Switching waves in the course of elastic deformation by twisting

Yu D Zavorotnev\textsuperscript{1}, L S Metlov\textsuperscript{1,2}, A Yu Zakharov\textsuperscript{3} and E Yu Tomashevska\textsuperscript{4}

\textsuperscript{1}Donetsk Institute for Physics and Engineering named after A.A. Galkin, Donetsk, Ukraine
\textsuperscript{2}Donetsk National University, 83055 Donetsk, Ukraine
\textsuperscript{3}Yaroslav-the-Wise Novgorod State University, ul. B. St. Petersburgskaya, 41 173003 Veliky Novgorod, Russia
\textsuperscript{4}Donetsk Educational Institute, 83055 Donetsk, Ukraine

E-mail: zavorotnev.yuri@mail.ru

Abstract. Kink solutions of the Landau-Khalatnikov equation have been calculated in the case when elastic deformation by twisting is applied to a semi-infinite rod and a finite one. As a crystal without an inversion center was considered, Lifshitz invariants were taken into account in the thermodynamic potential. The specific features of kink propagation at varied boundary conditions, phase velocities and modulus of the torsion moment have been studied.

1. Introduction

It is known that non-linear differential equations (DE) have a few types of solutions, as a rule. Among other possible solitary-wave solutions of relaxation equation by Landau-Khalatnikov \cite{1}, kinks are of special importance because these topological solitons are stable asymptotically \cite{2} and very often structurally \cite{3}. In the present work, a kink is interpreted as a step-like solution of the wave equation. Widely spread step-like changes in a parameter that characterizes the state of the system correspond to kink solutions of a differential equation. For instance \cite{4}, it is found in the course of studying of interaction between populations of phytoplankton and zooplankton that the process of destruction of a homogeneous state and formation of a statistically steady dissipative structure is of jump-like (kink) shape. A kink is an example of a solution of autowave type. Autowaves arise in a number of media of physical, chemical and biological origin. An examples are concentration waves by Belousov-Zhabotinskii \cite{5}, the waves of chemical signalization in colonies of some microorganisms \cite{6}, waves in interstellar gas resulting in formation of spiral galaxies \cite{7}. Important references of active media are biological tissues. Neural impulse propagation \cite{8} and excitations in myocard \cite{9} are of autowave nature. In physical systems, auto model solutions of the differential equation are related to the motion of an interphase boundary during phase transitions \cite{10} or describe flame propagation \cite{11}.

2. Theory

Let us consider a highly symmetrical crystal without an inversion center. Lifshitz invariants composed by the components of the structural order parameter (OP) are distinct from zero. The density of non-equilibrium thermodynamic potential of the system (NETP) subjected to the plastic deformation by twisting (PDT) with the torsion moment M oriented along OZ axis has the form \cite{16, 17}
\[
\Phi = \frac{b_1}{2} q^2(N) + \frac{b_2}{4} q^4(N) + \frac{b_3}{6} q^6(N) + \frac{\delta_i}{2} M' \left( q_x \frac{\partial q_x}{\partial z} - q_y \frac{\partial q_y}{\partial z} \right) + \\
\frac{\delta_i}{2} M' \left( \left( \frac{\partial q_x}{\partial z} \right)^2 + \left( \frac{\partial q_y}{\partial z} \right)^2 \right) + b_4 q_x^2 q_y^2
\]

where \( \delta_i \) are phenomenological constants, \( q \) is a vector of the structural order parameter with the components \( q_x \) and \( q_y \). The order parameter is a linear combination of the displacement of ions of a unit cell due to the phase transition, by definition. The component \( q_z \) is not taken into account because the torsion moment is aligned with \( \text{OZ} \) axis. Actually, only an opportunity of emergence of shear waves is considered here. As shown in [16], \( r = 2, s = 6 \). It should be noted that the potential \( (1) \) does not include a term related to the elastic interaction. The procedure of elimination is reported in [16]. A source of non-linearity is present in \( (1) \) that is determined by Lifshitz invariants.

