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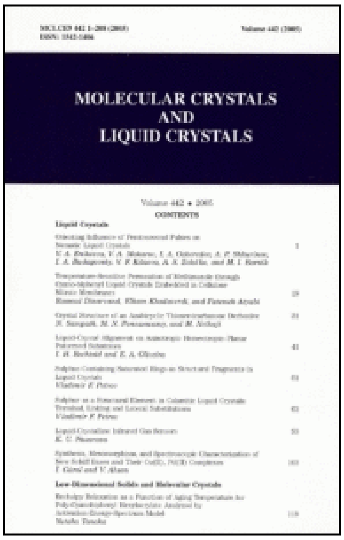

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Computing the Wave Speed of Soliton-Like Solutions in SmC* Liquid Crystals

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We present a novel method for numerically computing the wave speed of a soliton-like travelling wave in chiral smectic C liquid crystals (SmC) that satisfies a parabolic partial differential equation (PDE) with a general nonlinear term [1]. By transforming the PDE to a co-moving frame and recasting the resulting problem in phase-space, the original PDE can be expressed as an integral equation known as an exceptional nonlinear Volterra-type equation of the second kind. This technique is motivated by, but distinct in nature from, iterative integral methods introduced by Chernyak [2]. By applying a simple trapezoidal method to the integral equation we generate a system of nonlinear simultaneous equations which we solve for our phase plane variable at equally spaced intervals using Newton iterates. The equally spaced phase variable solutions are then used to compute the wave speed of the associated travelling wave. We demonstrate an algorithm for performing the necessary calculations by considering an example from liquid crystal theory, where a parabolic PDE with a nonlinear reaction term has a solution and wave speed which are known exactly [3,4]. The analytically derived wave speed is then compared with the numerically computed wave speed using our new scheme.*

Keywords Smectic C*; soliton; wave speed

1. Introduction

In this paper we consider the problem of determining the wave speed of travelling wave solutions satisfying parabolic PDE's of the form

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} - i(\phi), \tag{1}$$

where $i(\phi)$ represents a nonlinear reaction term. Nonlinear parabolic PDE's of the form (1) occur frequently in liquid crystal theory. For example the equation

$$\begin{aligned} 2\lambda_5 \frac{\partial \phi}{\partial t} = {} & B\frac{\partial^2 \phi}{\partial x^2} - P_0 E \cos\alpha \cos\phi \\ & - \varepsilon_0 \varepsilon_a E^2 \left(\frac{1}{4}\sin 2\alpha \sin 2\theta \sin\phi + \frac{1}{2}\cos^2\alpha \sin^2\theta \sin 2\phi \right), \end{aligned} \tag{2}$$

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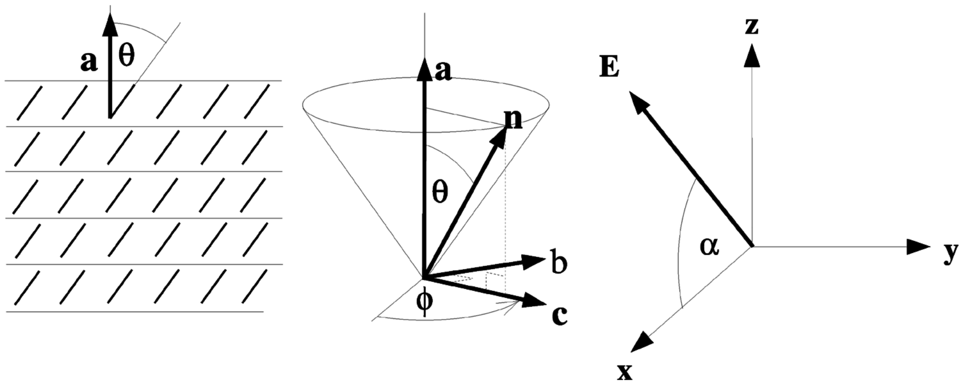

(a) (b) (c)

Figure 1. (a) The planar layer arrangement of the liquid crystal sample being considered. The molecules are tilted at a fixed angle θ to the layer normal **a** which is aligned with the z-axis. (b) The average molecular alignment is denoted by the unit vector **n**, called the director. The vector **c** is the unit orthogonal projection of **n** onto the smectic planes. The orientation angle of the c-director is ϕ. Note also that SmC* has a spontaneous polarisation which lies along the vector **b** and is denoted by $\mathbf{P} = P_0\mathbf{b}$ where $\mathbf{b} = \mathbf{a} \times \mathbf{c}$. (c) The electric field **E** at an angle of incline $\alpha \geq 0$ with respect to the smectic layers in the xy-plane.

