Kink and solitary waves may propagate together

A. V. Porubov and B. R. Andrievsky
Institute of Problems in Mechanical Engineering, Bolshoy avenue 61, V. O., Saint Petersburg 199178, Russia
(Received 22 October 2011; revised manuscript received 2 March 2012; published 13 April 2012)

It is shown numerically that kink-shaped and bell-shaped localized moving defects may coexist in a biatomic crystalline lattice. The shape and velocity of these waves are defined from a corresponding single wave exact traveling wave solution to the governing coupled nonlinear equations. The features of the initial conditions, or an external loading, are found that provide simultaneous propagation of these nonlinear moving defects, inputs, and their amplitudes.

DOI: 10.1103/PhysRevE.85.046604 PACS number(s): 46.40.Cd, 43.25.Dc, 43.25.Qp

I. INTRODUCTION

Knowledge of the evolution of localized defects along a crystalline structure due to an external loading is important from many points of view (e.g., for an assessment of durability). These localized defects are highly nonlinear phenomena, and corresponding coupled nonlinear equations were obtained recently to account for large rearrangements in the complex crystalline lattice [1–3]. The similar governing equations arise for the description of nonlinear processes in biatomic lattices [1,2] as well as in a molecular chain when the rotatory molecular groups with large rotations [4,5]. Studying their exact traveling wave solutions, it was found in Ref. [3] that it is the *phase velocity* (not the equations' coefficients) that defines the existence of either bell-shaped or the kink-shaped wave solutions accounting for moving defects. This is not typical for the solutions of nonlinear wave equations. Indeed, both the bell-shaped and the kink-shaped waves of a permanent shape appear as a result of some balances, and the last are defined by the structure of the equation. In particular, the bell-shaped solitary wave arises due to a balance between nonlinearity and dispersion, the celebrated example is the Korteweg–de Vries (KdV) equation. The kink-shaped wave is usually supported by a balance between nonlinearity and dissipation, here the celebrated example is the Burgers equation. However, one cannot obtain a kink-shaped solution of permanent form for the KdV equation and the bell-shaped one for the Burgers equation. There exist equations, for example, the modified KdV (mKdV) equation, that admit either bell-shaped or kink-shaped solutions, but it is the sign of the cubic nonlinear term coefficient in the mKdV equation that defines the shape of the solution (see, e.g., [6]).

Dependence on the phase velocity for the solutions of the equations from Refs. [1–3] allows us to assume the possibility of simultaneous propagation of the bell-shaped and kink-shaped waves for one and the same set of the coefficients of the governing equations. As will be seen below, suitable initial and boundary conditions may be imposed. Since the equations under study are nonintegrable, such solutions may be obtained only numerically. As noted before, only single-wave exact traveling wave solutions are known; they describe only one kind of localized waves. Nevertheless, the solutions are employed for the verification of numerical solutions and an explanation of the results. Previously we used such an analysis for the explanation of the bell-shaped strain waves' evolution and interaction [7,8].

The plan of the paper is as follows. In Sec. II known results about exact solutions to the governing equations under study will be given. Then a numerical solution accounting for simultaneous existence of the bell-shaped and kink-shaped solutions will be presented in Sec. III together with a detailed comparison with the exact solutions. Section IV is devoted to the factors affecting simultaneous waves propagation. Some conclusions will summarize the results obtained.

II. GOVERNING EQUATIONS AND THEIR EXACT LOCALIZED TRAVELING WAVE SOLUTION

The one-dimensional limit of the equations from Refs. [1–3] reads

$$\rho v_{tt} - E v_{xx} = S\,[\cos(u)]_{xx}\,, \tag{1}$$

$$\mu u_{tt} - \kappa u_{xx} = (Sv - p)\sin(u), \tag{2}$$

where $v = U_x$ describes macrostrains, u accounts for nondimensional relative micro-displacement [1–3]. The choice of the trigonometric function allows us to describe the translational symmetry of the crystal biatomic lattice.

