Do shape invariant solitons in highly nonlocal nematic liquid crystals really exist?

Milan S. Petrović,1,2 Aleksandra I. Strinić,1,2 Najdan B. Aleksić,1,2 and Milivoj R. Belić2

1Institute of Physics, P. O. Box 68, 11001 Belgrade, Serbia
2Texas A&M University at Qatar, P. O. Box 23874, Doha, Qatar

We question physical existence of shape invariant solitons in three-dimensional nematic liquid crystals. Using modified Petviashvili’s method for finding eigenvalues and eigenfunctions, we determine shape invariant solitons in a realistic physical model that includes the highly nonlocal nature of the liquid crystal system. We check the stability of such solutions by propagating them for long distances. We establish that any noise added to the medium or to the fundamental solitons induces them to breathe, rendering them practically unobservable.

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The fundamental spatial optical soliton is a beam that propagates in a nonlinear (NL) medium without changing its transverse profile. Such shape-invariant solutions are easily identified in (1+1)-dimensional NL systems because the inverse scattering theory guarantees their existence. The situation is less clear in the multidimensional and multicomponent systems. No credible inverse scattering theory is formulated in more than one dimension and even when the localized solutions are found, no credible procedure for guaranteeing their stability is established (however, there are many credible linear stability analyses or stability criteria or numerical procedures, but not for rigorously proven stability.) In fact, wave instability and the collapse of solutions are overriding concerns in multidimensional NL systems. Additional compounding difficulties arise in the multicomponent vector models or in the scalar nonlocal models in which the medium response is driven by the optical field itself. Such are the models describing the generation of solitary waves – nematicons – in nematic liquid crystals (NLCs).

Nonlocality is an important characteristic of many NL media. A highly nonlocal situation arises in a nonlocal nonlinear (NN) medium when the characteristic size of the response is much wider than the size of the excitation itself. In NLCs both experiments and theoretical calculations demonstrated that the nonlinearity is highly nonlocal.

For more complex nonlinearities, numerical techniques are necessary to determine the soliton solutions. Soliton profile calculations in NN media have been presented in a number of papers, see for example [10–12]. The existence and stability of 2D solitons in media with NN response was discussed in [13]; even a high degree of nonlocality did not guarantee the existence of stable high-order soliton structures [14]. Orientational nonlinearity in NLCs is highly nonlocal but the NL response is not perfectly quadratic, implying that if one launches a Gaussian beam into the cell it is only possible to observe breathing solitons [3, 15].

In some publications soliton profiles were calculated using semi-analytical models [4, 16–18]. For the more general vectorial model, in which the order parameter in NLC is not constant, steady elliptical soliton profiles are found numerically [16]. To determine such profiles, the authors demonstrated that it is necessary to include all three components of the optical electric field.

However, what is puzzling is that even though everybody agrees that shape-preserving solitons do exist in highly nonlocal NLCs, practically nobody cared to present them explicitly. Experimental accounts profusely mention steady nematicons, but careful inspection of all published figures reveals self-focusing oscillations. True, experimental results may be of not much help in this regard, because all experimental setups feature a few mm long cells, which cannot capture slow (if any) convergence to a steady profile. In this paper we find a family of fundamental solitons for the same model and the same parameters: we check their stability in propagation and demonstrate that any small change in the input shape, as well as in the medium, leads to the soliton breathing. Consequently, we question the real physical observability of such shape-invariant solitons.

To find an exact fundamental soliton solution in a NLC model that is not vectorial, we use an iterative numerical eigenvalue technique. We consider widely accepted scalar model of beam propagation that is well suited for uniaxial NLCs and low-intensity optical fields, which correspond to most situations of practical interest. Also, we discuss the influence of boundary conditions (BCs) on the shape and power of solutions, and analyze soliton and Gaussian propagation using two different propagation methods.

We adopt the well-known NN 3D scalar model in NLCs, which provides good agreement with experimental data [6]. The optical beam polarized along the x axis
propagates in the $z$ direction, while the NLC molecules can rotate in the $x$-$z$ plane. The liquid-crystal cell of interest is sketched in Fig. 1. The total orientation of molecules with respect to the $z$ axis is denoted as $\theta(x, y, z)$, whereas the orientation induced by the static electric field only is denoted by $\theta_0$ (the pre-tilt angle). The bias field points in the $x$ direction and is uniform in the $z$ direction; hence the pre-tilt angle is uniform along the $z$ axis as well. The quantity $\hat{\theta} = \theta - \theta_0$ corresponds to the optically induced molecular reorientation.

The system of equations of interest consists of the scaled NL Schrödinger-like equation for the propagation of the optical field $A$, and the diffusion equation for the molecular orientation angle $\theta$ [7, 8, 15]:

$$
2i\frac{\partial A}{\partial z} + \Delta_{x,y}A + \alpha[\sin^2 \theta - \sin^2 \theta_0]A = 0, \quad (1)
$$

$$
2\Delta_{x,y}\theta + |\beta + \alpha A|^2 \sin(2\theta) = 0, \quad (2)
$$

where the coefficients $\alpha$ and $\beta$ are proportional to the optical and static permittivity anisotropies of the NLC molecules, respectively. Hard boundary conditions (BCs) on the molecular orientation at the NLC cell faces in the $x$ direction are assumed: $\theta(x = -D/2, y) = \theta(x = D/2, y) = \text{const.}$ [20]. In our calculations we use data corresponding to typical experimental conditions [8, 13, 20].

