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Solitons in highly nonlocal nematic liquid crystals: Variational approach

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We investigate numerically and theoretically solitons in highly nonlocal three-dimensional nematic liquid crystals. We calculate the fundamental soliton profiles using the modified Petviashvili method. We apply the variational method to the widely accepted scalar model of beam propagation in uniaxial nematic liquid crystals and compare the results with numerical simulations. To check the stability of such solutions, we propagate them in the presence of noise. We discover that the presence of any noise induces the fundamental solitons—the so-called nematicons—to breathe. Our results explain the difficulties in experimental observation of steady nematicons.

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I. INTRODUCTION

Spatial optical solitons are self-localized wave packets originating from a robust balance between dispersion and nonlinearity. They propagate in a nonlinear medium without changing their internal structure [1]. An important characteristic of many nonlinear media is nonlocality, which is known to strongly affect the propagation of beams through the medium. It tends to improve the stability of solitons, because of the diffusion mechanism in the underlying nonlinearity. When the characteristic size of the response is much wider than the size of the excitation, a highly nonlocal situation emerges in nonlocal nonlinear (NN) media. In this limit the system becomes effectively linear [2]. In nematic liquid crystals (NLCs), both experiments [3,4] and theoretical calculations [5] demonstrated that the nonlinearity is highly nonlocal.

For the more complicated nonlinearities, numerical methods are necessary to find soliton solutions; no analytical solutions are known for realistic multidimensional models. However, variational techniques are extremely useful in situations when one can expand about the fixed points in a nonlinear system. Such a situation naturally occurs in the highly NN model of NLCs.

If a Gaussian beam is launched into the NLC cell, it is only possible to observe breathing solitons [6], because the NLC orientational nonlinearity is highly nonlocal and the nonlinear response is not of a perfect parabolic shape. Breathers are natural extensions of the fundamental solitons in highly nonlocal systems, whenever, for whatever reasons, the conditions for the emergence of shape-invariant fundamental solitons are not met.

Soliton profile calculations in NN media have been presented in a number of papers [7–12]; for variational calculations see Refs. [13,14]. Criteria for the existence and stability of 2D solitons in media with spatially NN response were discussed in Ref. [15]; even a high degree of nonlocality may not guarantee the existence of stable high-order soliton structures [16]. In many publications semianalytical models were used for soliton profile calculations [17,18]; however, simplified models cannot describe all aspects of the reorientation dynamics. For the more general vectorial model, in which the order parameter in NLC is not constant, steady fundamental soliton profiles were found numerically [19], by including all three components of the optical electric field.

In this paper we use an iterative numerical technique to find exact fundamental shape-invariant solutions of a NLC model that is not vectorial. Also, we discuss the influence of boundary conditions (BCs) on the symmetry and power of solitons. Modulation equations for the beam and the reorientation angle evolution are derived using suitable trial functions in a Lagrangian formulation of the nematicon equations, and main results of variational approximation are presented. We confirm the stability of solitonic solutions by direct numerical simulations, with and without noise. The noise, which is inevitable in any real physical system, causes a regular oscillation of soliton parameters, with the period well predicted by our variational calculus.

II. THE MODEL

We start from the well-known NN three-dimensional (3D) scalar model for the wave propagation in uniaxial NLCs, since it provides very good agreement with the experimental data [4]. In this model, the optical beam polarized along the x axis propagates in the z direction, while the NLC molecules can rotate in the x-z plane only; the modeled liquid-crystal cell of interest is sketched in Fig. 1 [4]. The total orientation of the 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 θ_0 (the pretilt angle). The bias field points in the x direction and is uniform in the z direction; hence the pretilt 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 NL Schrödinger-like paraxial wave equation for the propagation of the optical field E, and the diffusionlike equation for the molecular orientation angle θ [4,5]. After the rescaling $x/x_0 \rightarrow x$, $y/x_0 \rightarrow y$, $z/L_D \rightarrow z$, where x_0 is the transverse scaling length and $L_D = kx_0^2$ is the diffraction length, the following model equations in the computational domain, in the steady state, are obtained [6]:

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

$$2\Delta_{x,y}\theta + [\beta + \alpha|E|^2]\sin(2\theta) = 0, \tag{2}$$

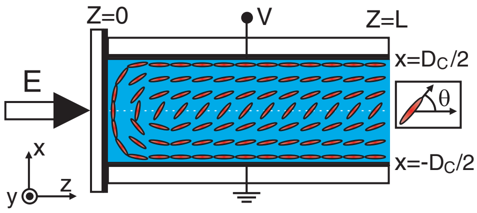

FIG. 1. (Color online) Liquid-crystal cell considered.

