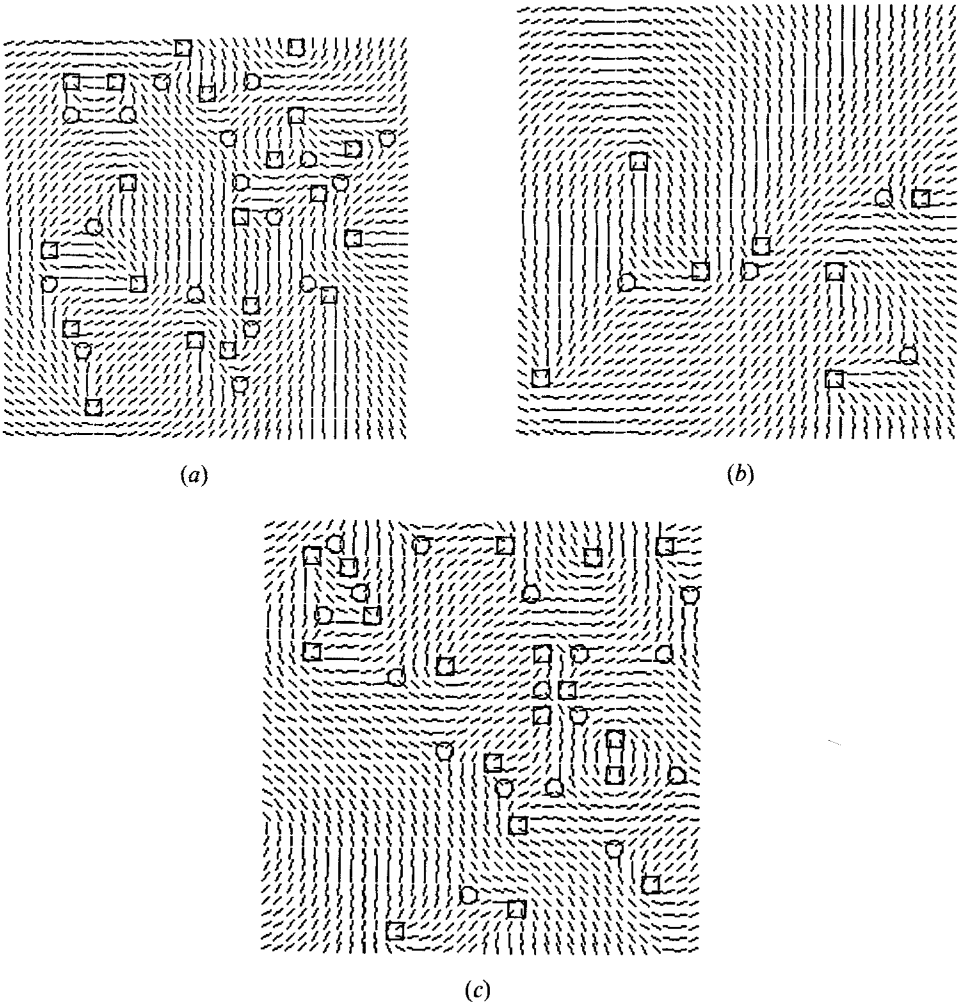


Figure 3. Texture patterns with fixed boundary condition of $S=3/2$, simulated by the quenching method (*a*) and by the annealing method (*b*). The periodic boundary condition was used for (*c*), where the disclination strength of the boundary is found to be $S=1/2$. Circles and squares indicate primitive disclinations of strength of $-1/2$ and $1/2$, respectively.

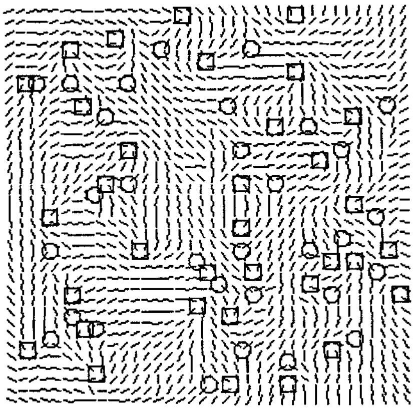

Figure 4. Texture patterns simulated by the quenching method with $S=3/2$ (as in figure 3 (*a*)), but with iteration truncated before the energy minimization is completed. Circles and squares indicate primitive disclinations of strength of $-1/2$ and $1/2$, respectively.



Even for these cases, the conservation law is satisfied by taking a circuit large enough to avoid discrete sampling errors.

### 3.2. *Matrix method solutions*

In figure 2 are reproduced the patterns obtained by the matrix method [8] for $S=3/2$ and $-2$ for the comparison with those by the continuum theory. The conservation law is evidently satisfied: $3/2=4\times(1/2)-1/2$, and $-2=4\times(-1/2)$. For the other values of $S$ in the previous study [8], the conservation law is also satisfied: for $S=-3/2$ and 2, we have $-3/2=4\times(-1/2)+1/2$ and $2=4\times(1/2)$, and for $S=\pm1$ with shifted centre, we have $-1=2\times(-1/2)$ and $1=2\times(1/2)$. Comparing the patterns between the two methods, we find that the topology of the primitive disclinations apparent in the core for the continuum theory seems to remain in the patterns of the matrix method, with the total energy decreased by decentralizing the apparent primitive disclinations. The same tendency is observed for other values of $S$. It should be noted that the solution by the matrix method corresponds to equation (3) where multiple disclination points are allowed to be located in an arbitrary way as long as the conservation is satisfied and $\phi_0$ is determined.

### 3.3. *Pattern obtained by simulation*

The simulation used to obtain the texture patterns shown in figure 3 is based on an iterative method of selecting a lattice site and minimizing the orientational energy of the site with respect to its four neighbours until the total energy becomes a minimum [9, 11]. The patterns shown here thus satisfy equation (1). Two types of boundary conditions are possible: fixed and periodic boundary conditions. In the case of fixed boundary conditions, two ways to select a lattice site are possible: random selection (quenching method) and selection from the boundary (annealing method [11]) In figure 3 (*a*) is shown a texture pattern obtained by the quenching method with the fixed boundary condition of $S=3/2$. We see that the conservation law is satisfied: $3/2=17\times(-1/2)+20\times(1/2)$. In figure 3 (*b*), a result for the annealing method for the same boundary condition is shown, where we see

$3/2=4\times(-1/2)+7\times(1/2)$. In figure 3 (*c*) a texture pattern for the periodic boundary condition is shown. (In the periodic boundary condition, directors on the boundary of the lattice are not fixed but are subjected to minimization with respect to their four neighbours: at a lattice site $(n,j)$, for example, on the boundary of the right edge of the system, one of these neighbours, i.e., $(n+1,j)$, is located outside the system. In the periodic boundary condition, this site is assumed to be identical with $(1,j)$, i.e. one on the left edge of the system. The same thing applies to the other edges.) In the figure, we see that the disclination strength around the boundary is 1/2 which is equal to the sum of the primitive disclinations, i.e. $17\times(-1/2)+18\times(1/2)$.

Figure 4 shows a texture for the quenching method with $S=3/2$ as the fixed boundary condition, but here the iteration is truncated before the energy minimization is completed, so that equation (1) is not satisfied. As proven in § 2, even under this condition, the conservation of the disclination strength is expected. Thus, we see that $3/2=31\times(-1/2)+34\times(1/2)$.

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