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which appears in [1], governs the temporal and spatial development of the usual c-director orientation angle $\phi(x, t)$ in a sample of SmC* in the planar layer arrangement of Figure 1(a), under the influence of an external electric field **E**, as shown in Figure 1(c). Introducing suitable dimensionless parameters χ and σ along with the scaled variables T and X

$$\chi = 2P_0(\varepsilon_0\varepsilon_a E \cos\alpha \sin^2\theta)^{-1}, \tag{3}$$

$$\sigma = \tan\alpha \cot\theta, \tag{4}$$

$$T = \frac{1}{4}t(2\lambda_5)^{-1}\varepsilon_0|\varepsilon_a|E^2\cos^2\alpha\sin^2\theta, \tag{5}$$

$$X = \frac{1}{2}xB^{\frac{1}{2}}(\varepsilon_0|\varepsilon_a|E^2\cos^2\alpha\sin^2\theta)^{\frac{1}{2}}, \tag{6}$$

and the transformation

$$\hat{\phi}(X, T) = 2\phi(X, T) - \pi, \tag{7}$$

permits (2) to be expressed as

$$\frac{\partial\hat{\phi}}{\partial T} = \frac{\partial^2\hat{\phi}}{\partial X^2} - 4\chi\sin\frac{\hat{\phi}}{2} - 4\sin\hat{\phi} + 8\sigma\cos\frac{\hat{\phi}}{2}, \tag{8}$$

and is typical of the type of equation we shall study in this paper. We note that P_0 represents the polarisation, B is an elastic constant, E the magnitude of the electric field, λ_5 is a rotational viscosity, ε_0 is the permittivity of free space, ε_a is the (unitless) measure of the dielectric anisotropy and θ is the (fixed) angle the director **n** makes with the layer normal **a**. If $\sigma \neq 0$ then no closed form solutions are known and therefore to solve such an equation we must resort to numerical methods. If, on the other hand, $\sigma = 0$, then (8) becomes

$$\frac{\partial \hat{\phi}}{\partial T} = \frac{\partial^2 \hat{\phi}}{\partial X^2} - 4\chi \sin\frac{\hat{\phi}}{2} - 4\sin\hat{\phi}, \tag{9}$$

which admits the travelling wave solution [4,8,9]

$$\hat{\phi}(X, T) = 4\arctan\{\exp[\mp 2(X + \nu T + c)]\}, \quad \nu = \pm\chi, \tag{10}$$

where c is an arbitrary constant. Note that for (9) the wave velocity is exactly $\nu = \pm\chi$ and that $\hat{\phi} \to 0$ as $X \to \infty$ while $\hat{\phi} \to 2\pi$ as $X \to -\infty$. Given this special solution for $\sigma = 0$, we conjecture that when $\sigma \neq 0$, (8) admits travelling wave solutions of the form

$$\psi(z) = \hat{\phi}(X, T), \quad z = X + \nu T, \tag{11}$$

where ν now represents a dimensionless wave speed. Justification for this stems from experimental observations, for example the work of Abdulhalim *et al.* [5]. By considering Eq. (1) we develop a simple numerical scheme which will, assuming the equation admits travelling wave solutions, allow us to compute the wave speed directly. We will demonstrate the technique by considering Eq. (9) (where $\sigma \neq 0$) and exploit the fact that it has the well-known solution and wave speed stated in Eq. (10) in order to demonstrate that the new method converges numerically and finds the known exact solution. We will then briefly examine the method applied to the full three term problem in (8) when $\sigma \neq 0$.