where we introduced the notation $\alpha = k_0^2 x_0^2 \Delta\varepsilon^{\mathrm{OPT}}$ and $\beta = \varepsilon_0 x_0^2 \Delta\varepsilon^{\mathrm{dc}} |E^{\mathrm{dc}}|^2/K$. We also scaled the optical field intensity $\frac{\varepsilon_0}{2Kk_0^2}|E|^2 \to |E|^2$. The wave numbers in the medium and vacuum are k and k_0, respectively. The amplitude of the static bias electric field is $E^{\mathrm{dc}} = V/D_C$, where V is the applied bias voltage and D_C is the cell thickness. $\Delta\varepsilon^{\mathrm{OPT}}$ and $\Delta\varepsilon^{\mathrm{dc}}$ are the optical and static permittivity anisotropies of the NLC molecules, respectively. K is Frank's elastic constant. The pretilt angle θ_0 is found from Eq. (2) in the absence of optical field: $2\Delta_{x,y}\theta_0 + \beta \sin(2\theta_0) = 0$. Hard BCs on the molecular orientation at the NLC cell borders in the x direction are applied: $\theta(x = -D_C/2) = \theta(x = D_C/2) = \mathrm{const}$ [20].

In all calculations the following data are kept constant: $L_D = 78.6\ \mu$m, the propagation distance $L = 20L_D$, $x_0 = 2\ \mu$m, $\lambda = 514$ nm, $n_0 = 1.53$, $D_C = 75\ \mu$m, $V = 1$ V, $\Delta\varepsilon^{\mathrm{OPT}} = 0.4$, $\Delta\varepsilon^{\mathrm{dc}} = 20$, $K = 12 \times 10^{-12}$ N, and $\theta_0(x = -D_C/2, y) = \theta_0(x = D_C/2, y) = 2^{\mathrm{o}}$. These data correspond to typical experimental conditions (optical power in the mW range, NLC parameters of commercially available liquid crystals).

III. THE EIGENVALUE PROCEDURE

The solitonic solutions can be found from the system of equations (1) and (2) by using the modified Petviashvili iteration method [21–23]. Equation (1) allows the existence of a fundamental soliton solution in the form $E = a(x,y)e^{i\mu z}$, where μ is the propagation constant. Then the real-valued amplitude function $a(x,y)$, after the separation of linear and nonlinear terms onto different sides of the equation, satisfies the following relation: $-\Delta a + (2\mu + \mathbb{P})a = \mathbb{Q}$, where $\mathbb{P} = \alpha \sin^2(\theta_0)$ and $\mathbb{Q} = \alpha \sin^2(\theta)a$. We perform Fourier transformation of that equation, to find:

$$\overline{a} = \frac{1}{|\mathbf{k}|^2 + 2\mu}(\overline{\mathbb{Q}} - \overline{\mathbb{P}a}), \tag{3}$$

where the overbar denotes the Fourier transform. Straightforward iteration of Eq. (3) does not converge in general, so we have to introduce the stabilizing factors of the form $\mathbf{a} = \int [(|\mathbf{k}|^2 + 2\mu)\overline{a} + \overline{\mathbb{P}a}]\overline{a}^*\, d\mathbf{k}$ and $\mathbf{b} = \int \overline{\mathbb{Q}}\overline{a}^*\, d\mathbf{k}$, into the equation. The following iteration equation is obtained:

$$\overline{a}_{m+1} = \frac{1}{|\mathbf{k}|^2 + 2\mu}\left[\left(\frac{\mathbf{a}_m}{\mathbf{b}_m}\right)^{3/2}\overline{\mathbb{Q}}_m - \left(\frac{\mathbf{a}_m}{\mathbf{b}_m}\right)^{1/2}\overline{\mathbb{P}a_m}\right]. \tag{4}$$

For each iteration step given by Eq. (4), Eq. (2) is treated using a successive over-relaxation (SOR) method, until its convergence. In this manner, stable self-consistent solutions are found. Our method is suitable for finding both fundamental and higher-order soliton solutions.

