Large amplitude nematicon propagation in a liquid crystal with local response

Catherine Garcia-Reimbert
*Universidad Nacional Autonoma de Mexico*

Antonmaria Minzoni
*Universidad Nacional Autonoma de Mexico*

Noel Smyth
*University of Edinburgh*

Annette L. Worthy
*University of Wollongong, annie@uow.edu.au*

Publication Details
Large amplitude nematicon propagation in a liquid crystal with local response

Abstract
The evolution of polarized light in a nematic liquid crystal whose directors have a local response to reorientation by the light is analyzed for arbitrary input light power. Approximate equations describing this evolution are derived based on a suitable trial function in a Lagrangian formulation of the basic equations governing the electric fields involved. It is shown that the nonlinearity of the material response is responsible for the formation of solitons, so-called nematicons, by saturating the nonlinearity of the governing nonlinear Schrödinger equation. Therefore in the local material response limit, solitons are formed due to the nonlinear saturation behavior. It is finally shown that the solutions of the derived approximate equations for nematicon evolution are in excellent agreement with numerical solutions of the full nematicon equations in the local regime.

Keywords
crystal, nematicon, local, response, large, liquid, propagation, amplitude

Disciplines
Engineering | Science and Technology Studies

Publication Details

This journal article is available at Research Online: http://ro.uow.edu.au/eispapers/2528
Large-amplitude nematicon propagation in a liquid crystal with local response

Cathy García Reimbert and Antonamaria A. Minzoni

Fenómenos No lineales y Mecánica (FENOMEC), Department of Mathematics and Mechanics, Instituto de Investigación en Matemáticas Aplicadas y Sistemas (IMAS), Universidad Nacional Autónoma de México, Apartado 20-726, 01000 México, Distrito Federal

Noel F. Smyth

School of Mathematics, The King’s Buildings, University of Edinburgh, Edinburgh, Scotland, EH9 3JZ UK

Annette L. Worthy

School of Mathematics and Applied Statistics, University of Wollongong, Northfields Avenue, Wollongong, New South Wales, Australia, 2522

Received June 15, 2006; revised August 24, 2006; accepted September 1, 2006; posted September 7, 2006 (Doc. ID 72009)

The evolution of polarized light in a nematic liquid crystal whose directors have a local response to reorientation by the light is analyzed for arbitrary input light power. Approximate equations describing this evolution are derived based on a suitable trial function in a Lagrangian formulation of the basic equations governing the electric fields involved. It is shown that the nonlinearity of the material response is responsible for the formation of solitons, so-called nematicons, by saturating the nonlinearity of the governing nonlinear Schrödinger equation. Therefore in the local material response limit, solitons are formed due to the nonlinear saturation equation. It is finally shown that the solutions of the derived approximate equations for nematicon evolution behavior. It is in excellent agreement with numerical solutions of the full nematicon equations in the local regime.

© 2006 Optical Society of America

OCIS codes: 190.5530, 190.5940, 160.3710, 190.4400, 190.5330

1. INTRODUCTION

In the present work, the propagation of solitons of coherent polarized light, so-called nematicons, in nematic liquid crystals with a local or Kerr response to reorientation is considered. The propagation of light in liquid crystals with local response has been considered by Khoo1 in several contexts. In particular, the nonlinear Schrödinger equation, which is valid for local response of a medium, has been derived for 5CB-type liquid crystals.2 Also, equations for stimulated orientational scattering in liquid crystals with local response have been derived by Sarkissian et al.3 Finally, the theoretical existence of nematicons in liquid crystals with a Kerr response is pointed out by Conti et al.4 These nematicons are denoted as T solitons.

