JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 12 No 4, 04016(4pp) (2020)
ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 12 № 4, 04016(4cc) (2020)

Influence of the Vector Order Parameter on the Dynamics of 3D Ultrashort Pulses in Carbon Nanotubes

N.N. Konobeeva*, M.B. Belonenko

Volgograd State University, 400062 Volgograd, Russia

(Received 23 March 2020; revised manuscript received 15 August 2020; published online 25 August 2020)

In this paper, we propose a model for taking into account the vector order parameter for studying the evolution of an ultrashort optical pulse in a medium with carbon nanotubes. We consider the electric field of the pulse in the three-dimensional geometry. To describe the dynamics of the considered system we use the phenomenological theory developed by A.Z. Patashinskii and V.L. Pokrovskii. Given the specificity of the problem at hand, it is assumed that the vector order parameter is related to the electric field directed along the nanotube axis. For the clarity, we consider a ferroelectric medium with the polarization, which has three nonzero spatial components. Based on the Ginzburg-Landau theory, we obtain the governing equation of motion for the vector order parameter. Based on Maxwell's equations, we obtain the effective nonlinear wave equation in a cylindrical coordinate system. We use the approximation when the accumulation of charge can be neglected. Therefore, the cylindrical symmetry in the field distribution is preserved. The system of these two equations allows us to analyze the dependence of the shape of three-dimensional ultrashort optical pulses on the distance from the critical point of phase transition. That important observation can in practice be used to identify experimentally the critical point. We show that ultrashort optical pulse propagates stably without secondary wave radiation. The energy of the electromagnetic pulse is preserved in a localized region. Also a comparative analysis of two models of the order parameter (scalar order parameter and vector order parameter) is performed. The influence of the order parameter model on the dynamics of the pulse is determined. The proposed technique allows us to carry out the spectroscopy by changing the order parameter when probing the medium with ultrashort pulses.

Keywords: Vector order parameter, Carbon nanotubes, Optical pulses.

DOI: 10.21272/jnep.12(4).04016 PACS numbers: 77.80.Bh, 78.67.Ch

1. INTORDUCTION

L.D. Landau has introduced a general approach to the description of phase transition, which is driven by the most fluctuating parameter called the order parameter [1]. The order parameter is a value different from zero at a temperature less than critical ($T < T_{cr}$) and tending to zero at $T \geq T_{cr}$. This value can be the magnetization in a ferromagnet, the polarization vector in a ferroelectric, etc. The increased interest of researchers in phase transition media is primarily due to the large number of practical applications [2-4]. In this case, a very important problem is the studying the dynamics of the order parameter in the presence of strong external variable fields [5]. From this point of view, it seems relevant to consider a composite medium, which consists of a medium with a phase transition and carbon nanotubes (CNTs) [6-8]. This fact is due to both the ability of carbon nanotubes to withstand electric fields of high intensity and their stabilizing effect on the propagation of electromagnetic field pulses (for example, light bullets) [9, 10]. It should be noted that CNTs are sensitive to the electric field orientation due to the structure anisotropy.

The interaction of the order parameter with the medium implies the choice of a model to describe this parameter. Some phase transitions may have an order parameter with more than one degree of freedom. In this case, it can take the form of a complex number, a vector, or even a tensor, the magnitude of which tends to zero during the phase transition. The authors previously studied the possibility of spectroscopy of a scalar order parameter [11]. In this paper, a model for the vector case is constructed.

Thus, the statement of the problem is to determine the possibility of using light bullets for spectroscopy of the vector order parameter in composite nonlinear media with CNTs.

2. BASIC EQUATIONS

As an object of study, we choose a medium containing CNTs. We can write down the equations of motion using the phenomenological approach developed in [1, 12]:

$$\frac{d\mathrm{P}}{dt} = -\Gamma \frac{\delta \Phi}{\delta \mathrm{P}}, \quad (1)$$

where Γ is the kinetic coefficient (further it is equal to 1), $\mathbf{P}$ is the order parameter, Φ is the functional density of free energy.

Further, we assume that the vector order parameter $\mathbf{P} = (P_x(x, y, t), P_y(x, y, t), P_z(x, y, t))$ is connected with an electric field whose vector potential has the following form: $\mathbf{A} = (0, 0, A(x, y, z, t))$. For definiteness, we consider a ferroelectric with a polar axis coinciding with the CNT's axis.