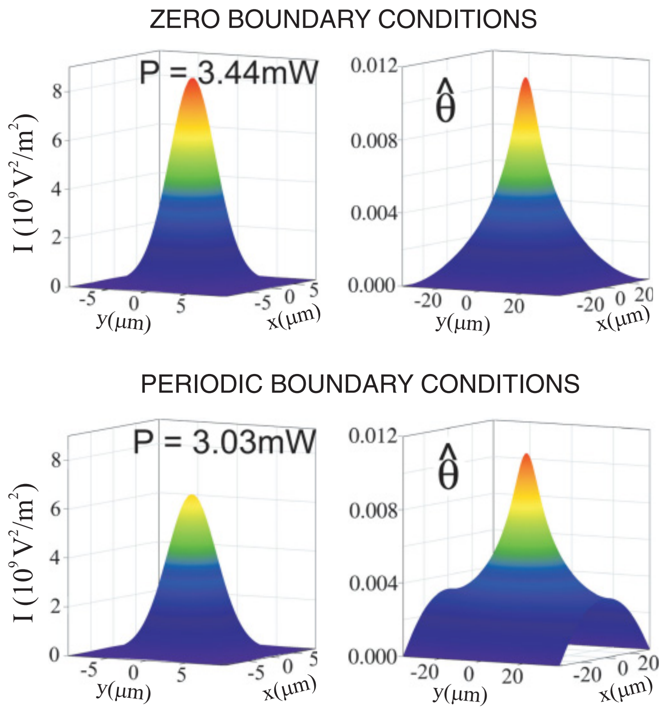

FIG. 2. (Color online) Possible solitonic solutions for $\mu = 1L_D^{-1}$. Two cases of intensity profiles and reorientation angles are presented for zero and mixed BCs.

In fact, a family of fundamental solitons is found, depending on the BCs applied. Examples of such fundamental solitonic solutions are presented in Fig. 2, where the optical field intensity is denoted as $I = |E|^2$. Shape and power of spatial shape-invariant solutions depend on the BCs applied to the optically induced molecular reorientation angle $\hat{\theta}$. Zero BCs ($\hat{\theta} = 0$ on all boundaries) present Dirichlet BCs. Periodic BCs correspond to the mixed BCs, in which along the y direction $\hat{\theta}(-D_C/2, y) = \hat{\theta}(D_C/2, y) = 0$ (Dirichlet BC) and along the x axis $\partial\hat{\theta}(x, -D_C/2)/\partial y = \partial\hat{\theta}(x, D_C/2)/\partial y = 0$ (Neumann BC). Evidently, the solution with the periodic BCs is more appropriate to the geometry and symmetry of the problem (see the figure for $\theta_0(x,y)$ in Ref. [6]). It is also more acceptable on physical grounds, since it requires less beam power for the same value of the propagation constant. An approximation used in many publications $\theta_0 = \pi/4$ leads to the solution with zero BCs.

Thus, for each set of reasonable physical parameters one can find a family of fundamental solitonic solutions, depending on the BCs applied, with different propagation constants and beam powers (see Fig. 3).

IV. VARIATIONAL CALCULUS

There are no known exact analytical solitonic solutions of the nematicon equations. A powerful approximate technique for studying this problem is based on the variational approach

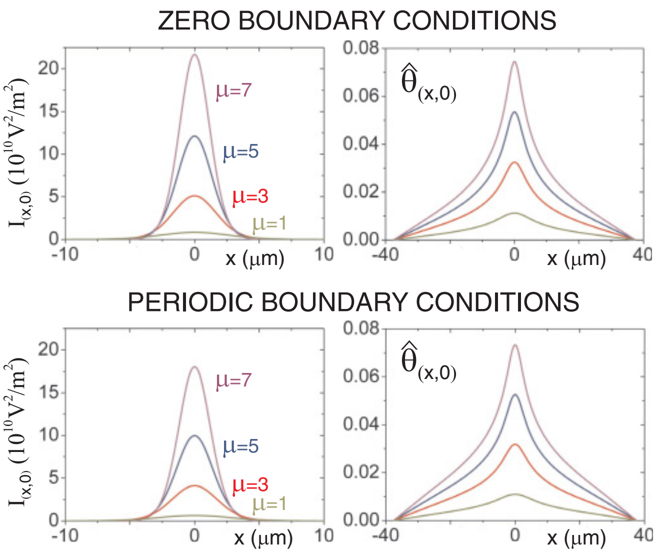

FIG. 3. (Color online) Fundamental soliton intensity profiles (left) and the corresponding profiles of the optically induced molecular reorientation (right) at y = 0, in the case of zero BCs (top) and periodic BCs (bottom).