In García Reimbert et al.5 the propagation of nematicons in a nematic with a local or Kerr response was studied in the limit of a low power input optical field using a nonlinear Schrödinger (NLS) equation modified by a higher-order nonlinearity. Modulation equations for the evolution of a nematicon, which included the effect of the effect of the dispersive radiation, were derived and their solutions were found to be in good agreement with full numerical solutions of the governing nematicon equations. However, as the power of the input optical field was increased, the modulation equations lost accuracy. Therefore a description of nematicon evolution in a Kerr-like nematic is needed that is valid for arbitrary optical power. This is the subject of the present work. In detail, a saturable NLS equation is studied both asymptotically and numerically. To enable the appropriate modulation equations for the nematicon evolution to be derived, the idea of an "equivalent Gaussian" is introduced. This equivalent Gaussian is needed in order to evaluate the saturation effects in an averaged Lagrangian. The resulting modulation equations are found to have solutions in excellent agreement with numerical solutions.

This paper is organized as follows: Section 2 formulates in detail the nematicon equations and summarizes previous results in this area. Section 3 develops the modulation equations using an averaged Lagrangian and the use of the equivalent Gaussian. This section also includes a discussion of the modification of the modulation equations due to the dispersion of numerical solutions. Section 4 presents results, and we present our conclusions in Section 5.

2. NEMATICON EQUATIONS FOR LOCAL RESPONSE

Let us consider coherent polarized light propagating through a nematic liquid-crystal slab as in Conti et al.4 and Assanto et al.6 The basic configuration is shown in Fig. 1. The axes are orientated such that the z-axis is the direction of light propagation, with the x-axis in the direction of the electric field of the light. The nematic is taken to be anchored at the cell walls and the cell lies in the region $-L \leq x \leq L$. The director angle $\varphi$ of the nematic mol-
ecule is measured from the \( z \) axis in the \( x,z \) plane. To overcome the Fréedericksz threshold, a static electric field is applied parallel to the \( z \) axis in order to pretilt the nematic. In this manner low power light can self-focus since the total electric field will be above the Fréedericksz threshold. A typical distribution of the pretilt angle \( \theta \) is shown in Fig. 1. Note that the director is horizontal at the boundary, which is not illustrated. In the absence of the optical field, \( \varphi = \hat{\theta} \).

As in Conti et al.\(^4\) and Assanto et al.,\(^6\) the slowly varying envelope \( E \) of the electric field satisfies the Foch–
Leontovich equation

\[
\frac{i}{\varepsilon} \frac{\partial E}{\partial z} + \frac{1}{2} \nabla^2 E - \cos(2\varphi)E = 0.
\]

The equation for the optical axis \( \varphi \) is obtained from the extremization of the free energy of the nematic. This free energy contains the elastic energy and dipole energy due to the interaction between the molecules and the electric fields. This equation is given in Conti et al.\(^4\) and in non-dimensional form is

\[
u \nabla^2 \varphi + 2p \sin(2\varphi) + 2|E|^2 \sin(2\varphi) = 0,
\]

with \( \varphi = 0 \) at the boundaries of the cell. The parameter \( p \) is related to the strength of the external static electric field. While the nematic equations (1) and (2) could now be solved to study the propagation of a nematic, a further simplification can be made by explicitly invoking the prettilt background.

When the optical field \( E = 0 \), the director angle satisfies

\[
\frac{\partial^2 \varphi}{\partial z^2} + 2p \sin(2\varphi) = 0, \quad \varphi(L) = \varphi(-L) = 0.
\]

Depending on the external field \( 2p \), the profile of the pretilt angle \( \hat{\theta} \) can be adjusted.\(^3,7\) Moreover it is possible to adjust \( p \) so that \( \varphi > \pi/4 \) in the central region of the cell since for large \( p \) the director axis away from the boundaries is aligned with the field with \( \varphi = \pi/2 \). In the center of the cell the director angle is then decomposed as \( \varphi = \hat{\theta}(x) + \theta(x,y) \), so that the director equation (2) takes the exact form

\[
u \nabla^2 \theta + \nu \nabla^2 \hat{\theta} + 2p \sin(2\hat{\theta})\cos(2\hat{\theta}) + 2p \cos(2\hat{\theta})\sin(2\hat{\theta}) + 2|E|^2 \sin(2\hat{\theta})\cos(2\hat{\theta}) + 2|E|^2 \cos(2\hat{\theta})\sin(2\hat{\theta}) = 0.
\]

