The effect of elastic anisotropy on nematic disclination lines

Gavin Kelly, Nigel Mottram, Alison Ramage
Department of Mathematics, University of Strathclyde, Glasgow G1 1XH, United Kingdom.

Introduction

Under a polarising microscope, liquid crystals exhibit beautiful optical patterns such as the Schlieren texture of a nematic, the fingerprint texture of a cholesteric and the focal conic structure of smectics. These textures are due to an assembly of topological defects and are determined by the molecular ordering of the particular mesophase [1]. Such defect textures are useful in identifying liquid crystal phases but are generally an unwanted effect causing a reduction in contrast of a liquid crystal display. Whether needed for identification or unwanted in displays, a clear understanding of defects will be extremely useful. Figure 1 shows a typical Schlieren texture, in the xy coordinate plane, of a

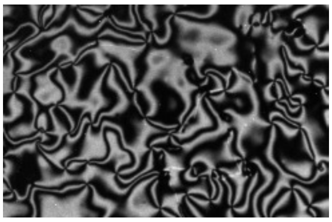

Figure 1: Schlieren texture of a nematic liquid crystal (from Date et al. [2])

nematic sample when it is placed between crossed polarisers (two polarisers with polarising directions perpendicular to each other) and light is shone through the cell in the z direction. The presence of crossed polarisers means that, at any point in the sample where the average molecular direction (the *director*) is aligned with either one of the polarisers, the transmission of light through the cell is blocked resulting in a dark area. When the director is not aligned with a polariser a lighter region is visible. The lightest regions in Figure 1 occur when the director is at 45 degrees to both polarisers. We can see from Figure 1 that there are points in the cell where the director orientation changes as we trace a path around that point. In fact each such point is a line perpendicular to the xy-plane called a disclination or defect line. For example, if we pick any point in Figure 1 where four dark regions merge then trace a path around that point, in going from one dark region to another the director has changed alignment from one polariser direction to the other polariser direction, in other words by 90 degrees. In a full circuit the director must have rotated by 360 degrees. A full rotation by 360 degrees indicates a disclination line of strength $S = +1$ or $S = -1$ (depending on whether the director rotated clockwise or anti-clockwise as we went round the disclination). When two dark regions merge at a point (usually a little harder to see) a defect of strength $S = +\frac{1}{2}$ or $S = -\frac{1}{2}$ occurs.

In this paper we will consider the director structure around disclination lines of strength $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$. Analysis has shown that only defects of half-integral strength are singular because defects with integral strength can escape into the third dimension, the z direction in our case [3]. Figures 2(c) and 3(c) show director configurations for $S = +\frac{1}{2}, -\frac{1}{2}$. The director distortion that occurs around these defects can be characterised by bend and splay distortion. When $S = +\frac{1}{2}$, bend is dominant when $x < 0$, and splay is dominant when $x > 0$. When $S = -\frac{1}{2}$ there are three regions where bend is dominant, and three regions where splay dominates.

The lower plots in Figures 2 and 3 show the calculated transmission through the cell if the director structure is placed between crossed polarisers which are aligned with the x and y axes. For a director at an angle ϕ to the x-axis the transmission will be proportional to $\sin^2(2\phi)$.

The properties of defects in liquid crystals have been discussed by many authors (see the reviews by Chandrasekhar and Ranganath [1] and Klèman [3]) and have been described in terms of continuum mechanics and in terms of topology. In this paper, we solve the Euler-Lagrange equations, derived from a continuum description of the nematic material in terms of the director $\mathbf{n}$, (whose solution will be a minimum energy configuration) using analytic and numerical methods.