to the governing equations (1) and (2). We start from the model equations in the lowest-order approximation for the fields:

$$2i\frac{\partial E}{\partial z} + \Delta E + \bar{\alpha}\hat{\theta}E = 0, \tag{5}$$

$$2\Delta\hat{\theta} + \bar{\beta}\hat{\theta} + \bar{\alpha}|E|^2 = 0, \tag{6}$$

where we introduced abbreviations $\bar{\alpha} = \alpha\ \sin(2\theta_0)$ and $\bar{\beta} = 2\beta\ \cos(2\theta_0)$, and assumed $\hat{\theta} \ll 1$. The term proportional to $|E|^2\hat{\theta}$ is eliminated from Eq. (6) on account of presenting a higher-order term in the system of equations (5) and (6). We also assumed the notation $\theta_0 = \theta_0(x=0,y=0)$, for simplicity. The Lagrangian density for the system of equations (5) and (6) is given by:

$$L = i\left(\frac{\partial E^*}{\partial z}E - \frac{\partial E}{\partial z}E^*\right) + |\nabla E|^2 + |\nabla\hat{\theta}|^2 - \frac{\bar{\beta}}{2}\hat{\theta}^2 - \bar{\alpha}\hat{\theta}|E|^2. \tag{7}$$

An appropriate choice of trial functions is most important for the success of variational techniques. In the case of zero BCs (see Fig. 2), the trial function should possess radial symmetry. As the most appropriate localized solution in a highly nonlocal system, we choose the Gaussian trial function for the electric field:

$$E = A\ \exp\left[-\frac{r^2}{2R^2} + iCr^2 + i\psi\right], \tag{8}$$

where r is the distance from the z axis in cylindrical coordinates, A is the amplitude, R is the width of the beam, C is its curvature, and ψ is the peak-intensity phase. We assume $R \ll D_C$. The trial function for the reorientation angle is composed of the nonlocal (the first two terms) and the local (the last term) contributions:

$$\hat{\theta} = B[\mathrm{Ei}(-r^2/W^2) - \ln(r^2/d^2)] + D\ \exp[-r^2/W^2], \tag{9}$$

where B and D are the amplitudes, W is the width of the nonlocality, $d = D_C/2$, and Ei is the exponential integral function, defined as $\mathrm{Ei}(z) = -\int_{-z}^{\infty}\exp(-t)/t\,dt$. The nonlocal part of the ansatz in Eq. (9) represents the solution of Eq. (6) when $\bar{\beta} = 0$ and E is given by the ansatz in Eq. (8). We see that the trial function for the reorientation angle satisfies zero BCs.

Substituting the trial functions [Eqs. (8) and (9)] into the Lagrangian [Eq. (7)] and integrating over r, we obtain the averaged Lagrangian (still in the limit $R \ll d$):

$$\begin{aligned}\langle L\rangle \approx{}& 2P\psi' + 2PR^2(C' + 2C^2) + \frac{P}{R^2}\\ &+ \pi B^2\left[4\ \ln\left(\frac{d^2e^\gamma}{2W^2}\right) - \beta d^2\right] - \bar{\alpha}PB\ \ln\left(\frac{d^2e^\gamma}{R^2+W^2}\right)\\ &- D\left(4\pi B + \frac{\bar{\alpha}PW^2}{R^2+W^2}\right) + O(\delta^2),\end{aligned} \tag{10}$$

where the prime denotes the derivative with respect to z, γ is Euler's constant, and $\delta = \max\{\beta,(R/d)\ln(d/R)\}$. The main quantity characterizing the spatial soliton is its power $P = \pi A^2R^2$, which also represents an integral of motion. We have used it to eliminate $A(z)$ from Eq. (10).