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2. Theory

We begin by considering (1). We shall employ a technique motivated by, but distinct in nature from, iterative integral methods introduced by Chernyak [2]. Our aim is to express the PDE as an integral equation. Then we may apply boundary conditions and treat the problem approximately using discrete rather than continuous methods. The first step is to recast (1) using the transformation

$$\psi(z) = \phi(x, t) \quad z = x + \nu t, \tag{12}$$

to obtain the equivalent expression

$$\frac{d^2\psi}{dz^2} - \nu\frac{d\psi}{dz} - i(\psi) = 0. \tag{13}$$

By making the substitution

$$p(\psi) = \frac{d\psi}{dz}, \tag{14}$$

we can transform (13) to $p - \psi$ phase space by noting that

$$\frac{d^2\psi}{dz^2} = \frac{dp}{dz} = \frac{d\psi}{dz}\frac{dp}{d\psi} = p\frac{dp}{d\psi}. \tag{15}$$

Then Eq. (13) becomes

$$p\frac{dp}{d\psi} - \nu p - i(\psi) = 0. \tag{16}$$

Now, we seek solutions for $\psi(z)$ connecting two constant states a and b say, such that the solution satisfies the boundary conditions

$$\lim_{z\to-\infty}\psi(z) = a, \quad \lim_{z\to\infty}\psi(z) = b. \tag{17}$$

Since the solution $\psi(z)$ approaches constant values for large $|z|$ we expect

$$p(a) = \lim_{z\to-\infty}\psi'(z) = 0, \quad p(b) = \lim_{z\to\infty}\psi'(z) = 0, \tag{18}$$

where the prime denotes differentiation with respect to z. Integrating with respect to ψ and noting that $p(a) = 0$ and $p(b) = 0$, we find that (16) may be written in the form of an integral equation,

$$p^2(\psi) - \lambda\int_{t=a}^{\psi} p(t)dt = f(\psi), \tag{19}$$

where $\lambda = 2\nu$ and

$$f(\psi) = 2\int_{t=a}^{\psi} i(t)\ dt. \tag{20}$$

Equation (19) is known as an exceptional nonlinear Volterra-type equation of the second kind [6]. Our aim is to use (19) to determine the wave speed ν of the travelling wave connecting the steady states obtained by considering zeros of the nonlinear term $i(\psi)$. To solve (19) we assume that for $\psi < a$ and $\psi > b$, $p(\psi) = 0$, whereas we expect $p(\psi) \neq 0$ in the interval $a \leq \psi \leq b$. Based on this assumption, and using the fact that $p(a) = p(b) = 0$, we shall construct a numerical scheme for the solution $p(\psi)$ using a simple trapezoidal quadrature rule in place of the integral. This in turn will lead us to an iterative procedure which we shall use to numerically calculate an accurate approximation to the actual wave speed ν.

3. Numerical Method

We proceed as follows. Firstly, suppose that between $\psi = a$ and $\psi = b$ we divide the interval into $N - 1$ equally spaced strips of width

$$h^{(N)} = \frac{b-a}{N-1}, \tag{21}$$

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where $h^{(N)}$ denotes the strip width for an interval with N node points. The variable ψ is defined discretely as

$$\psi_i = a + ih^{(N)},\ i = 0, \ldots, N-1. \tag{22}$$

Then we can compute the discrete solution p_i at N points giving the set of solutions

$$p_i = p(\psi_i),\ i = 0, \ldots, N-1. \tag{23}$$

Denoting $f(\psi_i)$ by f_i and using (19) to generate our N solutions for p_i at equally spaced values of ψ between a and b via

$$p^2(\psi_j) - \lambda \int_{t=a}^{\psi_j} p(t)dt = f(\psi_j),\ j = 0, \ldots, N-1, \tag{24}$$

we obtain the following N equations

$$\begin{aligned}
&p_0^2 = f_0, \\
&p_1^2 - \lambda\left[\frac{1}{2}p_0 + \frac{1}{2}p_1\right]h^{(N)} = f_1, \\
&p_2^2 - \lambda\left[\frac{1}{2}p_0 + p_1 + \frac{1}{2}p_2\right]h^{(N)} = f_2, \\
&\vdots \\
&p_{N-2}^2 - \lambda\left[\frac{1}{2}p_0 + p_1 + \ldots + \frac{1}{2}p_{N-2}\right]h^{(N)} = f_{N-2}, \\
&p_{N-1}^2 - \lambda\left[\frac{1}{2}p_0 + p_1 + p_2 + \ldots + \frac{1}{2}p_{N-1}\right]h^{(N)} = f_{N-1}.
\end{aligned} \tag{25}$$