Theory

The bulk free-energy density of a deformed liquid crystal relative to an undeformed one was given by Frank [4] as

$$F = \frac{1}{2}[k_{11}(\nabla \cdot \mathbf{n})^2 + k_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + k_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2], \tag{1}$$

where k_{11}, k_{22} and k_{33} are the elastic constants which refer to *splay*, *twist* and *bend* distortions, respectively and $\mathbf{n}$ is the director. The director is chosen to be of unit length $|\mathbf{n}| = 1$ and to have the symmetry $\mathbf{n} = -\mathbf{n}$. The ∇ symbol denotes the usual gradient operator, $(\partial/\partial x,\ \partial/\partial y,\ \partial/\partial z)$ in cartesian coordinates, and $\cdot$ and $\times$ denote the scalar and vector products. The total free energy of the system is then $E = \int_V F \mathrm{dv}$, where the integration is over the volume of the liquid crystal region.
Consider a planar director structure in which $\mathbf{n}$ is confined to the xy-plane, so that

$$\mathbf{n} = (\cos\phi, \sin\phi, 0), \qquad \phi = \phi(x, y). \tag{2}$$

Using this expression for the director there will be no twist distortion in the region and thus the only elastic constants to enter the free energy are splay, k_{11}, and bend, k_{33}. We will seek director configurations which minimise the free energy of the system. In practice it is easier to work in cylindrical polar coordinates and we seek a solution $\phi(r, \theta)$ which depends on r, the distance from the origin ($x = 0$, $y = 0$), and θ, the angle from the x-axis. From now on we will measure the angles ϕ and θ in radians.
In this paper we consider how the minimum energy solution changes as the ratio of the elastic constants k_{11}/k_{33} is altered. We concentrate on the two most common half strength defects, $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$. As we will see, these defects have different amounts of splay and bend distortion and, although when $k_{11}/k_{33} = 1$ these defects look the same when viewed between crossed polarisers, we find that when $k_{11}/k_{33} \neq 1$ there is a significant difference.
Minimisation of the total free energy E yields the differential equation (the Euler-Lagrange equation) for the director angle ϕ

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial F}{\partial \phi_r}\right) + \frac{\partial}{\partial \theta}\left(\frac{\partial F}{\partial \phi_\theta}\right) - \frac{\partial F}{\partial \phi} = 0, \tag{3}$$

where F is the free energy density in equation (1) and $\phi_r = \partial\phi/\partial r$, $\phi_\theta = \partial\phi/\partial\theta$.
It should be noted at this point that for an infinite region of liquid crystal there is no intrinsic length scale in this problem. No combination of the parameters k_{11}, k_{22} and k_{33} will lead to a number with the dimensions of length. For this reason, the governing equation derived from equation (3) is unchanged under the transformation $r \to \alpha r$ for any scaling factor α. This indicates that the solution to the equation is independent of r. We will introduce boundaries into our problem in the form of a inner and outer cylindrical surfaces at $r = r_c$ and $r = r_\infty$ respectively, but since they preserve the circular symmetry, the r-independent solution remains the minimum energy configuration. With this assumption the director angle is now only dependent on the polar angle θ and $\phi(\theta)$ satisfies the equation

$$\Big[(k_{33} - k_{11})\sin^2(\phi - \theta) + k_{11}\Big]\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}\theta^2}\right) + (k_{33} - k_{11})\sin(2(\phi - \theta))\left(\frac{1}{2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\theta}\right)^2 - \frac{\mathrm{d}\phi}{\mathrm{d}\theta}\right) = 0. \tag{4}$$

Various solutions to this equation are immediately apparent (for example $\phi = \theta$ for any values of k_{11} and k_{33} or $\phi = S\theta + c$ when $k_{11}/k_{33} = 1$ if S and c are constant) but in general this equation cannot be solved analytically because of the nonlinearity involved.

We can however observe some inherent symmetries in equation (4). The rotational transformation $\theta \to \theta + \alpha$ with $\phi \to \phi + \alpha$ leaves equation (4) unchanged. This allows us to choose the boundary condition $\phi(0) = 0$ without loss of generality. If we were to want the more general condition $\phi(0) = \alpha$ we would solve the system with $\phi(0) = 0$, to obtain $\phi(\theta) = \phi_0(\theta)$ say, and then the solution with $\phi(0) = \alpha$ would be simply $\phi(\theta) = \phi_0(\theta) + \alpha$. A second transformation is $\theta \to -\theta$ with $\phi \to -\phi$