The external electric field is now adjusted to have a pretilt \( \hat{\theta}(x) \) above \( \pi/4 \), but close to it, in order to maximize the self-focusing response. In this case \( \theta \) can be taken to be small, so that the director equation (4) becomes

\[
u \nabla^2 \theta + 2p \cos(2\hat{\theta})\sin(2\hat{\theta}) + 2|E|^2 \sin(2\hat{\theta})\cos(2\hat{\theta}) = 0.
\]

The slowly varying functions \( \cos(2\hat{\theta}) \) and \( \sin(2\hat{\theta}) \) are now replaced by typical values in the center of the cell. It should be noted that it is important that \( \cos(2\hat{\theta}) < 0 \) since the external field is chosen to result in \( \theta > \pi/4 \), but close to \( \pi/4 \), in the center of the cell.

After rescaling the director equation (5) takes the form

\[
u \nabla^2 \theta - q \sin(2\hat{\theta}) + 2|E|^2 \cos(2\hat{\theta}) = 0.
\]

In a similar manner, the Foch–Leontovich equation (1) takes the form

\[
u \nabla^2 \theta + \nu \nabla^2 \hat{\theta} + 2\sqrt{2} \sin(2\hat{\theta})\cos(2\hat{\theta}) + 2p \cos(2\hat{\theta})\sin(2\hat{\theta}) + 2|E|^2 \sin(2\hat{\theta})\cos(2\hat{\theta}) = 0.
\]

It is noted that after another rescaling and linearization, the nematonic equations (6) and (7) are the equations studied by Conti et al.\(^4\) and Assanto and co-workers.\(^6\)

The nematonic equations (6) and (7) describe the full range of behavior of a liquid crystal from Kerr-like with \( \nu \to 0 \) to nonlocal crystals with \( \nu \to \infty \). In the local, Kerr limit, nonlinearity plays the dominant role in preventing the collapse of a nematic, as mentioned in Conti et al.\(^4\). Moreover, since \( q \) is related to \( \cos(2\hat{\theta}) \), which is small, large nonlinear effects are expected, even for moderate values of the power \( |E|^2 \) of the input light.

Therefore taking \( \nu \) small, we obtain to leading order

\[
\tan 2\theta = \frac{2|E|^2}{q}.
\]

Then eliminating \( \theta \) from the electric field Equation (7), we have
assuming radially symmetric nematics. The solitary wave solutions of this saturating NLS equation are the T solitons of Conti et al.\textsuperscript{4} In this work the evolution of input beams into T solitons will be studied.

3. MODULATION EQUATIONS AND RADIATION EFFECTS

Approximate solutions of the saturating NLS equation for a nematic will now be obtained using the Lagrangian based method of Garcia Reimbert et al.\textsuperscript{5} and Kath and Smyth.\textsuperscript{9} The initial condition used in the present work is for a solitonlike pulse at $z = 0$, so that

$$E(r, t) = A \text{sech} \frac{r}{W}. \quad (10)$$

The saturating NLS equation (9) has the Lagrangian

$$L = i r[E_x E_z - E_z E_x] - r[E_z]^2 + r[q^2 + 4|E|^4]^{1/2} - rq, \quad (11)$$

where the superscript $'$ denotes the complex conjugate and it has been assumed that the electric field $E$ is radially symmetric.

To obtain approximate equations describing the evolution of a nematic, the method of Garcia Reimbert et al.\textsuperscript{5} and Kath and Smyth\textsuperscript{9} will be used, whereby a suitable trial function for $E$ will be substituted into the Lagrangian [Eq. (11)] and the Lagrangian will then be averaged by integrating in $r$ from $0$ to $\infty$. It was found in Garcia Reimbert et al.\textsuperscript{5} that a trial function with a sech profile gave approximate equations whose solutions were in good agreement with full numerical solutions for low power optical fields. For this reason, a suitable trial function for the electric field $E$ is

$$E = a \text{sech} \frac{r}{w} e^{i\sigma t} + i\sigma e^{i\alpha t}. \quad (12)$$

The second term in this trial function accounts for the low wavenumber, low phase-space radiation shed by the evolving pulse, which forms a circular shelf (or pedestal) under it.\textsuperscript{9} This shelf is assumed to form in the circular region $r < l$.