Imposing the boundary conditions given by (18) implies $p_0 = p_{N-1} = 0$, allowing us to eliminate the first equation in (25). The last equation in (25) can be used to obtain an expression for $\lambda h^{(N)}$, namely,

$$\lambda h^{(N)} = -\frac{f_{N-1}}{p_1 + p_2 + \ldots + p_{N-2}}. \tag{26}$$

Substituting this into the remaining equations and defining

$$\alpha = \sum_{i=1}^{N-2} p_i,\ \beta = \sum_{i=1}^{N-3} p_i. \tag{27}$$

we are left with $N-2$ nonlinear simultaneous equations to solve for p_i, $i = 1, 2, \ldots, N-2$

$$\begin{aligned}
&2p_1^2\alpha + f_{N-1}p_1 - 2f_1\alpha = 0, \\
&2p_2^2\alpha + f_{N-1}(2p_1 + p_2) - 2f_2\alpha = 0, \\
&2p_3^2\alpha + f_{N-1}(2(p_1 + p_2) + p_3) - 2f_3\alpha = 0, \\
&\vdots \\
&2p_{N-2}^2\alpha + f_{N-1}(\alpha + \beta) - 2f_{N-2}\alpha = 0.
\end{aligned} \tag{28}$$

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Solving this system involves employing Newton's iterative method [7] for $N-2$ nonlinear equations. At this stage we may compute an approximate value for λ from (26). Alternatively, after refining the values of p_i for some value of N, we can pursue a better approximation by constructing linear interpolants connecting the points p_i. We increment the number of node points by one to $N+1$ and calculate new approximate values $\hat{p}_i$ at new node values $\hat{\psi}_i$ over the interval with $N+1$ node points and spacing

$$h^{(N+1)} = \frac{b-a}{N}. \tag{29}$$

The node points are calculated from

$$\hat{\psi}_i = a + ih^{(N+1)},\ \ i = 0, \ldots, N, \tag{30}$$

and the rule for computing new interpolated points becomes

$$\hat{p}_{i+1} = \left(\frac{p_{i+1} - p_i}{\psi_{i+1} - \psi_i}\right)(\hat{\psi}_{i+1} - \psi_i) + p_i. \tag{31}$$

At the endpoints of the interval we make $\hat{p}_0 = 0$ and $\hat{p}_N = 0$. In addition we compute $\hat{f}_i = f(\hat{\psi}_i)$. The procedure is then repeated iteratively until a sufficiently accurate approximation is achieved.

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4. Zero Angle of Inclination

We demonstrate the method on the aforementioned PDE (9) with the known solution and wave speed in (10). The numerical method was implemented using MATLAB, but could in principle be coded using any suitable package or programming language. Consider (9), which we recall is equivalent to (8) with $\sigma = 0$. For clarity we drop the $\hat{\phi}$ notation and let $\hat{\phi} \to \phi$, $X \to x$ and $T \to t$ so that (9) becomes

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2 \phi}{\partial x^2} - 4\chi \sin\frac{\phi}{2} - 4\sin\phi. \tag{32}$$

Then, transforming according to Eqs. (12) to (16) and setting

$$i(\psi) = 4\chi \sin\frac{\psi}{2} + 4\sin\psi, \tag{33}$$

we arrive at the equation

$$4\left[\chi \sin\frac{\psi}{2} + \sin\psi\right] + p\left(\nu - \frac{dp}{d\psi}\right) = 0, \tag{34}$$

which is an Abel equation of the second kind, with solution

$$p(\psi) = \mp 4\sin\frac{\psi}{2}, \quad \nu = \pm\chi. \tag{35}$$

We chose to select $\chi = -2.154$ for our example problem, a choice motivated by Stewart and Momoniat [1]. The fixed points of (33) for $|\chi| > 2$, lie at even multiples of π, so that $\psi = 0, \pm 2\pi, \pm 4\pi, \ldots$ are solutions of $i(\psi) = 0$ when $\chi = -2.154$. We chose the interval over which we integrated the problem to be $\psi \in (a, b)$, where $a = -2\pi$ and $b = 0$ and calculated approximate solutions for $p(\psi)$ over a range of values of N.

