

Discrete solitons in Bragg environment with carbon nanotubes

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In this paper, we study the propagation of ultrashort optical pulses, which can be regarded as discrete solitons in this case, when the medium with carbon nanotubes (CNTs), has spatially modulated refractive index. As a result we were able to obtain the effective equation, which represents an analog of the classical sine-Gordon equation. A detailed analysis of the dependence on various parameters of the problem has been performed.

Keywords: Ultrashort optical pulses; Bragg environment.

1. Introduction

Nowadays we observe an increased interest in the nonlinear propagation of light in discrete waveguide structures. This is due to the possibilities of practical use of nonlinear optical effect and to the fact that the propagation of light beams in these structures is similar to the motion of an electron in a crystal lattice. We can also highlight the existence of forbidden and allowed bands, as well as the fact that the pulse propagates with the group velocity which is much lesser than the speed of light in vacuum. Similar physical phenomena are observed in other systems, e.g. in semiconductor superlattices, biological molecular structures, Bose–Einstein condensates with a periodic potential etc.¹

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The first theoretical justification of the possibility of nonlinear light localization in periodic structures of coupled optical waveguides has been given in Ref. 2, published back in 1988. However, the experimental confirmation of the existence of such spatially localized states, also known as discrete solitons, has been done 10 years later.^{3–5} The latter study dealt with waveguide grates based on gallium arsenide (GaAs), bearing a positive Kerr nonlinearity. Since this breakthrough, the study of the effects of the interaction of light beams in nonlinear periodic structures became widespread. Most importantly, the nonlinearity associated with the material properties should be properly chosen, so that it allows for at least theoretically possible existence of discrete solitons. Among various nonlinear materials, intensively studied in recent years, especially allocated one is an ensemble of carbon nanotubes (CNTs), whose preparing technique is now practically available worldwide.

Unique physical and chemical properties of CNTs, largely related to the periodicity of the dispersion law, make them promising materials for the formation of the nonlinear Bragg media in which the refractive index is periodically spatially modulated (see Refs. 6–8). Because the medium has a periodically alternating refractive index, the light pulse propagates therein slower than in any medium with a fixed refractive index. This makes it possible to build the delay lines which have important applications, e.g. in the femtosecond spectroscopy. Qualitatively, this behavior can be understood if we assume that the light pulse undergoes reflection and subsequent interference at the interface of different refractive index. Additional introduction of nonlinearity in such environments leads to qualitatively new effects (see Refs. 9–11). In particular, these systems allow for the formation of Bragg solitons (gap solitons), which represent particular combinations of counterpropagating waves thereby combining in a way that they move together with a reduced speed.

All of the above circumstances provided us an impetus for the study of the dynamics of propagation of extremely short optical pulses in a system of CNTs, which can lead to new effects useful in a wide range of practical applications. Namely, they include manufacturing of repeaters and inverters used in optical computers.

2. General Equations

Dispersion law, which describes the properties of single-walled CNT without the Coulomb interaction between electrons on the same site (which is a good approximation for the band structure of the nanotube) reads¹²

$$E(\mathbf{p}) = \pm\gamma\sqrt{1 + 4\cos(ap_z)\cos(\pi s/m) + 4\cos^2(\pi s/m)}, \quad (1)$$

where $\gamma = 2.7\text{ eV}$, $a = 3b/2h$, $b = 0.142\text{ nm}$ is the distance between adjacent carbon atoms, p_z is the projection of the electron momentum onto the CNT and s corresponds to the quantization along the CNT's circumferential. Hereinafter, only the semiconductor CNTs of zigzag type are considered. Different signs relate to the conduction and valence bands.

Accepting the gauge $\mathbf{E} = -\partial\mathbf{A}/c\partial t$, the Maxwell's equations with account for the dielectric and magnetic properties of the system can be written as (see Ref. 13),

$$\frac{\partial^2 \mathbf{A}_k}{\partial x^2} - \frac{n^2(x)}{c^2} \frac{\partial^2 \mathbf{A}_k}{\partial t^2} + \frac{4\pi}{c} \mathbf{j}_k - \frac{4\pi}{c} \frac{\partial \mathbf{P}_k}{\partial t} = 0. \quad (2)$$

Here, the vector potential \mathbf{A}_k , which corresponds to the electromagnetic field in the k th layer consisting of a CNT, is considered to have the form $\mathbf{A}_k = (0, 0, A_k(x, t))$. \mathbf{j}_k is the current flowing in the k th layer consisting of CNT graphene, $n(x)$ defines the spatial variation of the refractive index, i.e. Bragg grating and \mathbf{P}_k is the polarization induced in the k th layer by the electromagnetic field and currents of adjacent nanotubes. Note that we take a very simple model in which $\mathbf{P}_k = \alpha(\mathbf{E}_{k-1} + \mathbf{E}_{k+1})$, where α is the coupling coefficient, and $\mathbf{E}_{k\pm 1}$ stands for the electric field.