In principle the trial function [Eq. (12)] is now substituted into the Lagrangian [Eq. (11)] and the result averaged by integrating in $r$ from $0$ to $\infty$ to obtain the averaged Lagrangian,\textsuperscript{5,9} from which variational equations for the nematic parameters can be obtained. There is one difficulty which arises in this averaging, which is that the integral

$$\int_0^{\infty} r(\sqrt{q^2 + 4|E|^4} - q)dr = \int_0^{\infty} \frac{4r|E|^4}{\sqrt{q^2 + 4|E|^4}}dr, \quad (13)$$

cannot be evaluated exactly. In principle, this integral could be evaluated numerically, but this would defeat the purpose of using a trial function to obtain simple approximate equations describing the evolution of the nematic as the integral is not a fixed number, but a function of $a$.\textsuperscript{9}

One simple way around this difficulty is to replace the sech function in this integral by an equivalent Gaussian, which is meant to replace

$$E = a \text{sech} \frac{r}{w} \quad (14)$$

by

$$E = a\sigma e^{-2\sigma^2(q^2w^2)} \quad (15)$$

in the integral. The scaling parameters $\alpha$ and $\beta$ are then chosen by requiring that the resulting variational equations are the same of those of García Reimbert et al.\textsuperscript{5} in the small $E$ limit considered in that work. It is noted that there are other possible ways in which to determine the scaling parameters. The method used here has the benefit that it gives an averaged Lagrangian that, in the small amplitude limit, is the same as that of García Reimbert et al.,\textsuperscript{5} which gave excellent agreement with numerical solutions for small amplitude initial conditions. Furthermore, this choice of parameters gives very good agreement with numerical solutions for arbitrary amplitude initial conditions. Other matchings, such as to total power and the second moment, could be used, giving different values of $\alpha$ and $\beta$. However, due to good agreement with numerical solutions, we shall match to the low amplitude Lagrangian. The use of a Gaussian to evaluate the integral (13) suggests that a Gaussian rather than a sech should be used for the trial function. However if a Gaussian initial condition is used in numerical solutions of the nematic equations (7) and (6), or even the reduced equation (9), it is found that the initial condition breaks up into multiple nematics for the $O(1)$ amplitudes used in the present work and that there is a small initial amplitude window in which only a single nematic is formed. We therefore study initial conditions of the form (10) that do not readily split into multiple nematics for the wide range of initial parameters used in the present work.

Upon substituting the trial function [Eq. (12)] into the Lagrangian [Eq. (11)] and averaging by integrating in $r$ from $0$ to $\infty$, the averaged Lagrangian

$$\mathcal{L} = -2(a^2w^2I_2 + \Lambda g^2)\sigma' - 2aw^2I_1g' + 2gw^2I_1a' + 4awgI_1w'$$

$$- a^2I + \frac{1}{4}q\beta w^2 \left( \sqrt{\frac{4a^2w^2}{q^2} - 1} \right)$$

$$+ \frac{1}{4}q\beta^2 w^2 \ln \frac{2}{1 + \sqrt{1 + \frac{4a^2w^2}{q^2}}} \quad (16)$$

is obtained upon using the approximation (15) for the integral (13). Here

$$\Lambda = \frac{1}{2}l^2, \quad (17)$$

and the integrals $I, I_1,$ and $I_2$ are

$$I = \int_0^{\infty} x \text{sech}^2 x \tanh x dx - \frac{1}{3} \ln 2 + \frac{1}{6}. \quad (18)$$
\[ I_1 = \int_0^\infty x \text{sech}^2 x \, dx = 2C, \quad (19) \]
\[ I_2 = \int_0^\infty x \text{sech} x \, dx = \ln 2, \quad (20) \]

where \( C \) is the Catalan constant \( C = 0.915965594 \ldots \)