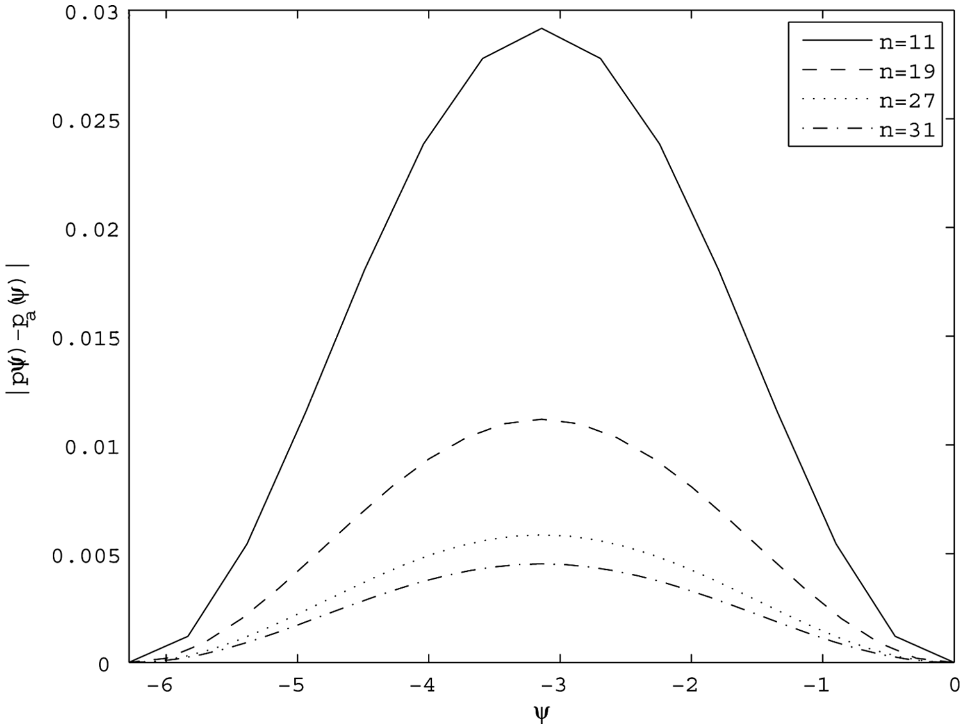

Figure 2. Plot of the relative error $|p(\psi) - p_a(\psi)|$ against ψ for a number of values of N with $\chi = -2.154$ and $\sigma = 0$.

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Starting with five equally spaced points satisfying (17), we have plotted the relative error between the numerically computed approximate values denoted by $p_a(\psi)$ and exact values of $p(\psi)$ computed at the same equally spaced points given by (35) in Figure 2. The graph demonstrates that as we increase the number of points N, the approximate solution $p_a(\psi)$ converges to the true solution $p(\psi)$. In other words, as N is increased the quality of the approximation $p_a(\psi)$ improves. Of course, as the approximation $p_a(\psi)$ improves, so does the quality of the approximated wave speed. The computed wave speeds ν for the values of N shown in Figure 2 are listed in Table 1. Compared to the magnitude of the exact wave speed for the problem which is $|\nu| = |\chi| = 2.154$, the computed wave speed for $N = 11$ is accurate to within about 1%. In addition we note that as the number of points N is increased the wave speed approximation does indeed converge to the exact value as expected. This confirms the validity of our proposed numerical scheme for $\sigma = 0$.

Table 1. Table of computed wave speeds

Data points N	Wave speed ν
11	2.17565
19	2.16249
27	2.15851
31	2.15750

5. Nonzero Angle of Inclination

To demonstrate the applicability of the method, we adapted the procedure to show how varying the angle α of inclination of the electric field affects the wave speed ν for fixed $\chi = -2.154$. It is important to bear in mind that although the dimensionless quantity χ is dependent on α, we treat it as fixed by supposing that E is allowed to vary to ensure χ remains constant. Recall that $\sigma = \tan\alpha\cot\theta$ and that θ is fixed and that σ is therefore dependent on α. When $\alpha \neq 0$ we have that $\sigma \neq 0$. This introduces a third term into the nonlinearity so that now

$$i(\psi) = 4\chi\sin\frac{\psi}{2} + 4\sin\psi - 8\sigma\cos\frac{\psi}{2}. \tag{36}$$

Note that the fixed points of (36) are no longer even multiples of π if $\sigma \neq 0$ for $\chi = -2.154$, and the fixed points change as α is varied. To take account of this a simple root finding scheme was implemented to determine the fixed points of (36) as α was slowly incremented. Initially the problem was solved for $\alpha = 0$ on the interval $\psi \in (a, b)$ with $a = 2\pi$ and $b = 4\pi$. Then as α was varied, new fixed points were computed and new values of a and b selected as appropriate for use in the numerical scheme. The inclination of the electric field was allowed to vary over the range $0 \leq \alpha \leq 22°$. The result is shown in Figure 3 below.