We choose Φ in the standard form taking into account the influence of the external field $\boldsymbol{E} = (0, 0, E(x, y, z, t))$:

$$\Phi = \Phi_0 + a \cdot \mathrm{P}^2 + b \cdot \mathrm{P}^4 - \mathrm{E} \cdot \mathrm{P}, \quad (2)$$

*yana_nn@volsu.ru

where a, b are the expansion coefficients. We also take into account that the medium field acts on the electrons of carbon nanotubes together with the electromagnetic field of the pulse $E_s = \delta\Phi/\delta P$.

We consider a propagation of the light bullets in the three-dimensional case. The electric field of the pulse is directed along the CNT's axis.

Let us write a standard expression for the current density [13]:

$$j = 2e\sum_{s=1}^{m}\int_{BZ} \upsilon_s(p)\cdot f(p,s)dp, \qquad (3)$$

where e is the electron charge, p is the component of the quasi-momentum of the conduction electron along the CNT's axis, $\upsilon_s(p) = \partial\varepsilon_s(p)/\partial p$ is the electron velocity, $f(p, s)$ is the Fermi distribution function, $\varepsilon_s(p)$ is the dispersion law which describes the properties of CNT's electrons and has the form [14, 15]:

$$\varepsilon_s(p) = \pm\gamma_0\sqrt{1+4cos(ap)cos\left(\frac{\pi s}{m}\right)+4cos^2\left(\frac{\pi s}{m}\right)}, \qquad (4)$$

where $s = 1, 2, \dots m$, CNT type is $(m, 0)$, $\gamma_0 = 2.7$ eV, $a = 3b/2\hbar$, $b = 0.142$ nm is the distance between adjacent carbon atoms.

During the propagation of an ultrashort pulse in a CNTs' array, due to the field inhomogeneity along some axis, the current is also inhomogeneous, which leads to charge accumulation in a certain region, which can be neglected for femtosecond pulses [13]. It can be assumed that cylindrical symmetry is preserved in the field distribution ($\partial/\partial\varphi \to 0$), then the effective equation for the vector potential has the form:

$$\begin{aligned}&\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right)+\frac{\partial^2 A}{\partial z^2}-\frac{\partial^2 A}{c^2\partial t^2}+\frac{4en_0}{c}\sum_{q=1}^{\infty}b_q sin\left(\frac{qae(A+A_s)}{c}\right)=0,\\&b_q=\sum_s a_{sq}\int_{BZ}dp\cdot cos(pq)\cdot f(p,s)\end{aligned} \qquad (5)$$

Here A_s corresponds to the electric field of the medium ($E_s = -\partial A_s/c\partial t$), k_B is the Boltzmann constant, T is the temperature, a_{sq} are the expansion coefficients of the electron dispersion law (4) in a Fourier series:

$$\varepsilon_s(p) = \frac{1}{2\pi}\sum_{s=1}^{m}\sum_{q=1}^{\infty}a_{sq}cos(pq), \qquad (6)$$

$$a_{sq} = \int_{BZ} dp\cdot cos(pq)\varepsilon_s(p). \qquad (7)$$

3. RESULTS AND DISCUSSION

The studied system of equations (1), (2) and (5) is solved numerically [16]. The initial condition is chosen in the Gaussian form:

$$\begin{aligned}&A(z,r,0) = Q\cdot exp\left(-\left(\frac{z-z_0}{\gamma_z}\right)^2\right)exp\left(-\frac{r^2}{\gamma_r^2}\right),\\&\frac{dA(z,r,0)}{dt} = 2Q\upsilon_z\frac{z-z_0}{\gamma_z^2}exp\left(-\left(\frac{z-z_0}{\gamma_z}\right)^2\right)exp\left(-\frac{r^2}{\gamma_r^2}\right)\end{aligned} \qquad (8)$$

where Q is the pulse amplitude; γ_z, γ_r determine the pulse width; z_0 is the initial displacement of the pulse center; υ_z is the initial pulse velocity along the z-axis.

The evolution of the electromagnetic pulse during its propagation through the sample is shown in Fig. 1. A broadening of the ultrashort optical pulse is observed, and a 300-fold decrease in the intensity of the electric field of the pulse occurs. Such behavior can be explained by the interaction of the current flowing through the CNTs with the subsystem described by the vector order parameter and is a consequence of the relaxation dynamics of the order parameter.