To obtain the scaling parameters \( \alpha \) and \( \beta \), the averaged Lagrangian [Eq. (16)] is linearized for small electric field amplitude \( a \), to give

\begin{multline}
\mathcal{L} = -2(a^2 w^2 I_2 + \Lambda g^2) \alpha' - 2aw^2 I_1 g' + 2gw^2 I_1 \alpha' + 4awg I_1 w' \\
- a^2 I + \frac{\alpha^4 \beta^2 a^4 w^2}{4q} - \frac{\alpha^8 \beta^2 a^8 w^2}{8q^3}.
\end{multline}

Now the averaged Lagrangian of García Reimbert et al. was derived in the limit of small electric field amplitude and was

\begin{multline}
\mathcal{L} = -2(a^2 w^2 I_2 + \Lambda g^2) \alpha' - 2aw^2 I_1 g' + 2gw^2 I_1 \alpha' + 4awg I_1 w' \\
- a^2 I - \frac{2}{q} I_1 a^4 w^2 - \frac{2}{q} I_1 a^8 w^2,
\end{multline}

where

\begin{align}
I_4 &= \int_0^\infty x \text{sech}^4 x \, dx = \frac{2}{3} \ln 2 - \frac{1}{6}, \\
I_8 &= \int_0^\infty x \text{sech}^8 x \, dx = \frac{16}{35} \ln 2 - \frac{19}{105}.
\end{align}

Matching these averaged Lagrangians then gives

\[ \alpha^4 = \frac{2I_8}{I_4} \quad \text{and} \quad \beta^2 = \frac{4I_4}{I_8}. \quad (25) \]

The amplitude scaling parameter \( \alpha = 0.9794 \ldots \), while the width scaling parameter \( \beta = 1.6027 \ldots \). So the amplitude of the equivalent Gaussian [Eq. (15)] is basically the same as that of the original \( \text{sech} \) [Eq. (14)], while there is a significant difference in width between these two profiles. The large change in the width to the equivalent Gaussian is the reason for the ready formation of multiple nematicons if a Gaussian initial condition were used.

The approximate equations describing the evolution of the nematicon can now be obtained as variational equations of this averaged Lagrangian. These variational equations are

\[ \frac{d}{dz} \left( a^2 w^2 I_2 + \Lambda g^2 \right) = 0, \quad (26) \]
\[ \frac{d}{dz} \left( aw^2 I_1 \right) = \Lambda g \alpha', \quad (27) \]
\[ I_1 \frac{dg}{dz} = \frac{Ia}{2w^2} + \frac{q \beta^2}{8a} \ln \frac{2}{1 + \sqrt{1 + \frac{4a^4 a'^4}{q^2}}} \quad (28) \]

\[ \frac{I_2}{dz} = - \frac{I}{w^2} - \frac{q \beta^2}{8a} \ln \left( \frac{2}{1 + \sqrt{1 + \frac{4a^4 a'^4}{q^2}}} \right) \quad (29) \]

The first of these variational equations [Eq. (26)] is the so-called mass conservation equation, as it describes mass conservation in the application of the NLS equation to fluid mechanics. In addition to this mass conservation equation, there is also an energy conservation equation that arises from Nöther's theorem as the Lagrangian [Eq. (11)] is invariant under shifts of the timelike variable \( z \). Nöther's theorem gives that the integrated energy conservation equation is

\[ \frac{dH}{dz} = \int_0^\infty r |E_r|^2 - \frac{1}{2} |E|^2 + |q| \, dr = 0. \quad (30) \]

Again using the approximation (15) for the second integral in the energy, the conserved energy is

\begin{multline}
H = \alpha^2 I - \frac{1}{4} q \beta^2 w^2 \left( \sqrt{1 + \frac{4a^4 a'^4}{q^2}} - 1 \right) \\
- \frac{1}{4} q \beta^2 w^2 \ln \frac{2}{1 + \sqrt{1 + \frac{4a^4 a'^4}{q^2}}}.
\end{multline}

The energy conservation equation is, of course, not independent of the variational equations [Eqs. (26)–(29)] and can be obtained from a suitable manipulation of these equations.