Let us write a standard expression for the current density:

$$\mathbf{j}_k = e \sum_{p_z, s} v_s \left(p_z - \frac{e}{c} A_k(t) \right) \langle a_p^+ a_p \rangle, \quad (3)$$

where $v_s(\mathbf{p}) = \partial E_s(p_z)/\partial p_z$, $\mathbf{p} = (p_z, s)$ and the angle brackets mean an average with the nonequilibrium density matrix $\rho(t): \langle B \rangle = \text{Sp}(B(0)\rho(t))$.

It turns that the current density becomes

$$\begin{aligned} \mathbf{j}_k &= -en_0 \sum_l D_l \sin\left(\frac{le}{c} A_k(t)\right), \\ D_l &= \sum_{s=1}^m \int_{-\pi/a}^{\pi/a} dp_z B_{ls} \cos(lp_z) \frac{\exp(-\varepsilon_s(p_z)/k_B T)}{1 + \exp(-\varepsilon_s(p_z)/k_B T)}, \end{aligned} \quad (4)$$

where k_B is the Boltzmann constant, T is the temperature and D_{ls} are coefficients of the expansion of velocity and the charge carriers in a Fourier series. The latter are explicitly given by

$$\begin{aligned} v_s(p) &= \sum_l B_{ls} \sin(lp_z), \\ B_{ls} &= \frac{1}{2\pi} \sum_p v_s(p) \sin(lp). \end{aligned}$$

Equation (4) can be represented in dimensionless form as

$$\begin{aligned} \frac{\partial^2 R_k}{\partial x'^2} - \frac{n^2(x)}{c^2} \frac{\partial^2 R_k}{\partial t'^2} - \text{sgn}(D_1) \sin(R_k) - \sum_{l=2}^{\infty} \left(\frac{D_l}{|D_1|} \sin(lR_k) \right) \\ + \frac{4\pi\alpha}{c} \frac{\partial^2 (R_{k-1} + R_{k+1})}{\partial t'^2} = 0, \\ R_k = \frac{eA_k}{c}, \quad x' = x \frac{2e}{c} \sqrt{\pi n_0 |D_1|}, \quad t' = t \frac{2e}{c} \sqrt{\pi n_0 |D_1|}. \end{aligned} \quad (5)$$

Note that Eq. (5) is a generalization of the well-known sine-Gordon equation for the case where the generalized potential is expanded in a full Fourier series. Due

to the fact that the coefficients D_l decrease with increasing l , a possible way to analyze the resulting system is to keep only the first nonvanishing terms of the sum in Eq. (5), which leads to the widely used double sine-Gordon equation, which cannot be integrated by the inverse scattering method.¹⁴

3. Numerical Results

For the numerical solution of Eq. (5), we have implemented explicit finite difference schemes for hyperbolic equations.¹⁵ Difference scheme steps in both time and space were iteratively decreased twice until the solution became unchanged in the eighth decimal place. Initial conditions for the vector potential have been chosen as

$$A_{t=0} = A_0 \exp \left\{ -\frac{x^2}{\gamma^2} \right\} \exp \{ -\beta(N - N_c)^2 \},$$

$$\left. \frac{dA}{dt} \right|_{t=0} = \frac{2vx}{\gamma^2} A_0 \exp \left\{ -\frac{(x - vt)^2}{\gamma^2} \right\} \exp \{ -\beta(N - N_c)^2 \},$$
(6)

where N_c is the number of central waveguide ($N_c = 6$), β , γ are the parameters determining the pulse width, N is the waveguide number and t_0 is the initial instant of time.

The refractive index was modeled as

$$n(x) = n_0(1 + \alpha \cos(2\pi x/\chi)).$$

Figure 1 shows that the pulses, in the system with a periodically varying refractive index, are slowed down, as required by the theory and at the same time there is an exchange of energy between the different layers of the CNT. Note that the energy (which is proportional to the square of the electric field amplitude, represented on the figure) is partially “pumped” from the central layer of the CNT to the neighboring ones and back. This exchange of energy is typical for discrete solitons.