Suppose that the temperature of the sample is below the second-order phase transition, the signs of coefficients \( b_1 \) and \( b_2 \) are different. The dynamics of the problem is described by the system of Landau-Khalatnikov equations [1]

\[
\frac{\partial q_i}{\partial t} = -\gamma_a \frac{\delta \Phi}{\delta q_i}; \quad (i = x, y)
\]

where \( \Phi \) is the free energy functional, \( \frac{\delta \Phi}{\delta q_i} = \sum_k (-1)^k \frac{d^k}{dz^k} \frac{\partial \Phi}{\partial \left( \frac{\partial^k q_i}{\partial z^k} \right)} \) is the functional derivative [18], \( t \) is time, \( \gamma_a (i = x, y) \) are the components of the parameter that characterizes the rate of the system relaxation to equilibrium. From this point on, we suppose these components to be constant and neglect non-diagonal components for the sake of simplicity. Note that dissipation is present in equation \( (2) \) because it is noninvariant with respect to time inversion. Combining of \( (1) \) and \( (2) \) results in the following system of equations

\[
\begin{align*}
\frac{\partial q_x}{\partial t} = & -\gamma_{xx} \left[ q_x \left( b_1 + b_2 q_x^2 + b_3 q_x^4 + 2b_4 q_x^2 \right) + 2\delta_x M' \frac{\partial q_x}{\partial z} - 2\delta_x M' \frac{\partial^2 q_x}{\partial z^2} \right] \\
\frac{\partial q_y}{\partial t} = & -\gamma_{yy} \left[ q_y \left( b_1 + b_2 q_y^2 + b_3 q_y^4 + 2b_4 q_y^2 \right) - 2\delta_y M' \frac{\partial q_y}{\partial z} - 2\delta_y M' \frac{\partial^2 q_y}{\partial z^2} \right]
\end{align*}
\]

(3)

Now we shall find the auto model solutions of the system. These solutions describe the effects generated by formation of a steady state under applied PDT. In particular, damped progressing waves and a kink can appear. For this purpose, we introduce a new autonomic variable (transition to a moving coordinate system)

\[
u = z - ct
\]

where \( c \) is “undisturbed” phase velocity of the wave propagation. Transformation \( (4) \) allows finding the solutions of progressing wave type. A specific feature of these solutions is that a profile of the solution can be transformed by shear transformation into another one associated with another time. If velocity \( c \) is constant, a Cartesian coordinate system can be introduced that moves at a constant speed. The profile of the sought-for value will be steady here. It should be noted that the solutions of progressive wave type allow only autonomic equations that do not explicitly depend on independent variables [2]. So the system of partial differential equations \( (3) \) after the transition to a new variable \( \nu \) is reduced to a system of ordinary differential equations.
\[
\begin{align*}
2\gamma_{xx}\delta_2 M' \frac{dq_x}{du} - 2\gamma_{xx}\delta M' \frac{dq_x}{du} + c \frac{dq_x}{du} &= \gamma_{xx}q_x (b_1 + b_2q^2 + b_4q^4) \\
2\gamma_{yy}\delta_2 M' \frac{dq_y}{du} + 2\gamma_{yy}\delta M' \frac{dq_y}{du} + c \frac{dq_y}{du} &= \gamma_{yy}q_y (b_1 + b_2q^2 + b_4q^4) 
\end{align*}
\]

(5)

It should be noted that (5) is a system of parabolic equations. Similar equations were studied in [3] at \( b_4 = 0 \) and \( \delta = 0 \). We consider a special case of \( b_4 \neq 0 \) and \( \delta \neq 0 \). As shown in [3], solution of system (5) without Lifshitz invariants exists only at \( \gamma_{xx} = \gamma_{yy} = \gamma \). It is a wave propagating to the right at speed \( c \). It is obvious that in an object described by system (5), due to the terms with the first derivatives, friction is present. Friction depends on both speed \( c \) and torsion moment. So, any oscillations should be damped. It was shown [3], that requirements imposed on the polynomial coefficients on the right sides of (5) to realize kink solutions coincided with the existence conditions of stable (with the minimum provided) \( \Phi \) solutions of Euler equilibrium equations [3] or the right sides of system (3) equal to zero, what is the same. It is seen that system (5) has two steady solutions: 1) \( q_x = q_y = 0 \); 2) roots of the equation

\[ b_1 + b_2q^2 + b_4q^4 = 0 \]