To obtain exact traveling wave solutions to Eqs. (1) and (2) depending on the phase variable $\theta = x - Vt - x_{11}$, x_{11} is a constant phase shift, one has to resolve Eq. (1) for u [3]

$$\cos(u) = 1 - \frac{(E - \rho V^2)v - \sigma}{S}, \tag{3}$$

where σ is a constant of integration. Then the exact bell-shaped localized solutions of two kinds for $v(\theta)$ are

$$v_1 = \frac{A}{Q\cosh(k\theta) + 1}, \tag{4}$$

$$v_2 = -\frac{A}{Q\cosh(k\theta) - 1}, \tag{5}$$

whose parameters are defined for two values of σ, $\sigma = 0$ and $\sigma = -2S$ [3]. Thus, for $\sigma = 0$ we obtain

$$A = \frac{4S}{\rho\left(c_0^2 + c_L^2 - V^2\right)}, \quad Q_{\pm} = \pm\frac{c_L^2 - V^2 - c_0^2}{c_L^2 - V^2 + c_0^2}, \quad k = 2\sqrt{\frac{p}{\mu\left(c_l^2 - V^2\right)}}, \tag{6}$$

where $c_L^2 = E/\rho$, $c_l^2 = \kappa/\mu$, $c_0^2 = S^2/(p\rho)$.

As follows from Eq. (3) the first derivative of u at $\theta = 0$ may exist or does not exist. In particular, this breaking happens

TABLE I. Wave shapes for $\sigma = 0$.

V^2	$(0; c_L^2 - c_0^2)$	$(c_L^2 - c_0^2; c_L^2)$	$(c_L^2; c_L^2 + c_0^2)$	$> c_L^2 + c_0^2$
Shape of v	Tensile v_1	Tensile v_1	Compression v_2	Compression v_1
Shape of u	Kink	Bell-shaped	Kink	Kink
Choice of $Q_\pm$	Q_+	Q_-	Q_+	Q_+

for $\theta = 0$ at $\sigma = 0$ and for $Q = Q_+$. In this case the correct solution for u should be written, for example, as

$$u = \pm 2\pi \mp \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \text{ for } \quad \theta \leqslant 0, \tag{7}$$

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \text{ for } \quad \theta > 0. \tag{8}$$

However, the first derivative is zero for $Q = Q_-$ at $\theta = 0$, and the expression for u reads

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right). \tag{9}$$

The solutions (7) and (8) accounts for the kink-shaped profile of the wave u, while the solution (9) describes the bell-shaped localized wave. The choice of Q_+ or Q_- follows from an analysis of the boundedness of the exact solution [3]. These findings for $\sigma = 0$ are summarized in Table I. Therefore, the shape of u depends upon the value of the phase velocity V. A similar analysis for $\sigma = -2S$ may be found in Ref. [3]. The sign $\pm$ in the above expressions means that one wave v may be accompanied by two different waves u. In the following only the upper sign will be used.

Therefore an analysis based on the single wave exact solution predicts the existence of either a bell-shaped, Fig. 1(a), or kink shaped, Fig. 1(b), wave u that accompanies the bell-shaped wave v depending on the phase velocity V. Exact solutions should satisfy specific initial conditions in the form of these solutions at $t = 0$. Also the maximum or minimum of the solitary wave solutions v (4) and u (9) should coincide, see Fig. 1(a), as well as the "middle" point ($\theta = 0$) of the kink solutions (7) and (8) should coincide with the maximum or minimum of the bell-shaped wave v as shown in Fig. 1(b).

III. SIMULTANEOUS PROPAGATION OF KINK-SHAPED AND BELL-SHAPED WAVES

Since the shape of the wave u is not fixed by coefficients of the equations, one can suggest that waves u of different shapes might coexist traveling with their own velocities from corresponding intervals from Table I. This solution may be obtained only numerically. The standard MATLAB routine ODE45 is used to solve Eqs. (1) and (2) numerically [9]. The "kink" interval $(0; c_L^2 - c_0^2)$ is studied, and the parameters are assumed to be $S = 1$, $p = 1$, $\rho = 1$, $c_0 = 1$, $c_L = 1.6$, $c_l = 2$. Following Table I, the initial condition for v is chosen in the form (4) with $Q = Q_+$. The condition for u is used in the form slightly differing from that described by Eqs. (7) and (8), namely, $u = \pi\{1 - \tanh[k(x - x_{12})]\}$ where $k = 0.25$ is chosen to be as close as possible to the shape of the solutions (7) and (8). This choice allows us to move the initial position of u relative to that of v.