The influence of the model of the order parameter on the propagation process of an ultrashort optical pulse is presented in Fig. 2.

As can be seen from Fig. 2, taking into account the order parameter has a stabilizing effect on the electromagnetic pulse shape (Fig. 2b, c compared to Fig. 2a), but leads to its attenuation in amplitude. Note that the more stable (from the point of view of concentrating most of the energy in the main pulse) is the pulse, which we considered in a medium with a scalar order parameter (Fig. 2b).

The influence of the equilibrium value of the order parameter a in the scalar and vector cases is presented in Fig. 3.

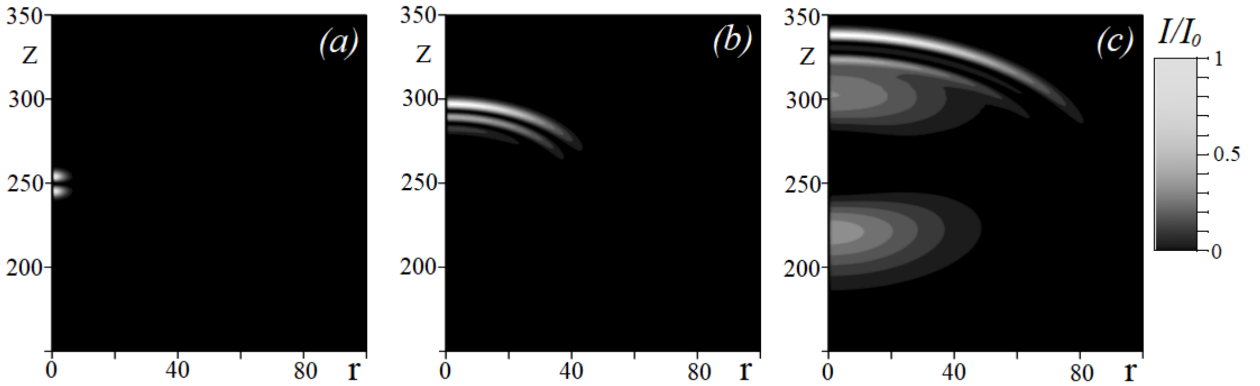

Fig. 1 – The intensity of 3D electromagnetic pulse $I(r, z, t) = E^2(r, z, t)$ (I_0 is the intensity maximum) at different time points ($\alpha = 0.1$, $\beta = -1$, $\Gamma = 0.1$): (a) $t = 0$ s; (b) $t = 5\cdot10^{-13}$ s; (c) $t = 10\cdot10^{-13}$ s

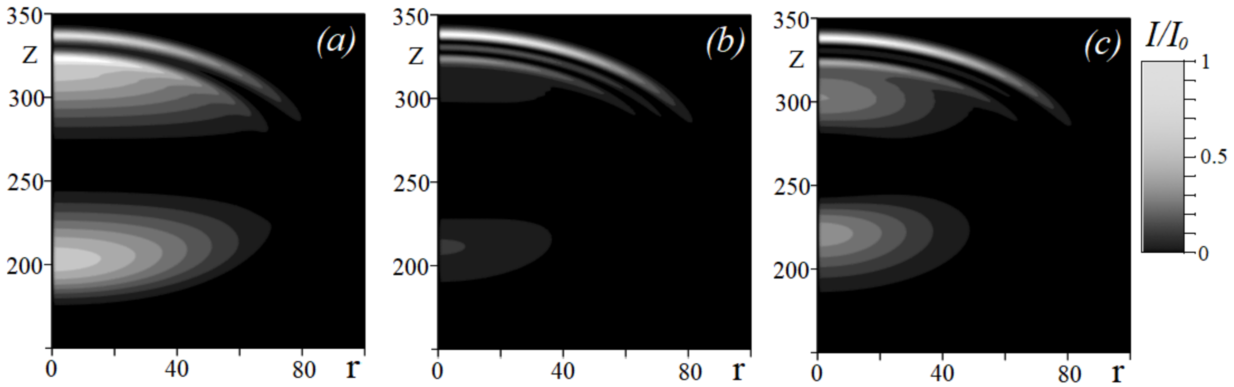

Fig. 2 – The intensity of 3D electromagnetic pulse $I(r, z, t) = E^2(r, z, t)$ (I_0 is the intensity maximum) for different values of the relaxation rate Γ ($\alpha = 0.1$, $\beta = -1$, $t = 10 \cdot 10^{-13}$ s): (a) excluding the order parameter; (b) scalar order parameter; (c) vector order parameter