Calculations were made for the CNTs of the type (7, 0) in the case of ambient temperature. Intel to medium pulse velocity is equal to $0.95c$ where c is light velocity. Modulation period χ is equal to $3 * 10^{-5}$ m, modulation depth α is equal to 0.05.

According to Fig. 2, this behavior is typical for Bragg gratings with different periods and the grating period only affects the deceleration of a pulse and the peculiarities of their form.

Similar behavior is detected for the depth of modulation of the refractive index, as shown in Fig. 3.

As can be seen from the figures, the pulse in the central waveguide hardly changes its shape depending on the initial pulse width, unlike the pulses in neighboring waveguides. Pulses on the side waveguides have the same shape as that of the center, but with a reduced amplitude. By changing the initial width of the central pulse, we can control the amplitude of the electromagnetic field in the adjacent

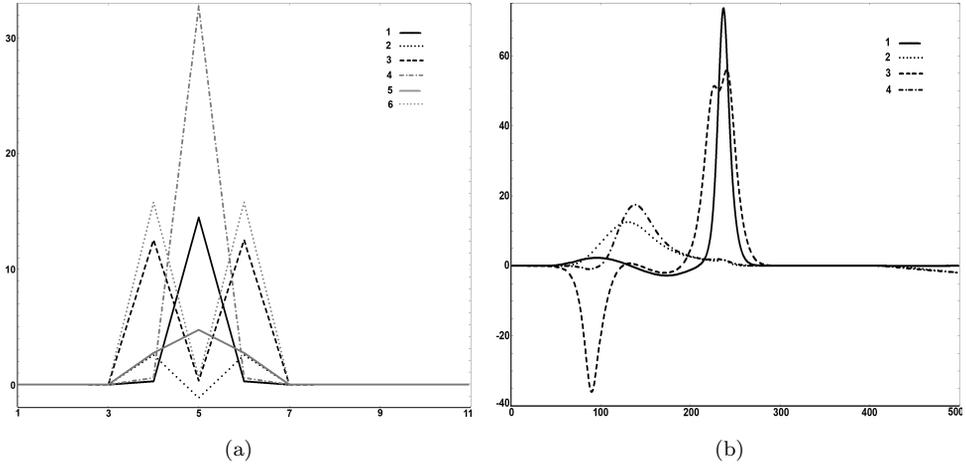


Fig. 1. (a) The dependence of the electric field, determined by the potential, on the number of the waveguide. Abscissa gives a number of the waveguide, N ; ordinate represents the dimensionless value of the electric field in the presence of a Bragg grating at times: $t = 2.5 \cdot 10^{-12}$ s (1-a), $t = 2 \cdot 10^{-12}$ s (2-a), $t = 1.3 \cdot 10^{-12}$ s (3-a) and without a grating at times: $t = 2.5 \cdot 10^{-12}$ s (4-a), $t = 2 \cdot 10^{-12}$ s (5-a), $t = 1.3 \cdot 10^{-12}$ s (6-a). (b) Dependence of the electric field on time. Abscissa gives a dimensionless time, ordinate represents the dimensionless electric field in the presence of a Bragg grating for the following numbers of waveguides: $N = 5$ (1-b), $N = 6$ (2-b) and without a grating: $N = 5$ (3-b), $N = 6$ (4-b).