We require the minimization of the averaged Lagrangian by the variational parameters $R(z)$, $C(z)$, $\psi(z)$, $B(z)$, $W(z)$, and $D(z)$, thereby obtaining three ODEs between them:

$$C = \frac{1}{2R}\frac{dR}{dz}, \tag{11}$$

$$\frac{dC}{dz} = -2C^2 + \frac{1}{2R^4} - \frac{\bar{\alpha}^2P}{32\pi R^2} + O(\delta^2), \tag{12}$$

$$\frac{d\psi}{dz} = -\frac{1}{R^2} + \frac{\bar{\alpha}^2P}{16\pi}\left[\ln\left(\frac{d^2e^{\gamma+1/2}}{2R^2}\right) + \frac{\bar{\beta}d^2}{8}\right] + O(\delta^2), \tag{13}$$

and three algebraic relations:

$$W = R\left[1 - \frac{1}{4}\bar{\beta}d^2\ \ln^{-1}\left(\frac{d^2e^{\gamma+3}}{2R^2}\right)\right] + O(\delta^2), \tag{14}$$

$$B = \frac{\bar{\alpha}P}{8\pi}\left[1 + \frac{1}{4}\bar{\beta}d^2\ \ln^{-1}\left(\frac{d^2e^{\gamma+3}}{2R^2}\right)\right] + O(\delta^2), \tag{15}$$

$$D = -\frac{\bar{\alpha}P}{8\pi}\bar{\beta}d^2\ \ln^{-1}\left(\frac{d^2e^{\gamma+3}}{2R^2}\right) + O(\delta^2). \tag{16}$$

From Eqs. (11) and (12) we obtain an equation that describes the dynamics of the beam width and (indirectly) the dynamics of all other quantities:

$$\frac{d^2R}{dz^2} = \frac{1}{R^3} - \frac{\bar{\alpha}^2P}{16\pi R} + O(\delta^2). \tag{17}$$

In the stationary state $dR/dz = dC/dz = 0$, so the fixed point of the system of equations (11)–(16) is:

$$R_0 = \frac{4}{\bar{\alpha}}\sqrt{\frac{\pi}{P}} + O(\delta^2), \tag{18}$$

$$C_0 = 0, \tag{19}$$

$$\left(\frac{d\psi}{dz}\right)_0 = \frac{\bar{\alpha}^2P}{16\pi}\left[\ln\left(\frac{d^2e^{\gamma-1/2}}{32\pi}\bar{\alpha}^2P\right) + \frac{\bar{\beta}d^2}{8}\right] + O(\delta^2), \tag{20}$$

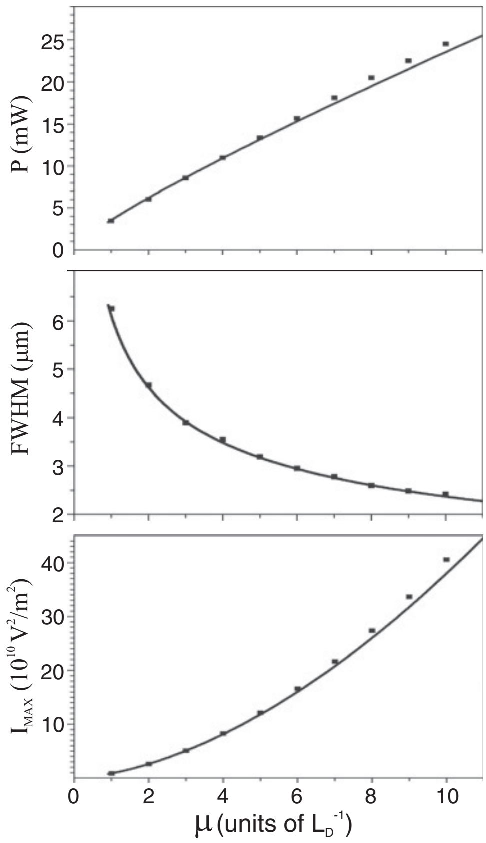

FIG. 4. Fundamental soliton power, width, and peak intensity as functions of the propagation constant, for zero BCs. Solid lines represent results of variational approach; dots represent numerical solitonic solutions.

and also $W_0 = W(R_0)$, $B_0 = B(R_0)$, and $D_0 = D(R_0)$. Note that the propagation constant $\mu = (d\psi/dz)_0$ is given by Eq. (20).