The final parameter to be determined for the approximate equations is the radius \( l \) of the shelf of radiation sitting under the evoking nematization. As was originally done by Kath and Smyth\(^a\) for the one space dimensional NLS equation and followed in García Reimbert et al.\(^5\) for the nematicon equations in the small amplitude limit, this parameter is determined by linearizing the approximate equations around their fixed point. The fixed point of the approximate equations [Eqs. (26)–(29)] is given by \( g = 0 \) with

\[ \frac{d}{dz} = - \frac{4I \dot{a}^2}{q \beta^2} \left[ \ln \left( \frac{2}{1 + \dot{S}} \right) \right]^{-1}, \quad (32) \]
\[ I_2 \frac{d\dot{a}}{dz} = - \frac{I}{2w^2} + \frac{\alpha^4 \beta^2 \dot{a}^2}{2q(1 + \dot{S})}, \quad (33) \]

with the amplitude at the fixed point \( \dot{a} \) determined from the initial conditions via the conserved energy [Eq. (31)]. Here

\[ \dot{S} = \sqrt{1 + \frac{4a^4 a'^4}{q^2}}. \quad (34) \]
Let us now linearize the variational equations (Eqs. (27)-(29)) plus the conserved energy (Eq. (31)) around the fixed point given by Eq. (32) using the expansions \(a = \tilde{a} + a_1, w = \tilde{w} + w_1\), and \(g = \tilde{g}_1\), with \(|a_1| \ll 1, |w_1| \ll 1, \text{ and } |\tilde{g}_1| \ll 1\). After some algebra, it is found that the approximate equations reduce to the simple harmonic oscillator equation

\[
\frac{d^2 \tilde{g}_1}{dz^2} + \frac{2 I}{\tilde{w}_1^2} \left[ \frac{\alpha^2 \beta \tilde{a}_0^2}{q \tilde{S}(1 + \tilde{S})} \right] \tilde{g}_1 = 0. \tag{35}
\]

As in García Reimbert et al.\(^5\) and Kath and Smyth,\(^8\) the frequency of this linear oscillator is now matched to the nematiclon oscillation frequency at the fixed point \(\dot{\sigma}'\), giving

\[
\Lambda = \frac{q I \tilde{S}(1 + \tilde{S}) \dot{\sigma}'}{2 q I \tilde{S}(1 + \tilde{S}) - \alpha^2 \beta \tilde{a}_0^2 \tilde{w}_1^2}. \tag{36}
\]

That the frequency of the shelf oscillation is equal to the soliton frequency was shown by Yang\(^13\) by considering the eigenfunctions for the equation governing a small perturbation from a soliton. In García Reimbert et al.\(^5\) and Kath and Smyth\(^8\), it was assumed that this expression for \(\Lambda\) is valid when the initial condition is not close to the fixed point value. In the present work, the variations in the pulse amplitude will be found to be large, so that keeping \(\Lambda\) fixed at the fixed-point value is not adequate and does not give good agreement with numerical solutions at large amplitudes. To overcome this, \(\Lambda\) is evaluated at the local values of \(a, w,\) and \(\dot{\sigma}'\), except for \(\tilde{S}\), which is kept at its fixed point value, as otherwise \(\Lambda\) was found to go negative, which is unphysical as this implies that the nematiclon is unstable. Hence the expression for \(\Lambda\) used in the present work is

\[
\Lambda = \frac{q I \tilde{S}(1 + \tilde{S}) \dot{\sigma}}{2 q I \tilde{S}(1 + \tilde{S}) - \alpha^4 \beta^2 \tilde{a}_0^2 \tilde{w}_1^2}. \tag{37}
\]