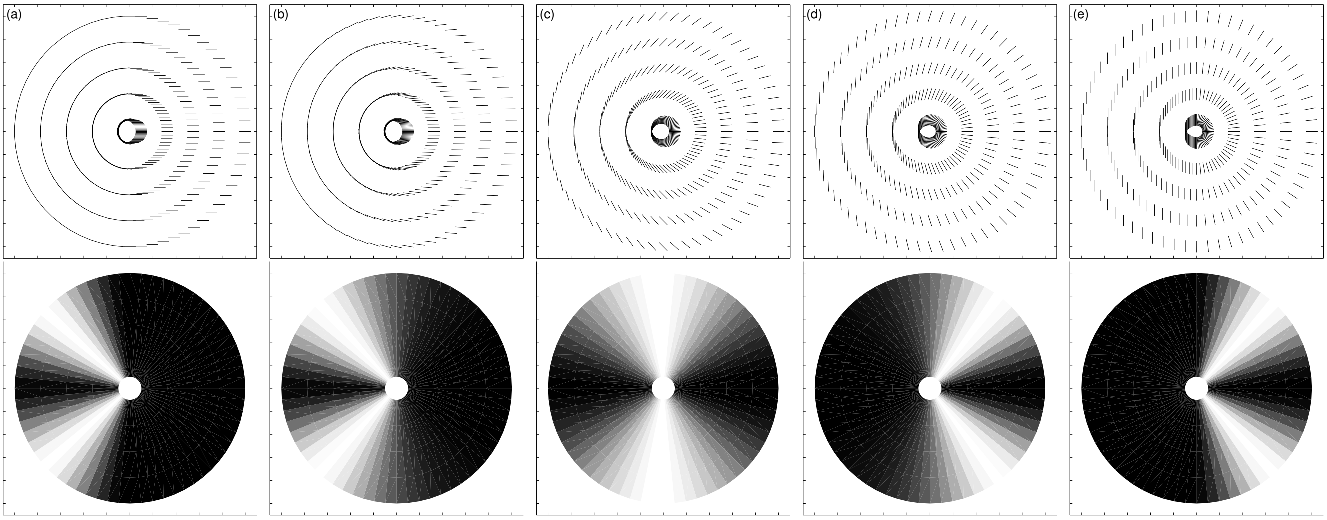

Figure 2: Director configurations for an $S = +\frac{1}{2}$ disclination line with (a) $k_{33}/k_{11} = 0$, (b) $k_{33}/k_{11} = 0.2$, (c) $k_{11}/k_{33} = 1$, (d) $k_{11}/k_{33} = 0.2$, (e) $k_{11}/k_{33} = 0$ (numerical results). The upper plots show the director configuration and the lower plots represent the transmission of such a structure when placed between crossed polarisers.

which leaves equation (4) unchanged and thus the director angle at the position $(r, -\theta)$ is simply the negative of the director angle at (r, θ). We therefore do not need to solve the equation over the full domain $(-\pi < \theta < \pi)$ but over the semi-infinite region $0 < \theta < \pi$. These two symmetries mean that, without loss of generality, we may take the boundary conditions to be $\phi(0) = 0$ and $\phi(\pi) = S\pi$ where S is the power of the defect, $\pm\frac{1}{2}$ in our case.

One last remark should be made about the size of the liquid crystal domain. We have assumed that our nematic liquid crystal is contained in the region $r_c < r < r_\infty$. It is not necessary to specify the values of r_c and r_∞ to solve equation (4) since this equation is independent of r. However, if the liquid crystal region was not bounded by the cylinder at $r = r_\infty$, the energy of the system would be infinite since we would have an infinite region of distorted liquid crystal. In reality, other defects or cell surfaces would influence the director orientation at a certain distance from the centre of the defect resulting in a finite energy. The region $r < r_\infty$ can be thought of as the 'zone of influence' of the defect, outside of which other effects influence the director structure. The inner boundary at $r = r_c$ is also necessary to achieve a finite energy. This is in fact the size of the 'defect core'. In this inner region the distortion is so high that a change in the nematic order occurs. An accurate model of the defect core must include this change in order and it has been shown by Schopohl and Sluckin [5] that there exists an amount of biaxiality in this region. In this paper, however, we are modelling the region outside the defect core assuming that the nematic order parameter/biaxiality remains constant and only the director varies.

