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Lattice modelling of nonlinear waves in a bi-layer with delamination

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Abstract

A lattice model consisting of two one-dimensional periodic chains with linear links between elements and nonlinear interaction between the chains is suggested to study nonlinear dynamics of a bi-layer. The properties of the model are discussed, and the influence of a delamination zone on the propagation of solitary waves is studied numerically.

Keywords: bi-layer, delamination, Frenkel-Kontorova model, coupled Klein-Gordon equations, nonlinear waves.

1 Introduction

Combination of two materials with different properties are broadly used to obtain a structure with the properties better than that of the parent constituents. Integrity of such layered structures is mainly determined by the quality of their interfaces. A sharp change in material properties at the interface and different deformation behavior under loading can result in considerable stress concentrations near interfaces leading to delamination and cracking. These processes not only affect functionality of structures but can also cause their total failure. The possibility of delamination zone development practically without any visible signs up to its catastrophic manifestation complicates the interface quality control and necessitates an elaboration of advanced detection methods for delamination zones and investigation of conditions for their propagation.

The problem of the interface crack growth belongs to the basics of the mechanics of fracture (see, for example, [1, 2]). Usually the possibility of the crack growth is related to the energy balance between the energy release due to cracking and crack resistance forces (known as fracture toughness). However, this purely phenomenological approach becomes rather cumbersome when applied to heterogeneous materials with different properties.

Another way of crack analysis based on a direct introduction of the atomic microstructure into consideration, which is now being actively developed [3], is still limited to relatively small volumes and selected types of materials. Expansion of this approach to macroscopic volumes of real materials with various relaxation properties is nowadays hardly possible.

To overcome limitations of both approaches, new ideas were suggested both in mechanical and physical communities based on lattice models representing solids as a lattice of elements larger than atoms and molecules. Here, fracture is introduced as vanishing links between respective elements ([4, 5, 6] and references there). An additional advantage of lattice models is their suitability for numerical simulations, with lattice algorithms being developed to solve various types of equations.

Design of new schemes of delamination diagnostics for bi-materials necessitates a considerable enhancement of existing methods of non-destructive evaluation. Recent developments in this area are linked with understanding nonlinear effects accompanying propagation of waves of finite amplitude in solids. Nonlinear methods are considerably more sensitive to damage-induced changes in structures than standard schemes using linear material parameters (wave speed, damping, etc.) [7].

A mathematical background of this study is rooted in the theory of nonlinear differential equations and respective numerical algorithms. After the intensive study of nonlinear wave processes in recent decades, it has become clear that the same equations such as, for instance, the Korteweg - de Vries equation or nonlinear Schrödinger equation, appear in many different physical situations (see, e.g., [8], [9] and the references there). Since heterogeneity constitutes an essential feature of many physical problems, it makes sense to try to find some suitable mathematical models which will allow us to study features of nonlinear wave processes in heterogeneous media. A possible way to derive such continuum models is to consider the long-wave dynamics of lattice models for bi-layers.

2 The model of a bi-layer

We study one-dimensional nonlinear dynamics of a bi-layer using the model of coupled chains of particles [10], i.e., two one-dimensional periodic chains aligned along the x-axis with linear links between elements and nonlinear interaction between the chains are considered, which is the natural generalization of the Frenkel-Kontorova (FK) model [11]. It is assumed that particles may move only parallel to the x-axis. The mass of any particle of the "upper" chain is m_1 and that of the "lower" chain is m_2. In equilibrium the distance between adjacent particles in each chain is a. Interaction between the nearest neighbors in the chains is considered in terms of the usual harmonic approximation (with different constants of interaction β_1 and β_2). The function determining interaction between the chains is assumed to depend on displacements of pairwise corresponding particles of the "upper" and the "lower" chains. The choice of this function is determined by the interface type.

Let u_n and w_n be displacements of the n-th particle of the "upper" and "lower" chains, respectively, and $H(u_n, w_n)$ be the energy of interaction between these particles. Dynamics of the system is described by the following equations

$$\begin{aligned} m_1\ddot{u}_n &= \beta_1(u_{n+1} - 2u_n + u_{n-1}) - H_{u_n}(u_n, w_n), \\ m_2\ddot{w}_n &= \beta_2(w_{n+1} - 2w_n + w_{n-1}) - H_{w_n}(u_n, w_n) \end{aligned} \tag{1}$$

(dots stand for differentiation with respect to time).