(6)

As a structural order parameter is defined as a linear combination of atom displacements from the equilibrium positions after phase transition, zero solution is related to the highly symmetric phase. We consider different types of progressive waves that can arise in a semi-infinite rod with PDT applied to the edge. In this case the state of the medium becomes metastable at \( z \to +\infty \), i.e. before the wave front, and stable away from the front. Suppose that at \( z \to +\infty \) highly-symmetrical phase is located, the boundary conditions should be formulated as \( q_x(+\infty) = 0, q_y(+\infty) = 0 \) to provide possible kink emergence. Torsion moment can be imposed to a crystal where a phase transition over the temperature has taken place. In this case, the boundary conditions at infinity can be non-zero solutions of equation (6). As the variables in (5) are the components of the modulus of the structural order parameter, indeterminateness of the initial conditions for \( q_x \) and \( q_y \) appears because these values are parts of a functional relation. For the sake of definiteness, suppose that the boundary conditions have the form

\[ q_x(\infty) = q_y(\infty) = \frac{q}{\sqrt{2}} \]

(7)

where \( q \) is a real root of the related algebraic equation. It means that the coordinate system is selected where the vector of the structural order parameter is directed in XOY plane at an angle of \( \pi/4 \) to the axis. It should be noted that further analysis is not limited by zero boundary conditions at \( z \to +\infty \). Evolution of a kink solution with respect to the boundary conditions is considered, too. Possible emergence of a solution of progressive wave type will be studied in the case of PDT applied after the phase transition from a high-symmetric phase to a low-symmetric one.

The state of the rod behind the front is stable. Thus, we can approximate the boundary conditions at \( z = 0 \) by transition from the system of differential equations to algebraic ones and finding of the steady state at a fixed modulus of the torsion moment. The transition can be performed if the right side part of equation (3) and the left one are set to zero. An approximate solution has the form

\[ q_x = q^* \cos(kz), q_y = q^* \sin(kz) \],
where \( k \) is the propagation vector that has the only one component. Defining \( k \) as a function of the moment modulus, we find the value \( q \) of the order parameter modulus at fixed \( M \).

It should be noted that the kink rate is uniquely determined by the medium characteristics. However, no analytical method of calculation of \( c \), at the arbitrary right side of the system of equations like (5) has been developed yet. As reported in [19], the velocity can be found on the base of assumption that the energy loss by friction should be exactly equal to the difference of potentials of the system state on either side far away from the kink front. This algorithm was realized in [19] for special cases of the right side of the one-dimensional equation with a single order parameter. Based on the aforesaid, velocity \( c \) is considered further as a phenomenological parameter varied in a wide range.

3. Results and discussion. Numerical experiment

A numerical experiment allows analysis of complex combinations of solutions, not the simplest solutions to be found analytically. We consider the case of \( \gamma_{xx} = \gamma_{yy} = \gamma, \ b_4 = 0 \) and find the dependence on the boundary conditions.

1) \( q_x(0) = q_y(0) = q/\sqrt{2}, \ q_x(\infty) = q_y(\infty) = 0 \).

It has been found that a solution of system (5) exists only if the right sides are of higher order of vanishing than the left ones. When the right sides are equal to zero, the system is linear and integrable. The solution can be derived in an analytical form that is formidable and we do not write it down here. These solutions for \( q_x \) and \( q_y \) are multiplied by \( \exp(-cu/(\delta_2 M^{'}) \), so they are fast underdamped oscillations with the wavevector written as \( k = \delta_1 M^{x{-t}}/\delta_2 \). The damping depends exponentially on the phase velocity \( c \) (4), and the value of the wavevector is increased along with the torsion moment. In the case of a half-infinite rod, the result is a kink (see the dashed line in figure 1). The related curve is descending. If the rod length is finite, i.e. \( q_x(L) = q_y(L) = 0 \), and the edge of the rod is close to the area of bending at \( t = 0 \), non-linear irregularities emerge in this range (see the solid line in figure 1). In this case, the rod edge is not located in the area where the solution for an infinite rod is steady. An increase in the kink rate results in a shift of the bend area to the left and in an increase of the distance between the rod edge and the bend at \( t = 0 \). So, the irregularities become smoothed and the kink curves is monotonic. An analogous result is provided by an increase in the rod size at a constant kink rate.