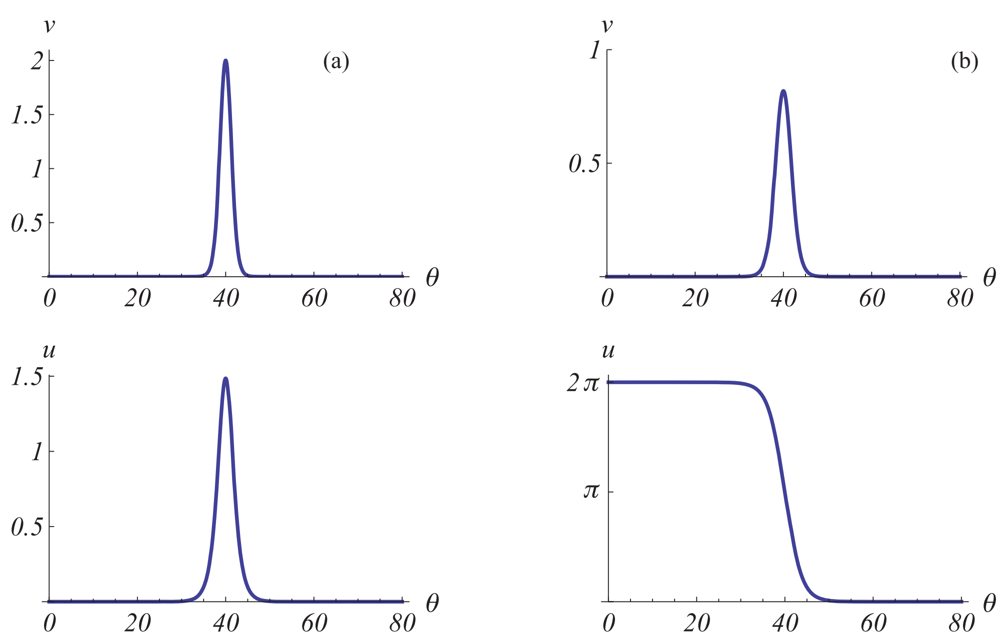

FIG. 1. (Color online) Shapes of the wave u corresponding to the bell-shaped wave v (4). (a) Bell-shaped wave (9) within the interval of velocities $(c_L^2 - c_0^2; c_L^2)$. (b) Kink-shaped wave (7) and (8) for the interval $(0; c_L^2 - c_0^2)$.

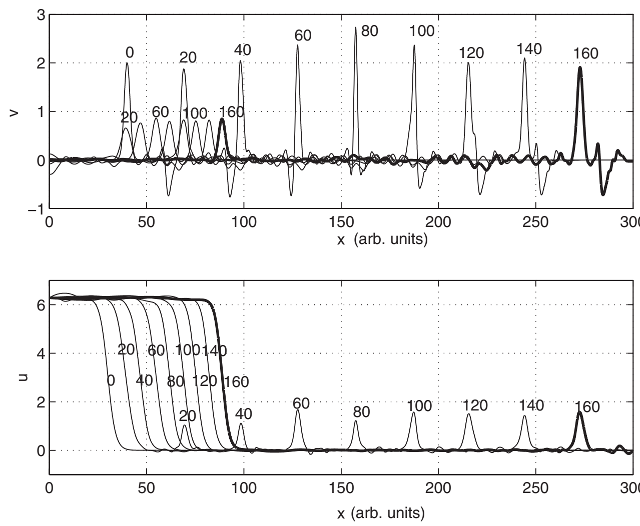

FIG. 2. Splitting of the input of u into the kink-shaped and bell-shaped parts. Initial position of the maximum of the input for v is equal to 40 ahead of that of the middle of u equal to 30. Initial velocity is chosen within the interval $(c_L^2 - c_0^2; c_L^2)$. Times are marked at the corresponding profiles. Last profiles are allocated in bold.