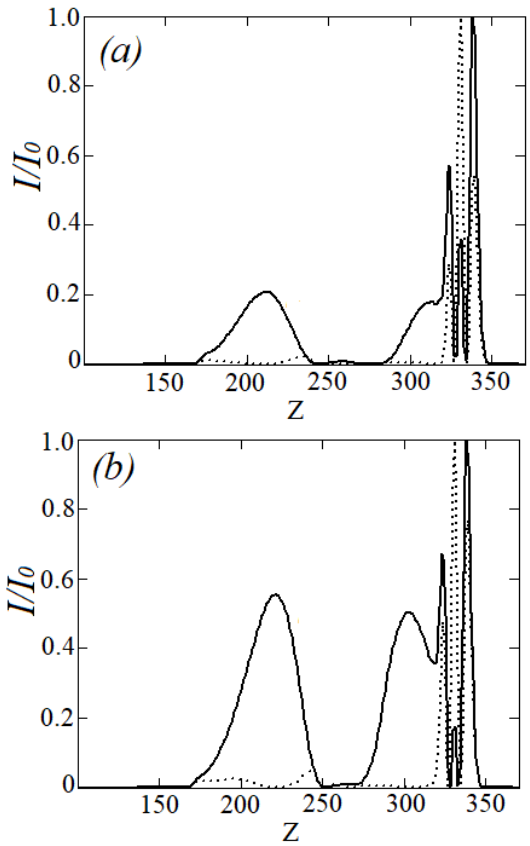

Fig. 3 – The intensity of 3D electromagnetic pulse $I(r, z, t) = E^2(r, z, t)$ (I_0 is the intensity maximum) for different values of parameter α ($\Gamma = 0.1$, $t = 10 \cdot 10^{-13}$ s: (a) scalar order parameter; (b) vector order parameter. Solid line: $\alpha = 0.1$, dotted line: $\alpha = 0.2$

An increase in the order parameter α contributes to the energy concentration in the main pulse and to a decrease in the "tail" following it. We also note that taking into account the order parameter (both scalar and vector) leads to a decrease in the pulse intensity.

It is known that, according to the Landau theory of phase transitions, the value of the parameter α is determined by the following dependence on the phase transition point: $\alpha \propto T_c - T$, where T is the phase transition temperature, T_c is the current temperature. Shown in Fig. 3 curves allow us to conclude that the pulse shape is directly determined by the distance from the phase transition point and can help to determine it. Thus, we can talk about the possibility of spectroscopy of not only the scalar, but also the vector order parameter using ultrashort electromagnetic pulses.

4. CONCLUSIONS

As a result, we can draw the following conclusions:

1. The model, which describes the evolution of three-dimensional ultrashort electromagnetic pulses in CNTs with the scalar order parameter, is generalized to the vector case.
2. It is shown, that an increase in the order parameter has a stabilizing effect on an ultrashort optical pulse, contributing to the conservation of the pulse energy in a localized region.
3. The possibility of spectroscopy of the vector order parameter using three-dimensional ultrashort optical pulses is demonstrated.

ACKNOWLEDGEMENTS

Belonenko M.B. thanks the Russian Foundation for Basic Research and the Volgograd Region Administration for support within the framework of the scientific project No. 19-43-340005; r_a. Konobeeva N.N. thanks the Ministry of Science and Higher Education of the Russian Federation for the numerical modeling and parallel computations support under the government task (no. 0633-2020-0003).