Introducing dimensionless variables

$$\tilde{t} = \frac{c_1}{a}t, \quad \tilde{x} = \frac{x}{a}, \quad \tilde{u} = \frac{u}{a}, \quad \tilde{w} = \sqrt{\frac{m_2}{m_1}}\frac{w}{a}, \quad \tilde{H} = \frac{H}{m_1 c_1^2},$$

and using the force function $f(\tilde{u}, \tilde{w}) = -\tilde{H}(\tilde{u}, \tilde{w})$, in the long-wave approximation we obtain from (1) the system of coupled Klein-Gordon equations (the tilde is omitted)

$$u_{tt} - u_{xx} = f_u(u, w), \quad w_{tt} - c^2 w_{xx} = f_w(u, w), \tag{2}$$

where $c = c_2/c_1 = \sqrt{\beta_2 m_1/\beta_1 m_2}$ is the ratio of acoustic velocities of non-interacting components, $c_i^2 = \beta_i a^2/m_i, i = 1, 2$, and $f(u, w)$ describes interaction between the chains.

Similar two-component models were proposed to describe dynamics of hydrogen-bonded chains, molecular crystals and polymer chains, etc. (see review [12]), and also in connection with the crack

propagation in solids (e.g., [6, 13, 14]). It's also worth noting that similar equations describe some processes in the DNA double helix [15] (see also [16] and the references there).

The function $f(u,w)$ in (2) describing the energy of the glue bond should be found experimentally, and therefore its analytic form is not unique. It makes sense to approximate, if possible, the experimental data by a function allowing a certain analytic study of the properties of equations. It is known that the existence of a sufficiently large group of symmetries allows such an investigation (see, for example, [19], [20]). Thus, the group classification problem for the coupled Klein-Gordon equations (2) naturally arises in connection with the above discussed model.

Equations of type (2) with $c=1$ (and arbitrary functions of u and w in the right-hand side) were studied in [17] where cases admitting Lie-Bäcklund symmetries were found, and completely or partially integrable examples were presented. If $f_{uw}(u,w)=0$, system (2) splits into two independent Klein-Gordon equations, whose group classification was given by S. Lie [18]. The Lie group classification of equations (2) for $c\neq 1$, $f_{uw}(u,w)\neq 0$ was carried out in [10].

It was proven that the admitted algebra of infinitesimal operators can only have dimension 2, 3, 6, 7 and be infinite-dimensional in the case of linear equations. The 6-dimensional algebra is admitted if the function $f(u,w)$ has one of the following forms (up to the equivalence transformations, see [10]):

- $f(u,w)=F(z)+Auw+(\varepsilon-\delta A)\dfrac{u^2}{2},\quad F'''(z)\neq 0;$
- $f(u,w)=F(z)+\varepsilon uw-\delta\varepsilon\dfrac{u^2}{2},\quad F'''(z)\neq 0;$
- $f(u,w)=F(z)+Au,\quad F'''(z)\neq 0.$

Here $z=\delta u-w$, A is an arbitrary constant, $\varepsilon=\pm 1$, δ is an arbitrary positive constant. The seven-dimensional algebra is admitted in the last case if, additionally, function $F(z)$ has one of the following four forms:

- $F(z)=\varepsilon z^{\sigma}+Bz,\quad \sigma\neq 0,1,2,$
- $F(z)=\varepsilon e^{z}+Bz,$
- $F(z)=\varepsilon\ln z+Bz,$
- $F(z)=\varepsilon z\ln z,$

where B and σ are arbitrary constants. The corresponding infinitesimal operators of the groups and the complete classification results can be found in [10].

System (2) with an arbitrary function $f(u,w)$ can be formulated by means of the Lagrangian principle from the density

$$L=\frac{1}{2}(u_t^2+w_t^2-u_x^2-c^2w_x^2)+f(u,w).$$

Therefore, knowing infinitesimal operators of the groups and using the Nöther theorem, one can find conservation laws (see, for example, [20]). The shifts in t and x are admitted with any function $f(u,w)$. The corresponding conservation laws for energy and momentum have the form

$$D_t[\frac{1}{2}(u_t^2+w_t^2+u_x^2+c^2w_x^2)-f(u,w)]-D_x[u_tu_x+c^2w_tw_x]=0,$$
$$D_t[u_tu_x+w_tw_x]-D_x[f(u,w)+\frac{1}{2}(u_t^2+w_t^2+u_x^2+c^2w_x^2)]=0.$$

In the cases with the dimension of the admitted algebra larger than 2, there are additional conservation laws, which can be easily written down explicitly (e.g. [20]) and that are useful for the application of various asymptotic methods and in numerical simulations.