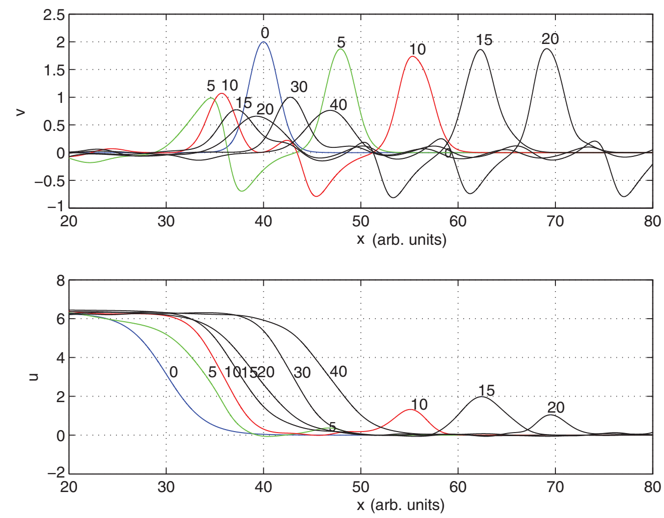

FIG. 3. (Color online) Initial stage of the waves splitting in the numerical solution. Times are marked at the corresponding profiles.

When the initial positions of the inputs coincide, $x_{11} = x_{12}$, an initial profile of u rapidly transforms to that of the exact solutions (7) and (8), and a pair of waves v and u, as in Fig. 1(b), propagates with the velocity within the interval $(0; c_L^2 - c_0^2)$ prescribed by the exact solution. Variation in the initial velocity does not affect significantly this scenario even if the square of the velocity turns out higher than $(c_L^2 - c_0^2)$. In this case the initial velocity decreases by that of the interval $(0; c_L^2 - c_0^2)$. However, the difference in the relative initial position $x_{11} \neq x_{12}$ together with the initial velocity within the interval $(c_L^2 - c_0^2; c_L^2)$ drastically changes the waves' evolution. Let us consider the case when the initial position x_{11} of the maximum of the input for v is equal to 40 ahead of that of the middle of u, x_{12}, equal to 30. The initial velocity for both inputs is chosen equal to 1.4 from the interval $(c_L^2 - c_0^2; c_L^2)$. The new phenomenon shown in Fig. 2 is that now initial profiles of u and v split into two parts. The input of u transforms into the kink-shaped part propagating with one velocity and the bell-shaped wave part whose velocity is higher. Accordingly, the input of v splits into two bell-shaped wave parts, the slower of them propagates together with the kink-shaped part of u while the faster one with the bell-shaped part of u. To study the process in detail the initial stage will be considered first, then the propagation of each part of the solution shown in Fig. 2 will be described separately, comparing it with the exact solutions.

Shown in Fig. 3 is the initial stage of splitting. One can see that the initial pulse v splits into two parts (times 5, 10, 15) around its initial position. The fast solitary wave part of v tries to propagate with the initial velocity $V_0 = 1.4$, but not with permanent amplitude, see the interval $x = 40 \div 70$. At the same time, the bell-shaped part of u is developing within the interval $x = 45 \div 75$, it propagates with the same velocity $V_0 = 1.4$, the position of its maximum coincides with that of the fast bell-shaped part of v. However, its amplitude varies in time trying to achieve some limit as seen for the following times in Fig. 2. The slow solitary wave part of v propagates together with the kink wave part of u within the interval $x = 30 \div 50$. Both the amplitude of the slower bell-shaped part of v and the slope of the kink part of u vary in time, the smaller the amplitude of v the smoother is the slope of u. The slow parts of u and v propagate with the same velocity approximately equal to 0.4. As seen in Fig. 2, further evolution (times higher than 120) demonstrates almost permanent amplitudes of the bell-shaped parts and the slope of the kink-shaped part of u. A small interaction between the bell-shaped and kink-shaped waves u happens due to coupling with the waves v, the last support corresponding waves u allowing them to survive.