REFERENCES

1. L.D. Landau, E.M. Lifshits, *Statistical Physics* (Moscow: Fizmatlit: 2002).
2. S. Arago, J.A. Gonzalo, J. Przeslawski, *Ferroelectrics* **304**, 125 (2004).
3. C.X. Zhang, K.L. Yang, P. Jia, H.L. Lin, C.F. Li, L. Lin, Z.B. Yan, J.-M. Liu, *J. Appl. Phys.* **123**, 094102 (2018).
4. G. Catalan, *Phase Transitions.* **81**, 729 (2008).
5. K.I. Zaytsev, I.N. Fokina, A.K. Fedorov, S.O. Yurchenko,

J. Phys.: Conf. Ser. **486**, 012024 (2014).
6. S. Iijima, T. Ichihashi, *Nature* **363**, 603 (1993).
7. J. Shi, H. Chu, Y. Li, X. Zhang, H. Pan, D. Li, *Nanoscale* **11**, 7287 (2019).
8. J. Wang, K.S. Liao, D. Fruchtl, Y. Tian, A. Gilchrist, N. Alley, E. Andreoli, B. Aitchison, A. Nasibulin, H. Byrne, E.I. Kauppinen, L. Zhang, W. Blau, S. Curran, *Mater. Chem. Phys.* **133**, 992 (2012).
9. M.B. Belonenko, N.G. Lebedev, A.S. Popov, *JETP Lett.* **91** No 9, 461 (2010).
10. A.V. Zhukov, R. Bouffanais, M.B. Belonenko, I.S. Dvuzhilov, Y.V. Nevzorova, *Appl. Phys. B* **123**, 196 (2017).
11. A.V. Zhukov, R. Bouffanais, N.N. Konobeeva, M.B. Belonenko, *J. Appl. Phys.* **121**, 084301 (2017).
12. A.Z. Patashinskii, V.L. Pokrovski, *Fluctuation Theory of Phase Transitions* (Oxford: Pergamon Press: 1979).
13. A.V. Zhukov, R. Bouffanais, E.G. Fedorov, M.B. Belonenko, *J. Appl. Phys.* **114**, 143106 (2013).
14. A.V. Eletskii, *Phys.-Usp.* **40**, 899 (1997).
15. M.S. Dresselhaus, G. Dresselhaus, P.C. Eklund, *Science of Fullerenes and Carbon Nanotubes* (Cambridge: Academic Press: 1996).
16. N.S. Bakhvalov, *Numerical Methods: Analysis, Algebra, Ordinary Differential Equations* (Moscow: Nauka: 1975).

Вплив векторного параметра порядку на динаміку 3D ультракоротких імпульсів у вуглецевих нанотрубках

N.N. Konobeeva, M.B. Belonenko

Volgograd State University, 400062 Volgograd, Russia

У роботі ми пропонуємо модель для врахування векторного параметра порядку у дослідженні еволюції ультракороткого оптичного імпульсу в середовищі з вуглецевими нанотрубками. Ми розглядаємо електричне поле імпульсу в тривимірній геометрії. Для опису динаміки системи, що розглядається, ми використовуємо феноменологічну теорію, розроблену А.З. Паташинським та В.Л. Покровським. З огляду на специфіку заданої проблеми, передбачається, що векторний параметр порядку пов'язаний з електричним полем, спрямованим уздовж осі нанотрубки. Для наочності ми розглядаємо сегнетоелектричне середовище з поляризацією, яке має три ненульові просторові компоненти. Спираючись на теорію Гінзбурга-Ландау, ми отримуємо основне рівняння руху для векторного параметра порядку. На основі рівнянь Максвелла ми знаходимо ефективне нелінійне хвильове рівняння в циліндричній системі координат. Ми використовуємо наближення, коли накопиченням заряду можна знехтувати. Тому в розподілі поля зберігається циліндрична симетрія. Система цих двох рівнянь дозволяє проаналізувати залежність форми тривимірних ультракоротких оптичних імпульсів від відстані від критичної точки фазового переходу. Це важливе спостереження на практиці може бути використане для експериментального визначення критичної точки. Показано, що ультракороткий оптичний імпульс поширюється стабільно без вторинного хвильового випромінювання. Енергія електромагнітного імпульсу зберігається в локалізованій області. Також проводиться порівняльний аналіз двох моделей параметра порядку (скалярний параметр порядку та векторний параметр порядку). Визначено вплив моделі параметра порядку на динаміку імпульсу. Запропонована методика дозволяє проводити спектроскопію шляхом зміни параметра порядку при зондуванні середовища ультракороткими імпульсами.

Ключові слова: Векторний параметр порядку, Вуглецеві нанотрубки, Оптичні імпульси.