When the potential function is $f(u,w)=\cos(\delta u-w)-1$, system (2) reduces to the coupled sine–Gordon equations:

$$u_{tt}-u_{xx}=-\delta^2\sin(u-w),\quad w_{tt}-c^2w_{xx}=\sin(u-w),\tag{3}$$

where the variable u replaces δu, compared to system (2). Although this case is not the most beneficial from the point of view of admitted symmetries (6-dimensional algebra of operators), it is interesting as

a possible generalization of the Frenkel–Kontorova model [11] (see also [12]). Unlike the latter, where the shear of one part of a crystal is considered with respect to the rigid base, system (3) is derived on the assumption that both parts of the crystal are deformable. In model (3) the dimensionless parameter $\delta^2 = m_2/m_1$ is equal to the ratio of masses of particles in the "lower" and "upper" parts of the crystal. For $\delta^2 \to 0$ and $u = 0$, system (3) reduces to the sine–Gordon equation for the variable w. Thus, there is a natural limit to the Frenkel–Kontorova model. Let also notice that system (3) with $c = 1$ was proposed to describe the open states in the DNA [15].

Invariant solutions for system (3) and solutions describing its dynamics in the presence of additional shear forces were constructed in [10]. The particular case of these solutions is periodic traveling-wave solutions, which have the following form:

$$u = U \arcsin\{k \text{ sn } [\sqrt{\lambda}(x - vt + x_0), k]\} = Ww, \quad 0 < k < 1,$$
$$U = \frac{2\delta^2(v^2 - c^2)}{\delta^2(v^2 - c^2) + v^2 - 1}, \quad W = \frac{\delta^2(v^2 - c^2)}{1 - v^2},$$

for "fast" waves, propagating with velocities $v^2 \in]S, M[\cup]L, +\infty[$, where $S = \min\{1, c^2\}, M = \frac{1 + \delta^2 c^2}{1 + \delta^2}, L = \max\{1, c^2\}$, and x_0 is a constant,

$$u = U \arcsin\{\text{dn } [\sqrt{|\lambda|}(x - vt + x_0), k]\} = Ww, \quad 0 < k < 1,$$

for "slow" waves, propagating with velocities $v^2 \in [0, S[\cup]M, L[$. In the limiting case of $k = 1$, "slow" periodic waves become solitary waves (kinks):

$$u = U \arctan\{\exp \sqrt{|\lambda|}(x - vt + x_0)\} = Ww. \tag{4}$$

Using the fact that equations (3) admit reflections

$$t \to -t, \quad x \to x; \qquad t \to t, \quad x \to -x; \qquad u \to -u, \quad w \to -w;$$

one can obtain solutions with other combinations of signs.

If $\delta \to 0$ ($m_1 \gg m_2$), solitary waves may propagate with velocities $v^2 \in [0, c^2[$. In that case the displacement of particles is independent of the wave propagation velocity. If the masses m_1 and m_2 are comparable, the solitary waves may propagate with velocities $v^2 \in [0, S[\bigcup]M, L[$. Therefore, if the acoustic velocities of non-interacting chains are different ($c^2 \neq 1$), a gap appears in the velocity spectrum of the solitary waves, i.e. the system acts as a filter of solitary waves. Here the relative displacement ("upper" particles relative to the "lower" ones) remains the same as in the FK model (per period of the chain), but the absolute displacement depends on the velocity of the wave.

Another essential feature of the considered system is a possibility of the energy exchange between its physical components (see [22]), in particular, in the situation when one component is initially excited (say, u) with another component (w) being initially at rest. Periodic and quasi-periodic processes in the wave system (3) are analogous to the energy exchange in a system of coupled pendulums in classical mechanics [23] (see also [24]).

The energy exchange between two components u and w of the system (3) takes place since different branches of the dispersion curve coexist for the same wavenumber k. Here we briefly discuss only a particular nonlinear solution of these equations for $c = 1$. Consideration of the general case and the analysis details, such as conditions of the full and partial energy exchange, can be found in [22].