The period of small oscillations around the fixed point (T) is calculated from Eq. (17). We assume $R = R_0 + \tilde{R}$, where $\tilde{R}$ is a small perturbation of the beam width, so that Eq. (17) becomes:

$$\frac{d^2\tilde{R}}{dz^2} + \frac{2}{R_0^4}\tilde{R} = 0, \tag{21}$$

which gives an expression for the period of oscillations:

$$T = \frac{16\sqrt{2}\pi^2}{\bar{\alpha}^2 P}. \tag{22}$$

V. RESULTS

The most important quantities of variational calculation are presented in Figs. 4 and 5. The fundamental soliton power, width, and peak intensity, as functions of the propagation constant, are shown in Fig. 4, respectively. We note very good agreement between the results of variational approach and the numerical solitonic solutions, obtained by integrating directly the system of equations (1) and (2). One can discern from Fig. 4 that the obtained variational solution is stable, according to the Vakhitov-Kolokolov stability criterion [24]. According

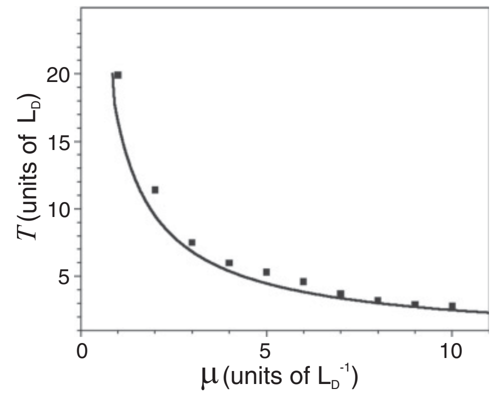

FIG. 5. Period of small oscillations T as a function of the propagation constant. Solid line represents results of variational approach; dots represent results obtained in numerical simulations.

to this criterion, the solitary wave should be stable as long as $dP/d\mu > 0$.

The period of small oscillations T as a function of the propagation constant is represented in Fig. 5 (solid line). To check this result, we propagate a fundamental soliton in the case of small perturbations, and find that it oscillates regularly with a period in good agreement with that obtained by the variational approach. Numerical procedure applied to the propagation equation is the split-step beam propagation method based on the fast Fourier transform (FFT); the diffusion-type equation for the optically induced molecular reorientation is treated using the SOR method.

Thus far we have presented the fundamental soliton solutions obtained by the Petviashvili eigenvalue procedure and the approximate Gaussian solutions obtained by the variational method. These two types of solutions are distinctly different. The Gaussian solutions can be considered as approximations to the fundamental solitons only up to a point. Their intensity profiles are similar, the difference being confined to the tails of the distributions. The basic difference between the two is the propensity of Gaussians to oscillate; the fundamental solitons, by definition, are shape invariant. However, upon closer inspection a more intimate connection between the two is discovered.

In fact, by conventional understanding of solitons in highly nonlocal media, the fundamental solitons are just a special case of nematicons, which appear for specific propagation constants and critical powers P_c [2]. Below and above critical powers, the proper localized solutions are breathers, whose profiles oscillate. As such, they can even better be approximated by propagating Gaussians. What we have discovered is that the propagating fundamental solitons very easily turn into breathers, by addition of any kind of perturbation or noise to the system.

The fundamental solitons are determined only up to an accuracy prescribed by the eigenvalue procedure. Usually, in such a procedure single-precision accuracy suffices. However, when we propagated a fundamental soliton obtained in single precision, we found that the profile slightly oscillates [Fig. 6(a)]; in double precision the oscillation is gone. This

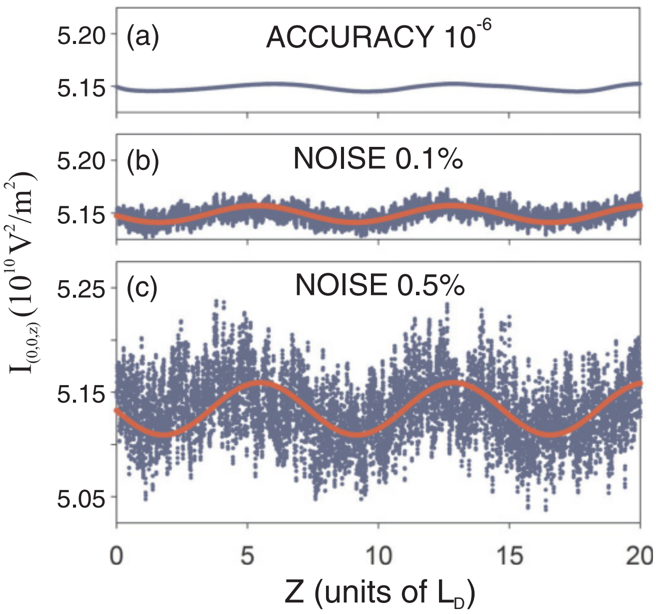

FIG. 6. (Color online) (a) Propagation of the nonideal soliton solution calculated with accuracy of 10^{-6}. [(b),(c)] Soliton peak intensity evolution in a noisy medium. The level of amplitude noise is indicated in each figure. Parameters: $\mu = 3L_D^{-1}$, $P = 8.6$ mW, $T = 7.5L_D$; zero BCs.