Analytic solutions

As mentioned above, it is possible to obtain exact or approximate analytic solutions for a variety of k_{11} and k_{33} values. With elastic isotropy, when $k_{11}/k_{33} = 1$, equation (4) simplifies significantly to $\frac{\mathrm{d}^2\phi}{\mathrm{d}\theta^2} = 0$ which, with the boundary conditions $\phi(0) = 0$ and $\phi(\pi) = S\pi$, has the solution $\phi = S\theta$. This is the solution for any disclination strength S. The director structures for $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$ are

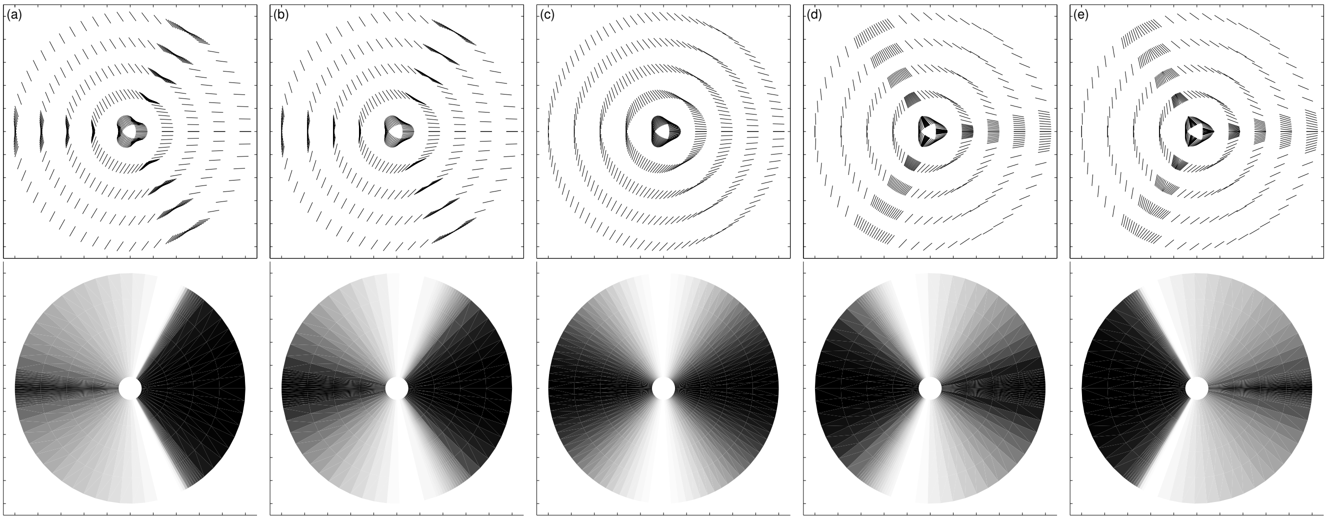

Figure 3: Director configurations for an $S = -\frac{1}{2}$ disclination line with (a) $k_{33}/k_{11} = 0$, (b) $k_{33}/k_{11} = 0.2$, (c) $k_{11}/k_{33} = 1$, (d) $k_{11}/k_{33} = 0.2$, (e) $k_{11}/k_{33} = 0$ (numerical results). The upper plots show the director configuration and the lower plots represent the transmission of such a structure when placed between crossed polarisers.