A more precise measurement of velocity of the fast bell-shaped parts u and v is possible at a further stage of evolution that gives rise to 1.45, corresponding to the interval $(c_L^2 - c_0^2; c_L^2)$ prescribed by the exact solution for the bell-shaped waves' propagation. The pair kink-shaped wave u and slow bell-shaped wave v propagate with the velocity equal to 0.34 that falls in the interval $(0; c_L^2 - c_0^2)$, in an agreement with the exact solution analysis. Let us see whether more similarity with the exact solutions may be revealed. For this purpose we separate the fast and slow parts of the profiles in Fig. 2 and compare them with the corresponding exact solutions. Thus, the exact solutions (4) and (9) calculated for $V = 1.45$ is added in Fig. 4 to numerical profiles so as to combine the analytical and numerical curves, placing the maximum of the exact profiles of v and u at the point 157.44 or choosing $x_{11} = 157.44$ and $t = 0$ in the expressions of the exact solutions. Then the sequence of the exact solution profiles are put on the numerical solution for times $t = 20,40,60,80$. We see rather good agreement between the solutions and tendency of the bell-shaped part of the numerical solution to the exact single traveling wave solution. This allows us to conclude that the fast bell-shaped wave parts of u and v are nothing but the bell-shaped traveling waves accounted for in the exact solutions (4) and (7).

Similarly, the last stages of the evolution of the slow parts of v and u are examined in Fig. 5. Now the exact solutions (4), (7), and (8) for $V = 0.34$ are installed choosing $x_{11} = 54.9$ for

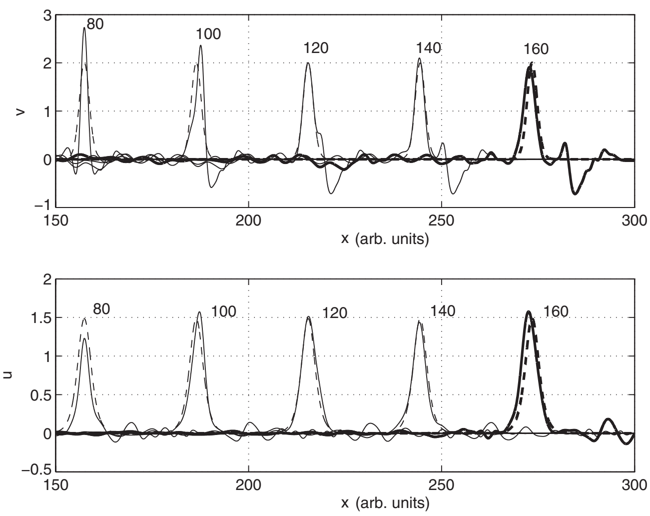

FIG. 4. Transition to the steady bell-shaped waves v and u with the velocity within $(c_L^2 - c_0^2; c_L^2)$. Shown by dashed lines are the exact traveling wave solutions (4) and (9). Times are marked at the corresponding profiles. Last profiles are allocated in bold.

their initial position. Again, further evolution demonstrates a good agreement between the exact and numerical solutions, in particular, the slope of the kink does not change anymore, contrary to the initial stage shown in Fig. 3. Then one can conclude that the slow parts of the profiles shown in Fig. 2 are recognized as the kink-shaped wave u and the bell-shaped wave v according to the exact traveling wave solutions (4), (7), and (8). Finally, simultaneous propagation of the kink-shaped and bell-shaped waves u is established where the kink-shaped and bell-shaped parts of u propagate with their own velocities according to theoretical intervals from Table I.