An exact solution describing the energy exchange between two components u and w of system (3) can be constructed if $c = 1$, i.e., if the acoustic velocities of both chains coincide. In this case, by introducing the new variables:

$$p = u - w, \ q = u + \delta^2 w,$$

system (3) can be transformed to the form:

$$p_{tt} - p_{xx} = -(1 + \delta^2) \sin p, \quad q_{tt} - q_{xx} = 0.$$

The system decomposes into the sine–Gordon equation uncoupled from the linear wave equation. As a result, the explicit two-wave solution describing the energy exchange between the two components u and w can be found in terms of Jacobi elliptic functions:

$$\begin{aligned} u &= \frac{2}{1+\delta^2}\left[\arcsin\,\phi_1 + \delta^2 \arcsin\,\phi_2\right], \\ w &= \frac{2}{1+\delta^2}\left[\arcsin\,\phi_1 - \arcsin\,\phi_2\right], \\ \phi_{1,2} &= \kappa\ \mathrm{sn}(kx - \omega_{1,2}t + \theta_0, \kappa). \end{aligned} \tag{5}$$

Here $\omega_1 = k, \omega_2 = \sqrt{1+\delta^2+k^2}$ are two branches of the dispersion curve, κ is the modulus ($0 < \kappa < 1$), and θ_0 is a constant. When $\delta^2 = 1$, it can be shown that the nonlinear solution (5) describes a full periodic exchange of energy between the two components of the system. Indeed, in this case, using the addition theorems for elliptic functions (e.g., [21]), (5) can be transformed to the form:

$$\begin{aligned} u &= \arcsin\left[2\kappa\ \mathrm{cn}(\gamma_- t, \kappa)\ F_1(t,x)/\Phi(t,x)\right], \\ w &= \arcsin\left[2\kappa\ \mathrm{sn}(\gamma_- t, \kappa)\ F_2(t,x)/\Phi(t,x)\right], \end{aligned} \tag{6}$$

where

$$\begin{aligned} F_1(t,x) &= \mathrm{dn}(kx - \gamma_+ t + \theta_0, \kappa)\ \mathrm{sn}(kx - \gamma_+ t + \theta_0, \kappa), \\ F_2(t,x) &= \mathrm{dn}(\gamma_- t, \kappa)\ \mathrm{cn}(kx - \gamma_+ t + \theta_0, \kappa), \\ \Phi(t,x) &= 1 - \kappa^2\ \mathrm{sn}^2(\gamma_- t, \kappa)\ \mathrm{sn}^2(kx - \gamma_+ t + \theta_0, \kappa). \end{aligned}$$

Here $\gamma_\pm = (\omega_2 \pm \omega_1)/2$. Since the Jacobi function $\mathrm{dn}(z,\kappa)$ has no zeros on the real axis, zeros of the nonlinear solution (6) coincide with zeros of the functions $\mathrm{cn}(z,\kappa)$ and $\mathrm{sn}(z,\kappa)$. Zeros of the function $\mathrm{sn}(z,\kappa)$ on the real axis are located at the points $z = 2mK$, while those of the function $\mathrm{cn}(z,\kappa)$ are located at the points $z = (2n-1)K$, where $m, n \in Z$, and

$$K = \int_0^{\pi/2} (1 - \kappa^2 \sin^2\phi)^{-1/2} d\phi$$

is the complete elliptic integral of the first kind. The real period of these functions is equal to $4K$. The time of the energy exchange from one component to another is $T = K/\gamma_-$. The nonlinear two-wave solution (6) is shown in Fig. 1 for $c = 1$, $\delta = 1$, $k = 1.6$, and $\kappa^2 = 0.99999$.

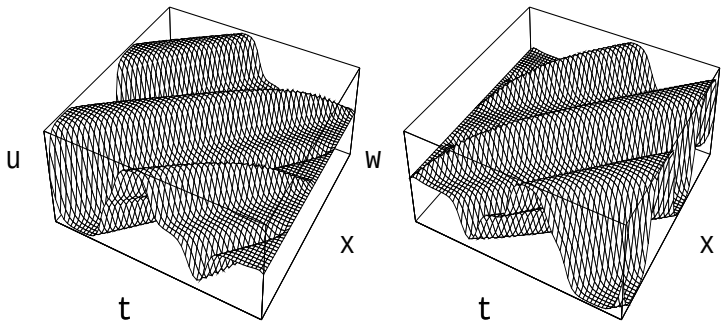

Figure 1: Energy exchange in the nonlinear two-wave solution (6).