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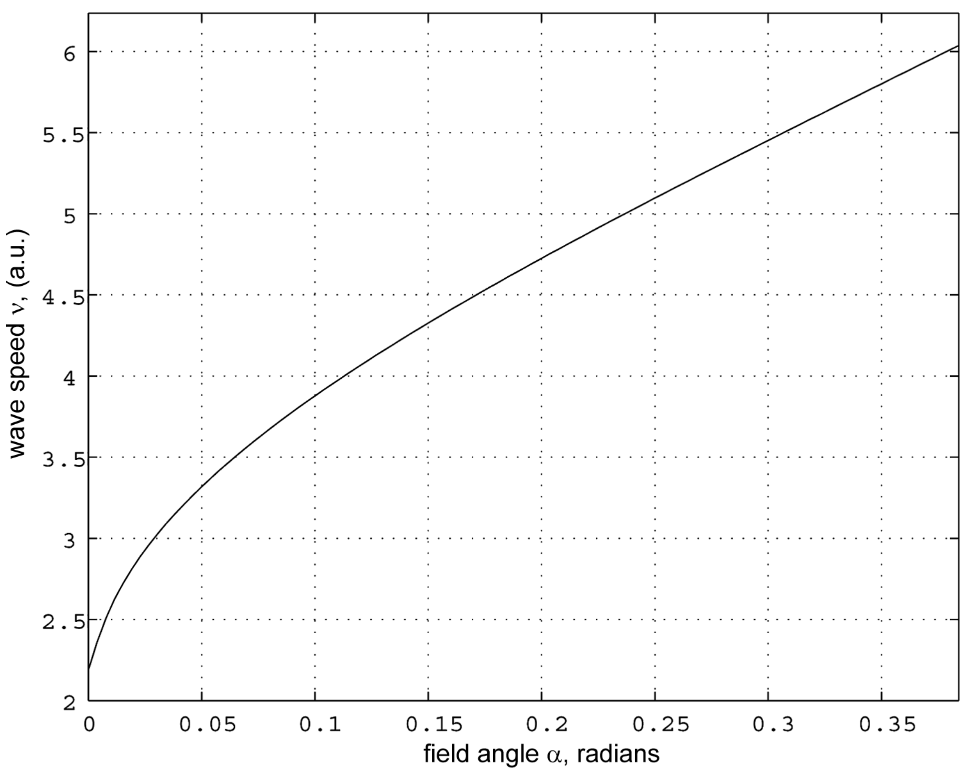

Figure 3. Field angle α versus wave speed ν for $\chi = -2.154$, $\theta = 22°$. Note the rate of change in wave speed is greatest for small inclinations of the applied field.

6. Conclusions

The technique described in the preceding sections provides a systematic and reliable method for the numerical determination of wave speeds for PDE's of the form (1), where a travelling wave solution may be assumed and $i(\phi)$ is taken to be a general nonlinear term. We chose to represent the problem as an integral equation and treated the equation discretely. We showed how, for a PDE with a nonlinear term which gives rise to an exact solution and analytically determined wave speed, it was possible to demonstrate convergence to the analytical wave speed using the numerical scheme. Furthermore, we demonstrated how the method may be extended to deal with problems where analytical solutions and wave speeds are not known explicitly. By developing the method of solution to the problem when $\alpha \neq 0$, we were able to extend our numerical procedure to construct a graph of wave speeds ν against the angle of inclination α for a range of values of α, and for the first time revealed for $\sigma \neq 0$ the nonlinear dependence of ν upon α. This was achieved despite there being no closed form solution to (1) when $i(\phi) = 4\chi \sin\phi/2 + 4\sin\phi - 8\sigma\cos\phi/2$.

Future work will improve the convergence rate and accuracy of the algorithm by employing a more sophisticated quadrature scheme. Making direct comparison of wave speeds observed in the laboratory with our numerical approximations, and applying the method to other types of nonlinear problem, will form the basis of further investigations.

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