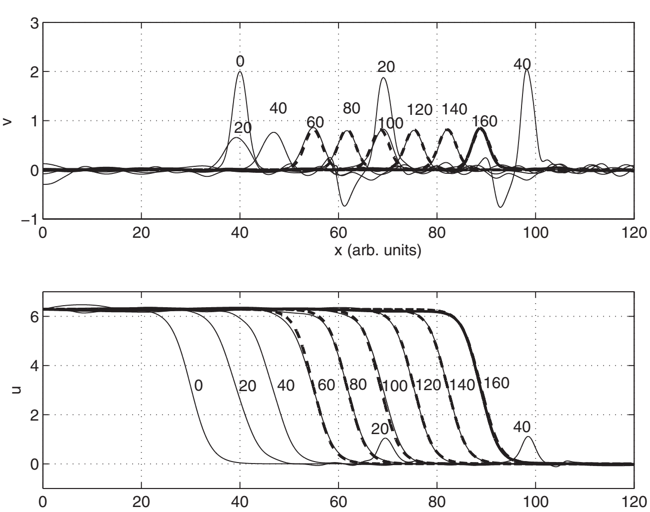

FIG. 5. Transition to the steady bell-shaped waves v and kink-shaped wave u propagating with the velocity within $(0; c_L^2 - c_0^2)$. Shown by dashed lines are the exact traveling wave solutions (4), (7), and (8). Times are marked at the corresponding profiles. Last profiles are allocated in bold.

A mathematical proof of the coexistence for long times is unlikely since the governing equations (1) and (2) are nonintegrable. Also the process shown in Figs. 2 through 5 is not governed by ordinary differential equation even at the final stage of coexistence of two waves that prevent employment of the phase portrait method. Nevertheless, we see in Figs. 4 and 5 rather stable and long time propagation of the waves; moreover, their shapes and velocities agree well with particular analytical solutions. The last exact solutions account just for thestable solitary (bell-shaped or kink-shaped) waves propagation with permanent shape and velocity.

IV. FACTORS AFFECTING SIMULTANEOUS PROPAGATION

It would be nice to present the areas of the parameters of the problem where our solutions exist. However, our equations are nonintegrable, and we have only particular traveling wave solutions that point to the possibility of the simultaneous existence of the waves of two kinds. The phase portraits analysis cannot help since the waves propagate with different velocities. Analytical solutions define only specific initial conditions required for their existence and say nothing about the deviations in them. Suitable variations in the initial conditions resulted in the simultaneous propagation of the waves of two kinds were found intuitively. Now we are going to examine the influence of variations in parameters of the initial conditions on the waves' coexistence.

As we know from the exact solution, see Table I, the kink-shaped wave u propagates provided that its velocity V (6) is less than 1.25 for our values of the parameters. However, we have chosen the initial velocity V both for u and v equal to $V_0 = 1.4$ or within the interval $(c_L^2 - c_0^2; c_L^2)$ corresponding to the bell-shaped wave propagation, see Table I. This is not fatal for the kink when $x_{11} = x_{12}$. In this case initial velocity is not kept; it decreases by the value $V_k = 1.15$ both for u and v. This velocity lies within the theoretically found interval $(0; c_L^2 - c_0^2)$. As a result, the stable propagation of the kink u and the bell-shaped solitary wave v with permanent shape and velocity is observed. Moreover, variation in the initial velocity V_0 does not affect the value of the final velocity V_k of the simultaneous propagation of the bell-shaped wave v and kink-shaped wave u. Therefore the first factor affecting the splitting is the relative distance between the inputs of u and v. When the input of v is slightly ahead that of u, only perturbations on the wave profiles are observed in comparison with the case $x_{11} = x_{12}$. An increase in the distance leads to a splitting, however, the fast solitary wave u does not propagate stably, contrary to what is shown in Figs. 2 and 4. A larger distance allows us to achieve stable propagation, but the further increase in the distance does not significantly affect the waves' evolution, only the amplitude of the fast part of v faster achieves the finite value.