shown in Figures 2(c) and 3(c). Because of the isotropic elastic constants, there is an equal amount of splay and bend distortion in these configurations. When $k_{11}/k_{33} \neq 1$ this will not be the case and the system will prefer either splay or bend distortion depending on which is smaller, k_{11} or k_{33}.
From the director configurations in Figures 2(c) and 3(c) we can also calculate the effect of rotation of the polarisers relative to the liquid crystal sample. If we rotate the polarisers anti-clockwise by $\pi/8$ radians (22.5 degrees) the direction of the polarisers will be $\pi/8$ and $5\pi/8$. The darkest regions will then occur when the director is oriented such that $\phi = \pi/8$, $\phi = 5\pi/8$, $\phi = 9\pi/8$ or $\phi = 13\pi/8$. For the $S = +\frac{1}{2}$ defect $\phi = \theta/2$ so this occurs at the values $\theta = \pi/4$ or $\theta = 5\pi/4$. The dark regions have rotated anti-clockwise by double the polariser rotation angle. However, for the $S = -\frac{1}{2}$ defect $\phi = -\theta/2$ so the new dark regions occur at the values $\theta = -\pi/4$ or $\theta = -5\pi/4$. The dark regions have rotated clockwise by double the polariser rotation angle. In this way it is possible to distinguish between positive and negative strength disclinations.
For the $S = +\frac{1}{2}$ defect it is also possible to write down the exact analytic solution for the two extreme cases of $k_{11}/k_{33} = 0$ and $k_{33}/k_{11} = 0$. When $k_{11}/k_{33} = 0$ splay distortion contributes nothing to the total energy and the liquid crystal will attempt to replace any bend distortion with splay distortion in order to reduce the total energy. For the $S = +\frac{1}{2}$ disclination it is possible to replace all bend distortion with splay and Figure 2(e) shows such a director configuration. The analytic solution is $\phi = \theta$ when $0 < \theta < \pi/2$, $\phi = \frac{\pi}{2}$ when $\pi/2 < \theta < 3\pi/2$ and $\phi = \theta - \pi$ when $3\pi/2 < \theta < 2\pi$. When $k_{33}/k_{11} = 0$ the opposite effect occurs: all of the splay distortion is replaced with bend distortion and Figure 2(a) shows the director configuration. The analytic solution is $\phi = 0$ when $0 < \theta < \pi/2$, $\phi = \theta - \frac{\pi}{2}$ when $\pi/2 < \theta < 3\pi/2$ and $\phi = \pi$ when $3\pi/2 < \theta < 2\pi$.
We can also determine an approximate analytic solution when the elastic constants are *nearly* equal. If we take $k_{11}/k_{33} = (1-\epsilon)$ where ϵ is a small positive number then, if ϵ is small enough, it is reasonable to assume that the solution to equation (4) is close to the solution $\phi_0 = S\theta$ (which is the solution when $k_{11}/k_{33} = 1$ or when $\epsilon = 0$). When we consider $k_{33}/k_{11} < 1$ we will take $k_{33}/k_{11} = (1 - \epsilon)$, although in this case the equation and solution changes slightly. We use the Taylor series expansion of the solution at $\epsilon = 0$ in powers of ϵ

$$\phi = \phi_0 + \sum_{i=1}^{\infty} \epsilon^i \phi_i \tag{5}$$

where $\epsilon = 1 - \frac{k_{11}}{k_{33}}$. Substituting $\frac{k_{11}}{k_{33}} = 1 - \epsilon$ into equation (4) gives

$$\left[1 - \epsilon\cos^2(\phi - \theta)\right]\left(\frac{\mathrm{d}^2\phi}{\mathrm{d}\theta^2}\right) - \epsilon\sin(2(\phi - \theta))\left(\frac{1}{2}\left(\frac{\mathrm{d}\phi}{\mathrm{d}\theta}\right)^2 - \frac{\mathrm{d}\phi}{\mathrm{d}\theta}\right) \;=\; 0. \tag{6}$$

By substituting equation (5) into equation (6) and equating coefficients of powers of ϵ we get a series of equations for the functions ϕ_i. Recall that, if we consider a strength S defect then the boundary conditions require $\phi(0) = 0$ and $\phi(\pi) = S\pi$. We can satisfy these boundary conditions using only the first order term since $\phi_0(0) = 0$ and $\phi_0(\pi) = S\pi$. Therefore, the higher order terms in equation (5) must have zero boundary conditions, $\phi_i(0) = 0$ and $\phi_i(\pi) = 0$. The first four functions in the expansion are

$$\begin{aligned}
\phi_0(\theta) &= S\theta \\
\phi_1(\theta) &= \frac{S(S-2)}{8(S-1)^2}\sin(2(S-1)\theta) \\
\phi_2(\theta) &= \frac{S(S-2)}{16(S-1)^2}\sin(2(S-1)\theta) \\
&\quad \frac{S(S-2)(5S^2-10S+4)}{256(S-1)^4}\sin(4(S-1)\theta) \\
\phi_3(\theta) &= \frac{S(S-2)(71S^4-284S^3+440S^2-312S+80)}{2048(S-1)^6}\sin(2(S-1)\theta), \\
&\quad + \frac{S(S-2)(5S^2-10S+4)}{256(S-1)^4}\sin(4(S-1)\theta) \\
&\quad + \frac{S(S-2)(29S^4-116S^3+160S^2-88S+16)}{6144(S-1)^6}\sin(6(S-1)\theta).
\end{aligned} \tag{7}$$