The approximate equations are not as close yet as the effects of the dispersive radiation shed by the evolving pulse has not been included. As the effect of this shed linear radiation was determined in García Reimbert et al.,\(^5\) only the final result of the analysis will be given here. This work found that when the effect of the shed dispersive radiation is added, the only equation changed is that for \(g\), Eq. (28), which becomes

\[
I_1 \frac{dg}{dz} = \frac{Ia}{2 \omega^2} + \frac{q I \beta}{8a} \ln \frac{2}{1 + \sqrt{1 + \frac{4 \alpha^4 a^4 \omega^4}{q^2}}} - 2 \dot{g}, \tag{38}
\]

where the loss coefficient \(\delta\) is

\[
\delta = \frac{2 \pi R \Lambda}{32 e R \Lambda} \left[ \int_0^{\frac{\pi R(z') \ln((z-z')/\Lambda)}{\Lambda}} \left( \frac{1}{4 \ln((z-z')/\Lambda)} \right)^2 + \frac{3 \pi^2/16}{\Lambda} \left( \frac{\pi^2}{16} \right)^2 \right] \left( \frac{z-z'}{\Lambda} \right)^2. \tag{39}
\]

The variable \(R\) measures the difference between the mass of the nematiclon at \(z\) and its mass at the fixed point.

The full set of approximate equations describing the evolution of a nematiclon is then Eqs. (27), (29), (31), and (38). Solutions of these approximate equations will be compared with full numerical solutions of the nematiclon equations (7) and (6) in the next section.

4. RESULTS

In this section, full numerical solutions of the nematiclon equations (7) and (6) will be compared with numerical solutions of the approximate equations (27), (29), (31), and (38). The mass equation (26) has been replaced by the energy equation (31) since, to leading order, energy is conserved by the evolving nematiclon, while mass is lost. The electric field equation (7) was solved using a pseudospectral method based on that of Fornberg and Whitham.\(^{13}\)

The main difference with the scheme of Fornberg and Whitham\(^{13}\) was that the stepping in the \(z\) direction was performed in Fourier space using a fourth-order Runge-Kutta method, rather than in physical space using a second-order method. The \(r\) derivatives were calculated using fast Fourier transforms. To numerically solve the Poisson equation (6), it was rewritten in the form

\[
\frac{\varphi \theta}{\varphi \varphi} \frac{\partial \varphi}{\partial r} + \frac{\varphi \theta}{\varphi \theta} = q \sin(2\varphi) - 2 q \theta - 2 |E|^2 \cos(2\varphi). \tag{41}
\]

The derivatives were then calculated using standard second-order finite differences, resulting in a tridiagonal system when the boundary conditions \(\varphi, \theta = 0\) at \(r = 0\) and \(\varphi \rightarrow \infty\) as \(r \rightarrow \infty\) were implemented. This nonlinear boundary value problem was then solved using a Picard iteration with the right-hand side of Eq. (41) being evaluated at the previous iteration. The director equation (6) was rewritten in the form of Eq. (41) as this re-expressed equation was found to have better convergence properties. The value \(r = 0.01\) has been used for the numerical solutions in this section. For this small value of \(r\), the solution of the full nematiclon equations (7) and (6) is the same to graphical accuracy as the numerical solution of the reduced saturating NLS equation (9), obtained using the same pseudospectral method as for the NLS equation (7).
Figure 2 shows a comparison between the amplitude of the nematon as given by the full solution of the nematon equations (7) and (6) and the solution of the approximate equations for the initial amplitude $A=0.3$ and initial width $W=4.0$ for $q=2$. Also shown is the amplitude as given by the solution of the approximate equations of García Reimbert et al.\textsuperscript{5} The one difference between this example and the following ones is that $A$ had to be kept fixed at the value (36) as the varying value (37) was found to go negative initially, which is unphysical. It can be seen that the approximate equations of the present work give results in excellent agreement with the numerical solution, both in amplitude and period. It can be further seen that the radiation loss analysis of Section 3 gives a decay rate onto the steady state in excellent agreement with the numerical rate. The amplitude oscillations shown in Fig. 2 are large, with the maximum amplitude of the oscillations being nearly triple the initial pulse amplitude. This is a manifestation of the instability of solitons for the standard two space dimensional NLS equation

\[ i \frac{\partial E}{\partial z} + \frac{1}{2} \nabla^2 E + |E|^2 E = 0, \tag{42} \]