The above-mentioned evolution is not realized when the kink u is initially put ahead of the bell-shaped wave v. In this case again only the disturbances on the profiles are observed at small relative initial distances. However, an increase in the distance does not lead to the formation of the stable fast bell-shaped solitary part of u. After the splitting of u and v, the fast part of v has a more or less localized character while the corresponding part of u propagates, changing not only its shape but even the sign of the amplitude.

By now the initial condition for v has been chosen in the form of the exact bell-shaped solution. Let us multiply this condition by some constant amplitude factor to see how the amplitude of v affects the splitting. The initial positions are kept $x_{11} = 40$, $x_{12} = 30$ like in Fig. 2. The factor higher than unity gives rise to a decrease in the phase velocity and an increase in the amplitude of the fast solitary wave part of u in an agreement of the exact solution. However, a decrease in the phase velocity leads to its shift into the kink-shaped wave interval $(0; c_L^2 - c_0^2)$ that results in the termination of the splitting at some value of the amplitude factor. Then only the pair of kink-shaped wave u bell-shaped wave v propagates. The factor less than unity or a decrease in the amplitude of the input for v gives rise to a gradual decrease in the amplitude of the fast wave part of u and its disagreement with the exact solution. Finally, due to the decay of it, the splitting of the inputs of u and v disappear, and only the kink u and corresponding bell-shaped solitary wave v remain.

V. CONCLUSION

The new effect, simultaneous propagation of the bell-shaped and the kink-shaped moving defects in a biatomic lattice is established. It happens because the existence of one or another wave is defined by the value of the phase velocity, not by the coefficients of the governing equations, as happens for many celebrated equations. Despite this the whole process cannot be described by the exact single traveling wave solutions, the bell-shaped and the kink-shaped parts of the numerical solutions are successfully compared separately with corresponding exact solutions. Besides a qualitative analysis, an agreement with the exact solution allows us to predict the conditions when this moving localized defect may arise and propagate along the lattice. The exact solutions account for stable wave propagation, hence the agreement with these solutions lets us hope for the stable waves' coexistence in numerical solutions for a long time. The nonintegrability of the governing equations does not allow us to provide a general mathematical analysis of simultaneous waves' evolution.

The fast bell-shaped parts u and v of the solution shown in Figs. 2 and 3 arise as a result of the evolution of the initial conditions which do not contain them at $t = 0$. Since equations (1) and (2) were obtained in Refs. [1,2] for a description of dynamic rearrangements in biatomic lattices, the appearance of the bell-shaped part of the relative distance between atoms in a lattice u accounts for the arising of a localized moving defect. Our results show that this bell-shaped localized moving defect may arise or decay in a lattice due to the propagation of a macrostrain wave v or an external loading. Variations in the loading, or variations in the amplitude of v, in its initial velocity or in its initial position relative to the input of u provide the appearance or an absence of the bell-shaped localized defect u.

ACKNOWLEDGMENTS

The work has been supported by the Russian Foundation for Basic Researches, Grants No. 12-01-00521-a and No. 10-01-00243-a.

[1] E. L. Aero, J. Eng. Math. **55**, 81 (2006).
[2] E. L. Aero and A. N. Bulygin, Mechanics of Solids **42**, 807 (2007).
[3] A. V. Porubov, E. L. Aero, and G. A. Maugin, Phys. Rev. E. **79**, 046608 (2009).
[4] G. A. Maugin, J. Pouget, R. Drouot, and B. Collet, *Nonlinear Electromechanical Couplings* (John Wiley & Sons, Chichester, England, 1992).
[5] M. K. Sayadi and J. Pouget, J. Phys. A: Math. Gen. **24**, 2151 (1991).
[6] M. J. Ablowitz and H. Segur, *Solitons and the Inverse Scattering Transform* (SIAM, Philadelphia, 1981).
[7] A. V. Porubov and B. R. Andrievsky, Commun. Nonlinear Sci Numer Simulat **16**, 3964 (2011).
[8] A. V. Porubov, G. A. Maugin, and B. R. Andrievsky, Wave Motion **48**, 773 (2011).
[9] L. F. Shampine and M. W. Reichelt, SIAM J. Sci. Comput. **18**, 1 (1997).