The solitary eigen-solutions are determined from the system of Eqs. (1,2) using the modified Petviashvili’s iteration method [21, 22]. Equation (1) suggests the existence of a fundamental soliton of the form $A = a(x, y)e^{i\mu z}$, where $\mu$ is the propagation constant. The real-valued function $a(x, y)$ satisfies the equation: $-\Delta a + (2\mu + P)a = Q$, where $P = \alpha \sin^2(\theta_0)$ and $Q = \alpha \sin^2(\theta) a$. After Fourier transforming the equation for $a$, we get:

$$
\overline{\sigma} = \frac{1}{|k|^2 + 2\mu} (\overline{Q} - \overline{Pa}), \quad (3)
$$

where overbar denotes Fourier transform. Straightforward iteration of Eq. (3) does not converge in general, so the stabilizing factors had to be introduced [22, 28]. In each iteration step of Eq. (3), Eq. (2) is treated using a successive overrelaxation (SOR) method, until convergence is achieved.

Stable soliton solutions are presented in Fig. 2 for two different BCs. The shape and the power of fundamental shape-invariant solutions naturally depend on the BCs applied. Zero BCs ($\hat{\theta} = 0$ on all boundaries) correspond to the Dirichlet BCs. Periodic BCs correspond to the mixed BCs – Dirichlet along the $y$ axis and Neumann along the $x$ axis. The solution with the periodic BCs is more appropriate to the geometry of the problem; furthermore, it is more acceptable on physical grounds. The fundamental soliton so obtained requires less beam power...
for the same value of the propagation constant and identical other parameters. In identical conditions (but for BCs) the solution requiring less power should be favored. The often used $\theta_0 = \pi/4$ approximation leads to the solution with zero BCs, and consequently such a soliton is less appropriate.

Spatial solitons in highly nonlocal media with quadratic response possess Gaussian profiles \cite{4,5}. However, the fundamental soliton profile is not Gaussian. The soliton intensity profile compared to a Gaussian is shown in Fig. 3(a); the difference is confined to the tails. To check the stability of fundamental solitons, we propagate them numerically; the results are presented in Fig. 3(b). Also included in Fig. 3(b) is a case presenting propagation of a Gaussian with similar parameters, but obtained using two different numerical methods. In both methods a split-step beam propagation procedure based on the fast Fourier transform (FFT) is used for the propagation of the optical field. In the first method the diffusion equation for the optically induced molecular reorientation is treated using the SOR method. In the second method the diffusion equation is treated using the split-step procedure again. One can see that the methods provide similar results; however the first method is more accurate.

The problem with the FFT procedure is that it treats an array of \textit{transversely} periodic cells. Since the molecular reorientation is wide, it tends to slightly spill over into the adjacent cells, i.e. back onto itself, adding to the optical field. This is not an overriding problem in the propagation of a Gaussian, as it only leads to a slightly amplified oscillation of the breathing solution. However, it makes huge difference in the propagation of the fundamental soliton – it makes it impossible for the field to keep the shape-invariant input profile and therefore should be discarded. Even the SOR solution slightly oscillates at lower accuracy; this, however, becomes imperceptible as the accuracy is improved. In Fig. 3(b) we show a case where the oscillation of the amplitude is still perceptible. This brings us to an important point.

When one considers the propagation of a Gaussian beam using the two propagation methods, the results are close. The propagation of Gaussians invariably leads to breathing beams, regardless of the method of integration. By the same token, when the fundamental soliton is propagated through the medium in which a small random noise added to the underlying molecular orientation $\theta_0$, a breathing solution is also obtained. The same phenomenon happens as well when a small intensity noise is added to the fundamental profile, but $\theta_0$ kept unchanged. This phenomenon is confirmed in our computations (Fig. 4) and is not difficult to understand. In a highly NN medium any additional energy from noise, no matter how small, cannot be radiated away and the solution has no way to relax to the fundamental soliton. Therefore, it keeps oscillating about the fundamental soliton, forming a \textit{stable} breathing soliton. Since noise is unavoidable in any realistic set-up, be it experimental or numerical, this fact opens the question of the physical observability of shape-invariant fundamental solitons in highly NN media.

In conclusion, we have presented calculations of shape-invariant fundamental solitons in a highly nonlocal 3D scalar NCLs, for a realistic physical model. Using modified Petviashvili’s iterative scheme we numerically determined the fundamental spatial soliton profiles and found a family of solutions, depending on BCs. We depicted stable propagation of such solitons. We then demonstrated that upon propagation, any amount of noise transforms the fundamental soliton into a breather, making shape-invariant nematicons practically unobservable.

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