for which, above a critical threshold, a pulse initial condition will blow up in amplitude in finite $z$. The initial pulse in Fig. 2 is then starting to blow up and reaches a relatively large amplitude before the saturation stops the amplitude increase and reverses it. We remark that since $q=2$, $|E|^2/q$ is relatively small, so that it is expected that the small amplitude theory of García Reimbert et al.\textsuperscript{5} will be in good agreement with the numerical solution, as shown in Fig. 2. Even though the amplitude rises to near 1, the small amplitude analysis of García Reimbert et al.\textsuperscript{5} remains valid as $q=2$. Let us now consider results for $q=1$, in which case the small amplitude approximation is not valid.

Figure 3 shows a similar amplitude comparison for the initial amplitude $A=0.4$ and initial width $W=2.5$ for $q=1$. It can be seen that reducing $q$ to 1 has had a major effect on the agreement between the numerical solution and the solution of the approximate equations of García Reimbert et al.\textsuperscript{5} with the amplitude, mean, and period of the solution of these approximate equations not being in accord with the numerical solution. However, the mean of the solution of the present approximate equations, which can be obtained from the conserved energy [Eq. (31)], is in excellent agreement with the mean of the numerical solution. This agreement is remarkable in that the pulse has nearly doubled in amplitude over that of the initial condition. The numerical and approximate solutions are then tending to the same steady nematon amplitude. The amplitude decay of the approximate equations is slightly greater than that of the numerical solution, resulting in a disagreement with the numerical amplitude at large values of $z$. This is because the radiation analysis of Section 3 and García Reimbert et al.\textsuperscript{5} is based on the asymptotic evaluation of the inversion of an integral for large $z$, so that small errors compound over large $z$. As the approximate equations (27), (29), (31), and (38) form a nonlinear oscillator, there is also a period difference due to the amplitude difference for large $z$.

Figure 4 shows a comparison between the amplitude of the nematon as given by the full numerical solution and the solution of the approximate equations for the higher initial amplitude $A=0.5$ with the same initial width $W=2.5$ and $q=1$. The solution of the approximate equations of García Reimbert et al.\textsuperscript{5} is not shown as these equations fail for the high amplitudes of this figure. Again there is good agreement in the mean of the amplitude oscillation, so that the approximate equations give the same amplitude of the final steady nematon as the numerical solution. However, for this example, the decay rate of the oscillations of the approximate solution is initially significantly lower than that of the numerical solution, which results in the large $z$ disagreement in the amplitude, even though the decay rates are in broad agreement for large $z$.

Figure 5 shows the amplitude comparison for the low initial amplitude $A=0.35$ with $W=2.5$ and $q=1$ as before.
the optical beam. It was then shown that in the Kerr regime the evolution of a nematic is governed by a saturable NLS equation. While previous work studied the small amplitude limit, the present analysis is valid for an arbitrary amplitude. The results of the present work stem from the use of an equivalent Gaussian to calculate certain integrals involved in the averaging of the saturating nonlinearity. The use of this equivalent function gives a closed form for the averaged Lagrangian. The resulting modulation equations were found to give solutions in very good agreement with full numerical solutions.

The analytical results of this work demonstrate the possibility of nematicon propagation in liquid crystals for which the local or Kerr regime is the relevant one. This could be tested experimentally in liquid crystals which have a local or Kerr response, such as 5CB.

ACKNOWLEDGMENTS

The authors would like to thank the three referees for their constructive comments that substantially improved this paper. This research was supported by the Engineering and Physical Sciences Research Council (EPSRC) under grant EP/C548612/1.

C. García Reimbert's e-mail address is cgr@mym.IMATE.unam.mx. A. A. Minzoni's e-mail address is tim@mym.IMATE.unam.mx. N. F. Smyth can be contacted by e-mail, N.Smyth@ed.ac.uk, or by phone, (44) (131) 650 5080. A. L. Worthy's e-mail address is Annette_Worthy@uow.edu.au.

REFERENCES

10. M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables (Dover, 1972).