Here we can see that an extra mode is added in each of the terms. When $\epsilon \ll 1$, we expect a truncated expansion series (we later consider the first six terms) to give a reasonably accurate solution since higher order terms will be negligible. However, when $\epsilon \approx 1$, the truncated approximation is no longer accurate unless the number of terms used in equation (5) is large.

Numerical Results

We can solve equation (4), for any value of k_{11}/k_{33}, using a standard numerical method. Discretising equation (4) on a non-uniform grid and approximating derivatives with central finite differences, we form a set of nonlinear equations $F(\Phi) = 0$ where Φ is the vector of ϕ values at each grid node. A non-uniform grid is necessary in some cases when the director distortion becomes large and would lead to significant discretisation errors on a uniform grid. The system of equations $F(\Phi) = 0$ is solved using the NAG routine c05nbf [6] by a modification of the Powell hybrid method.

In order for the NAG routine to work, we need a good initial guess. Since the analytic solution is known for $\epsilon = 0$, we use this as an initial guess, and step up the value of ϵ in discrete steps, using each solution as an initial guess for the next calculation, until we reach the required value of ϵ.

The numerical solutions for various values of ϵ are shown in Figures 2 and 3. Figure 4(a) and (c) shows a comparison of the approximate analytic solution equation (5) with the numerical solution when $\epsilon = 0.8$ and $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$, respectively. Here only six terms of the analytic solution are used, and we can see clearly that this gives very good agreement with the numerical solution.

Figure 4(b) and (d) shows the same comparison with $\epsilon = 1$. We can see that in this case the analytic solution (again with six terms) does not match up well with the numerical solution, and, in fact, an infinite number of terms of the analytic solution would be required for good accuracy.