The exact solution of system (3) for the periodic energy exchange is found only for $c = 1$. This condition is very restrictive. In general case, it is possible to construct weakly nonlinear two- and four-wave (for two pairs of counter-propagating waves) solutions describing the energy exchange between

two components u and w. In [22] the weakly nonlinear solutions are found with the use of asymptotic methods [25] by reduction of the coupled sine–Gordon equations (3) to the coupled nonlinear Schrödinger equations, which are derived for a slow spatio-temporal evolution of wave amplitudes.

The situation when the linear dispersion relation has two or more branches for the same wavenumber is typical in composites. The energy exchange between the physical components of the system (the layers) constitutes the essential feature of dynamics of bi-layered structures. It would be interesting to study the energy exchange processes in other physical systems admitting a similar dispersion relation. For example, the attractive candidate is the sine-Gordon–d'Alembert systems introduced in the study of the propagation of magnetoacoustic domain walls in elastic ferromagnets [26] and electroacoustic walls in elastic ferroelectrics [27] (see also [28]).

3 Kink in a bi-layer with delamination

We now suppose that a bi-layer has a delamination zone and are going to study its influence on nonlinear dynamics of a bi-layer. As an example, we have chosen the propagation of the solitary wave (kink) discussed in Section 2.

It should be noted that many features of the soliton-impurity interaction have been extensively studied within the framework of such models as the sine-Gordon equation or the discrete FK model with local or extended inhomogeneities (see review [12] and the references there). Soliton scattering by impurities in hydrogen-bonded chains has been studied in [32]. In recent years there has been an increasing interest to the behavior of breathers in presence of a defect ([29, 30, 31] and references there) in connection with the processes in DNA.

A major difficulty in the application of lattice models to real physical or biological processes is in the derivation of the interaction potentials and parameters of the model. In the case of bi-layers, this should (and can) be done experimentally. In this paper, we consider a simple model situation close to the FK model to study the potential applicability of nonlinear waves to the problems of the interface control in bi-layers.

Any of the known solutions of (3), appropriately rewritten, yields an approximate solution of the corresponding discrete equations, which are written bellow. In the case of a kink described by (4), such an approximate solution has the form

$$u_n \approx \tilde{u}_n = \frac{a}{\pi} U \arctan\{\exp[\varepsilon\alpha(n - v\sqrt{\frac{\beta_1}{m_1}}t + n_0)]\}, \quad w_n \approx \tilde{w}_n = \tilde{u}_n/W,$$
$$\alpha = \sqrt{|\lambda|\frac{2\pi\tau m_1}{a\beta_1 m_2}}, \quad \lambda = \frac{\delta^2(v^2-c^2)+v^2-1}{(v^2-1)(v^2-c^2)}, \quad \varepsilon = \pm 1, \tag{7}$$

where $\alpha a \ll 1$ to provide the condition $|u_{n+1} - u_n| \ll 1$ (the long-wave solution) and n_0 is a constant. Here τ is the constant of the chain interaction, $\varepsilon = -1$ corresponds to the kink, and $\varepsilon = 1$ corresponds to the antikink.

Using solution (7) with $\varepsilon = -1$ and $n_0 = 40$ as the initial condition for the corresponding discrete equations, we study numerically the following problem:

$$m_1\ddot{u}_n = \beta_1(u_{n+1} - 2u_n + u_{n-1}) - \tau\sin(2\pi\frac{u_n - w_n}{a}),$$
$$m_2\ddot{w}_n = \beta_2(w_{n+1} - 2w_n + w_{n-1}) + \tau\sin(2\pi\frac{u_n - w_n}{a}),$$
$$\text{for} \quad -N-1 \le n \le -K-1 \quad \text{and} \quad K+1 \le n \le N-1;$$

$$m_1\ddot{u}_n = \beta_1(u_{n+1} - 2u_n + u_{n-1}),$$
$$m_2\ddot{w}_n = \beta_2(w_{n+1} - 2w_n + w_{n-1}),$$
$$\text{for} \quad -K \le n \le K;$$