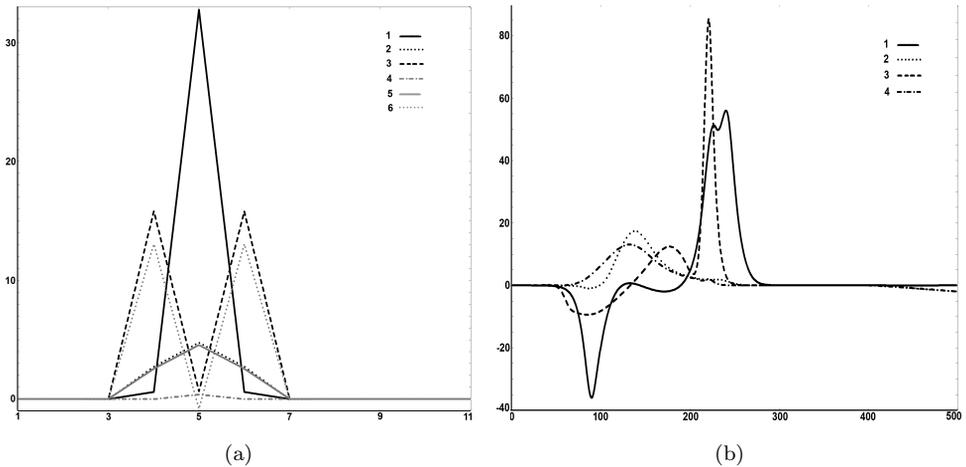


Fig. 2. (a) The dependence of the electric field, determined by the potential, on the number of the waveguide. Abscissa gives a number of the waveguide, N ; ordinate represents the dimensionless value of the electric field in the presence of a Bragg grating of a modulation period χ at times: $t = 2.5 \cdot 10^{-12}$ s (1-a), $t = 2 \cdot 10^{-12}$ s (2-a), $t = 1.3 \cdot 10^{-12}$ s (3-a) and the same for a period 2χ at times: $t = 2.5 \cdot 10^{-12}$ s (4-a), $t = 2 \cdot 10^{-12}$ s (5-a), $t = 1.3 \cdot 10^{-12}$ s (6-a). (b) Dependence of the electric field on time. Abscissa gives a dimensionless time, ordinate represents the dimensionless electric field in the presence of a Bragg grating of a period χ for the following numbers of waveguides: $N = 5$ (1-b), $N = 6$ (2-b) and the same for a period 2χ : $N = 5$ (3-b), $N = 6$ (4-b).

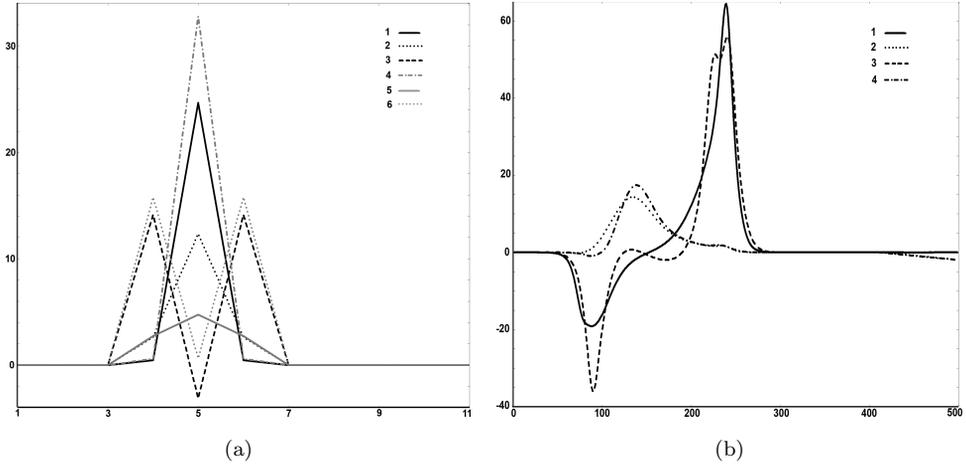


Fig. 3. (a) The dependence of the electric field, determined by the potential, on the number of the waveguide. Abscissa gives a number of the waveguide, N ; ordinate represents the dimensionless value of the electric field in the presence of a Bragg grating with the modulation depth α at times: $t = 2.5 \cdot 10^{-12}$ s (1-a), $t = 2 \cdot 10^{-12}$ s (2-a), $t = 1.3 \cdot 10^{-12}$ s (3-a); and with the modulation depth 2α at times: $t = 2.5 \cdot 10^{-12}$ s (4-a), $t = 2 \cdot 10^{-12}$ s (5-a), $t = 1.3 \cdot 10^{-12}$ s (6-a). (b) Dependence of the electric field on time. Abscissa gives a dimensionless time, ordinate represents the dimensionless electric field in the presence of a Bragg grating with the modulation depth α , for numbers of waveguides: $N = 5$ (1-b), $N = 6$ (2-b) and with the modulation depth 2α for numbers of waveguides $N = 5$ (3-b), $N = 6$ (4-b).

waveguides. Moreover, the wider the pulse supplied to a system of CNTs, the greater the amplitude of the neighboring pulses. This, in turn, makes it possible to control the shape of an extremely short pulse by changing the number of CNTs' layers and the distance between them, which determines the coupling coefficient.

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