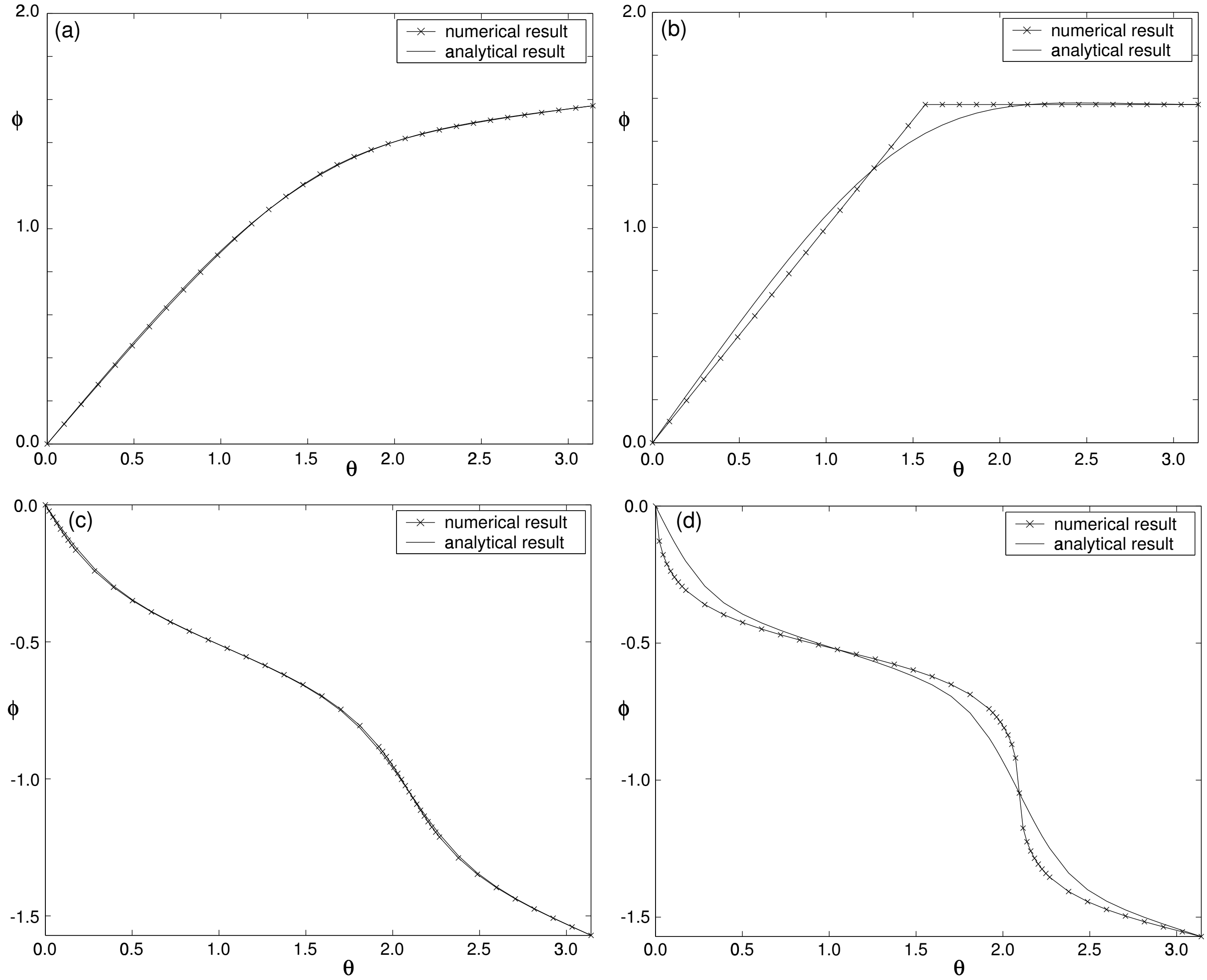

Figure 4: Comparison between the approximate analytic solution equation (5) with six terms and the numerical solution for (a) $S = +\frac{1}{2}$, $k_{11}/k_{33} = 0.2$, (b) $S = +\frac{1}{2}$, $k_{11}/k_{33} = 0.0$ and for (c) $S = -\frac{1}{2}$, $k_{11}/k_{33} = 0.2$, (d) $S = -\frac{1}{2}$, $k_{11}/k_{33} = 0.0$. For $k_{11}/k_{33} = 0.2$ the analytic solution is a good approximation to the exact solution.

There are two important points to consider regarding the director configurations in Figures 2 and 3. Firstly, it is clear that for a specific nematic material at a constant temperature (so that k_{11}/k_{33} takes a fixed value) the Schlieren pictures for $k_{11}/k_{33} \neq 1$ will appear different for the two defects $S = +\frac{1}{2}$ and $S = -\frac{1}{2}$ (consider for example Figures 2(d) and 3(d)). Secondly, for a single defect (for example $S = +\frac{1}{2}$ in Figures 2(c) and 2(d)) the Schlieren picture may be significantly different for different values of k_{11}/k_{33}. It is possible to calculate the angle between the regions of maximum transmission in Figures 2 and 3 as a function of k_{11}/k_{33} and also the rate of rotation of the maximum transmission angle as the polarisers are rotated. It is therefore theoretically possible for the ratio k_{11}/k_{33} to be found by examining the Schlieren texture. However, to perform such a calculation accurately the disclination line should have few external influences such as nearby defects and it would be extremely difficult to make a measurement from a sample such as the one shown in Figure 1. Similar calculations can be carried out for integer strength defects although the differences in the Schlieren picture are not as obvious as for $S = \pm\frac{1}{2}$.

References

[1] S. Chandrasekhar and G.S. Ranganath Advances in Physics, 1986, Vol. 35, No. 6, p.507.

[2] R. W. Date, C. T. Imrie, G. R. Luckhurst and J. M. Seddon Liquid Crystals, 1992, Vol. 12, p.203.

[3] M. Klèman Points, Lines and Walls, John Wiley New York, 1983.

[4] F.C. Frank Disc. Faraday Soc., 1958, Vol. 25, p.19.

[5] N. Schopohl and T.J. Sluckin Physical Review Letters, 1987, Vol. 59, No. 22, p.2582.

[6] The Numerical Algorithms Group, *NAG Foundation Toolbox,* http://www.nag.co.uk.