$$\ddot{u}_{-N} = \ddot{\tilde{u}}_{-N}(t), \quad \ddot{u}_N = \ddot{\tilde{u}}_N(t),$$

$$\ddot{w}_{-N} = \ddot{\tilde{w}}_{-N}(t), \quad \ddot{w}_N = \ddot{\tilde{w}}_N(t);$$

$$u_n|_{t=0} = \tilde{u}_n(0), \dot{u}_n|_{t=0} = \dot{\tilde{u}}_n(0),$$
$$w_n|_{t=0} = \tilde{w}_n(0), \dot{w}_n|_{t=0} = \dot{\tilde{w}}_n(0),$$
$$\text{for} \quad -N \le n \le N.$$

Here N and K correspond to half-lengths of a bi-layer and crack (delamination), respectively. The boundary conditions are chosen in accordance with the approximate solution (7).

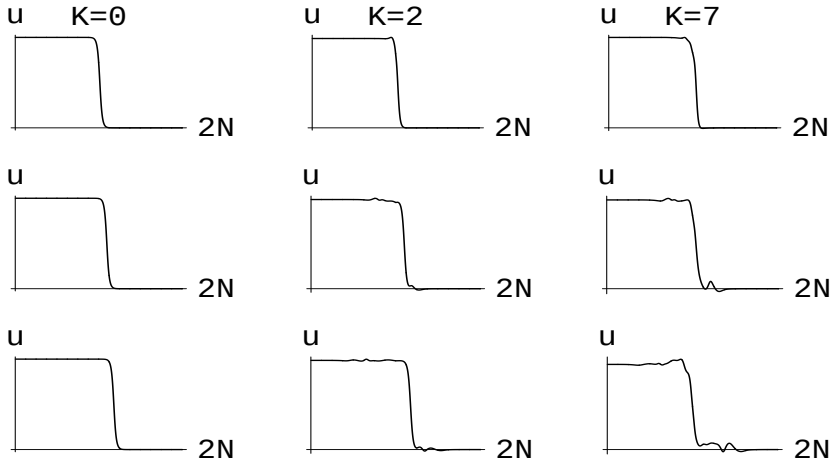

Figure 2: The u-wave for $v = 0.5$ at three consecutive moments of time ($t = 4, 7,$ and 10).

Numerical experiments show the sensitivity of the nonlinear wave to the length of the delamination zone. Fig. 2 and 3 demonstrate numerical results for u and w correspondingly for $K = 0$ (no crack), $K = 2$, and $K = 7$ (a longer crack). In all cases $N = 400$. In each figure we compare the wave propagating in an ideal bi-layer (without a defect) with the case of delamination for $c = 1.58114, \delta = 2$ ($m_1 = 0.02, m_2 = 0.08, \beta_1 = 10, \beta_2 = 100, \tau = 0.001, a = 0.05, v = 0.5$). Here $\alpha a \approx 0.00674 \ll 1$.

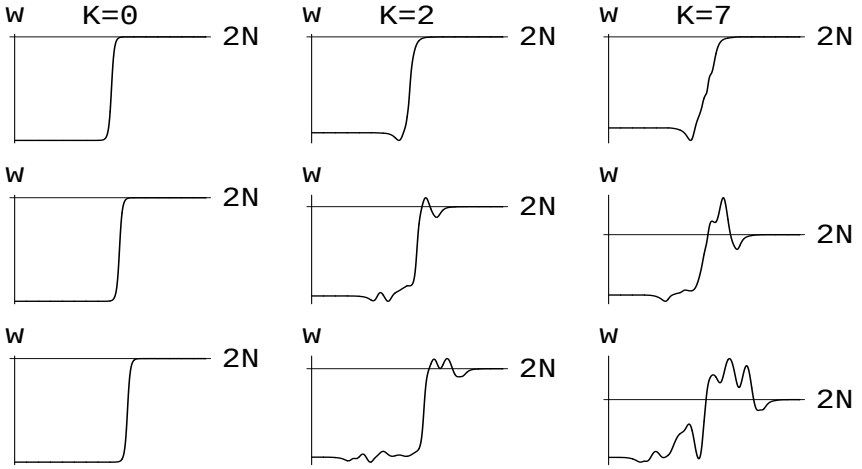

Figure 3: The w-wave for $v = 0.5$ at three consecutive moments of time ($t = 4, 7,$ and 10).