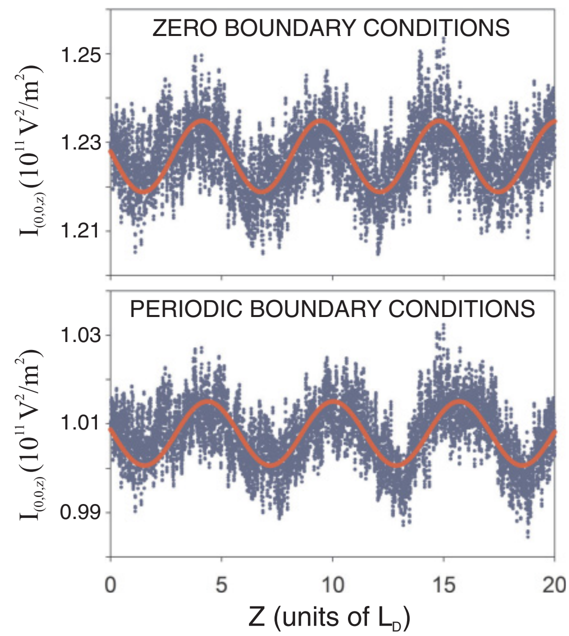

FIG. 7. (Color online) Peak intensity as a function of the propagation distance in the case of 0.5% noise added to the pretilt angle θ_0 (dots), fitted with a sine function (red line). For zero BCs (top) the period of oscillation is $T = 5.3L_D$; for periodic BCs (bottom) the period is $T = 5.7L_D$. The propagation constant for input solitons is $\mu = 5L_D^{-1}$.

motivated us to consider the influence of noise on the propagation of fundamental solitons.

We investigate the influence of small perturbations on the propagation of fundamental soliton solutions by monitoring the peak intensity as a function of the propagation distance (Figs. 6 and 7). A nonideal fundamental soliton oscillates regularly during propagation, as in Fig. 6(a), where the numerical accuracy of the beam profile calculation is defined as the relative error between the last two iterations in the Petviashvili iterative procedure. To achieve more proper input soliton shape, we needed better numerical resolution in our numerics: as the accuracy of the eigenfunction profile improved, the amplitude of its oscillation diminished.

However, in all realistic media, noise is unavoidable. Thermal fluctuations of the director field are inherent to the nematic phase [25,26]. Even if one launches a perfect fundamental soliton, some noise in the medium is bound to influence its propagation. We introduce noise in our simulations by adding randomly distributed white noise to the pretilt angle θ_0 at each propagation step. Propagation of an ideal (double-precision) fundamental soliton solution in a noisy medium is presented in Figs. 6(b) and 6(c), where the red curve is a sinusoidal fit to the perturbed soliton. It is seen that the perturbed soliton propagates similar to a breather. For all three cases in Fig. 6, the period of oscillations is $7.5L_D$; Eq. (22) gives $T = 6.9L_D$. The results presented are obtained using the fundamental solitons with zero BCs; similar conclusions hold for the case of periodic BCs (Fig. 7), the only difference being the period of oscillation. Our variational approach is valid for the case of zero BCs, and for the case presented in Fig. 7, Eq. (22) gives $T = 4.4L_D$.

VI. CONCLUSIONS

In this work, we have investigated numerically and theoretically solitons in biased highly nonlocal 3D uniaxial NLCs. We have presented calculations of shape-invariant fundamental profiles, using the modified Petviashvili method. We discussed the influence of BCs on the symmetry and power of solitons, and identified two possible kinds of fundamental solitonic solutions. We developed a variational approach to describe basic characteristics of solitons analytically. We confirmed the stability of solitonic solutions by Vakhitov-Kolokolov stability criterion and by direct numerical simulations. Because of the inevitable presence of noise in any real physical system, we also checked the stability of such solutions by propagating them in the presence of noise in the medium. The noise causes regular oscillation of soliton parameters, with periods well predicted by our variational calculus. Our results naturally explain experimental difficulties in observing steady fundamental nematicons.

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