2) \( q_x(0) = q_y(0) = q/\sqrt{2}, \ q_x(\infty) \neq 0, \ q_y(\infty) \neq 0, \ q_x(\infty) < q_y(0), \ q_y(\infty) < q_x(0) \).

These initial conditions mean that the twisting deformation applied after a phase transition provides a jump to a state of lower symmetry, that is characterized by higher modulus of the structural order parameter. In this case, a kink becomes deformed even if the boundary conditions are imposed at infinity (figure 2).

![Figure 1](image1.png) **Figure 1.** The dotted line is a semi-infinite rod, the solid line is a rod of finite length.

![Figure 2](image2.png) **Figure 2.** Kink after the phase transition. The kink rate is small.
A higher rate of kink propagation is associated with a smoothed curve. An increment in the torsion moment enhances the frequency of spatial oscillations. An analogous effect of an increase of the phase velocity is observed (figure 3).

As a result of twisting, a transition accompanied by a decrease in the modulus of the structural order parameter takes place. In figure 4, dependence $q(u)$ at a small phase velocity of kink propagation at zero right sides of system (5) is presented. The found process is actually a slowly propagating kink that describes a switch from a low-symmetric state to the high-symmetric one. It is seen in figure 4 that a non-stationary process is registered for a certain short time. From the viewpoint of physics, the emerging oscillations are determined by the time response of the material. The kink parameters stay almost the same at the basic stationary area.

$$q_x(0) = q_y(0) = q/\sqrt{2}, q_z(L) \neq 0,$$

$$q_x(L) \neq 0, q_y(L) > q_z(0), q_x(L) > q_y(0)$$

As mentioned above, a solution of system (5) becomes possible only in the case when the right side is small. The proper account results in small modifications of $q(u)$, as shown in figure 5. It is seen that the propagation vector of the oscillation process is reduced and the modulus of the structural order parameter rises in the area of total damping. This fact is an evidence that the solution is unstable at high $u$, as confirmed by conclusions made in [3] after theoretical analysis. When the temperature approaches the line of the phase transition, i.e. the modulus of $b_1$ decreases, the rate of divergence is reduced but not vanished at $b_1 = 0$. In Fig. 6, dependence $q(u)$ in the vicinity of the phase transition line at high torsion moment $M$ is illustrated. It is seen that the solution becomes more stable at large $u$. Mathematical explanation is that the source of instability in the right side of system (5) can be neglected at large torsion moment. Far from the phase transition line, instability growths. Besides, application of a large moment results in a substantial rise in the number of damped oscillations. It should be noted that the fitting of the moment at $b_1 \neq 0$ does not provide achievement of a stable state if $u \to \infty$ and the torsion moment is small.

![Figure 3. Kink after phase transition. The velocity of the kink is large.](image)

$$0 \quad 1 \quad 2 \quad u$$

![Figure 4. The dependence of the structural order parameter on the variable $u$ at a small value of the propagation velocity and the zero right-hand side of system (5).](image)

![Figure 5. The dependence of the structural order parameter on the variable $u$ with a small value of the propagation velocity and a non-zero right-hand side of system (5).](image)
When the phase velocity of kink propagation rises, the number of oscillations and their amplitude are sharply decreased. At the same time, the magnitude of quasi-stationary state \( q(u) \) at high \( u \) is reduced, too. In figure 7, possible dependence of \( q(u) \) at some intermediate rate of kink propagation is illustrated. Additional increase in \( u \) makes \( q(u) \) monotonically ascending and does not further modify the configuration of \( q(u) \), but reduces \( q \) that is related to the horizontal area.

![Figure 6. The dependence of the structural order parameter on the variable \( u \) for large values of the torsion moment near the PT line.](image1)

![Figure 7. The dependence of the structural order parameter at the intermediate value of the velocity of propagation of the kink.](image2)

Moving off from the phase transition line is associated with increasing \( q(u) \) \( u \) and emergence of non-zero positive derivative \( \frac{dq}{du} \) at high \( u \), that is an evidence of the stability loss.

A higher relaxation constant \( \gamma \) results in appearance of the oscillation process under the same conditions, so the curve of \( q(u) \) is analogous to that presented in figure 4.

It is reported in [5] that in the case of two-component order parameter and \( b_4 \neq 0 \), the components of the relaxation coefficient should be different. This conclusion was made when analyzing the system of equations without Lifshitz invariants. It seems that the account of the invariants provides a solution appearing at \( \gamma_{xx} = \gamma_{yy} \). The numerical analysis demonstrates that the condition of \( \gamma_{xx} \neq \gamma_{yy} \) determines a change in the rate of divergence at \( u \rightarrow \infty \), and a reduction of the rate occurs only at \( \gamma_{xx} \) falling down and rising \( \gamma_{yy} \).

4. Conclusions
   a) Undisturbed kink (switching wave) emerges only in a semi-infinite rod.
   b) Kink in a finite rod has non-linear specific features that are damped when the phase velocity is increased.
   c) If plastic deformation be twisting is applied to a crystal below the second-order phase transition temperature, stable solutions of the kink form are possible only at high torsion moment.

Acknowledgments
One of the authors (A.Yu. Zakharov) has been supported by the Ministry of Education and Science of Russian Federation within the framework of the project part of the state order (project no. 3.3572.2017/4.6).
References

[1] Lifschitz E M and Pitaevskii L P 1981 Physical Kinetics. Course of Theoretical Physics. Vol 10 (Oxford, Pergamon)

[2] Polyanin A D, Zaitsev V F and Zhurov A I 2005 Methods for solving non-linear equations of mathematical physics and mechanics (Moscow, Fizmatlit) p 254

[3] Kashcheev V N 1987 Kinks with structural phase transitions in systems with a multicomponent order parameter (Salaspils, Preprint LI–107) p 22

[4] Kurushina S E, Ivanov A A, Zhelnov Yu V, Zavershinsky I P and Maksimov V V 2010 Izvestia of the Samara Scientific Center of the Russian Academy of Sciences 12 41–50

[5] Zaikin A N and Zhabotinsky A M 1970 Nature 225 535–537

[6] Alcantara F and Monk M 1974 Microbiology 85 321–334

[7] Madore B F and Freedman W L 1987 Am. Sci. 75 252–259

[8] Gorelova N A and Bures J 1983 J. Neurobiol 14 353–363

[9] Gray R A and Jalife J 1996 Int. J. Bifurcation and Chaos 6 415–435

[10] Kashcheev V N 1986 Auto-model solutions of the diffusion-type evolution equation (Salaspils, Preprint LI–098) p 21

[11] Zeldovich Ya B, Barenblat G I, Librovich V B and Makhviladze G M 1980 Mathematical theory of combustion and explosion (Moscow: Science)

[12] Kashcheev V N 1986 Dynamics of kinks and solitary waves in a linear chain with potential \( q^4 \), \( q^6 \) (Salaspils, Preprint LI–087) p 15

[13] Khare A, Christov I C and Saxena A 2014 Phys. Rev. E 90023208

[14] Krasnyuk I B, Stefanovich L I and Yurchenko V M 2005 Physics of the Solid State 47 1740

[15] Shnir Ya M 2012 Physics of Particles and Nuclei Letters 9 745

[16] Zavorotnev Yu D, Pashinskaya E G, Varjuchin V N and Popova O Yu 2014 J. Magn. Magn. Mater. 349 244

[17] Zavorotnev Yu D and Zakharov A Yu and Metlov L S 2017 Physics of the Solid State 59 2290

[18] Zakharov V E 1982 Inverse scattering method In: Kunin I A 1982 Elastic Media with Microstructure I: One-Dimensional Models (Berlin, Heidelberg: Springer)

[19] Polak L S and Mikhaiiov A S 1983 Self-organization in non-equilibrium physicochemical systems (Moscow: Nauka) p 286