The figures demonstrate typical distortions of the wave form and the kink trapping by a sufficiently long delamination zone (at the given wave speed), accompanied by a strong radiation. Note that for the

chosen values of parameters the w-wave, which is less intensive than the u-wave, is much more sensitive to the interface crack than the u-wave. However, the kink is able to pass the delamination zone and to propagate further at higher wave speed, as shown in Fig. 4 and 5 for u and w correspondingly for the same values of all the parameters but the wave speed: $v = 0.8$.

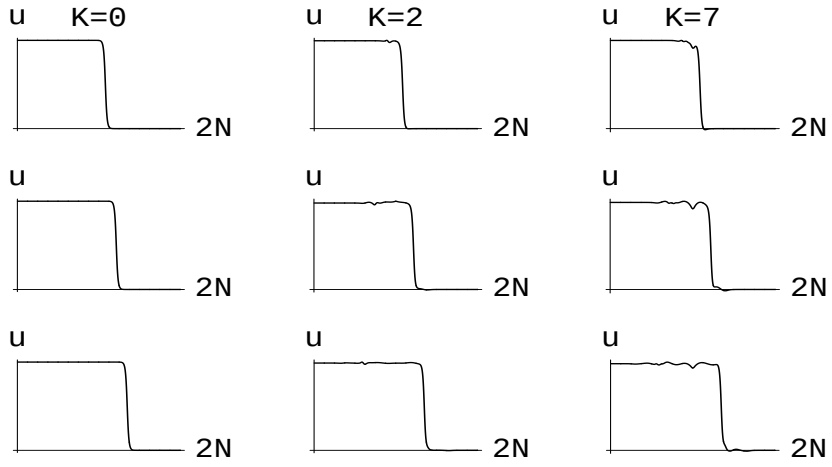

Figure 4: The u-wave for $v = 0.8$ at three consecutive moments of time ($t = 4, 7,$ and 10).

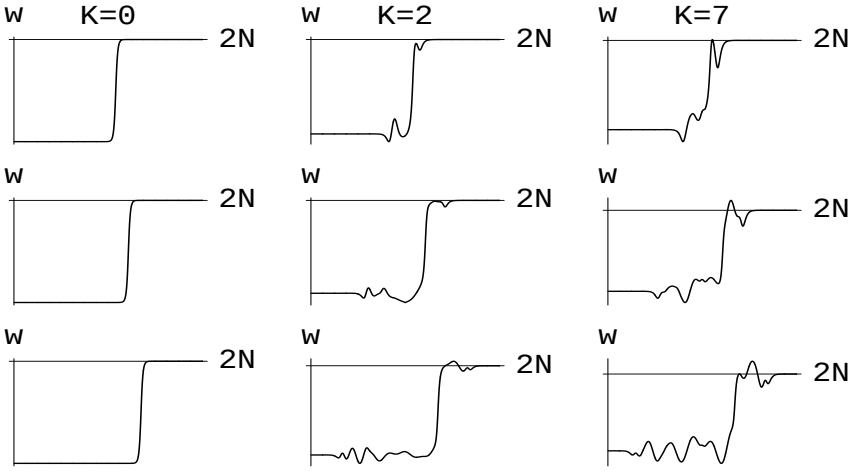

Figure 5: The w-wave for $v = 0.8$ at three consecutive moments of time ($t = 4, 7,$ and 10).

These results indicate the potential applicability of nonlinear waves to detection of delamination zones in bi-layers and invite further detailed studies (numerical, analytical and experimental). The problem of particular interest is the interaction of the wave propagating in the material with the separation wave. All this will be the topic of our further study.

4 Conclusion

The lattice model discussed here can be used to study characteristic features of propagation and interaction of nonlinear waves in bi-layers with delamination. The model can be modified to take

into account other degrees of freedom by considering the chains of interacting mechanical dipoles [33] instead of chains of point masses. It can also be two-dimensionalized.

Bi-material structures have been used for decades in various applications that need a combination of properties, which cannot be found in a single material. Now their increasing use is mainly due to new developments in aerospace industry and microelectronics. Composite-metal, polymer-metal, ceramic-metal, composite-composite bi-layers with various interfaces are hardly appropriate for a routine use of traditional modelling and diagnostic tools. On the other hand, nonlinear effects in such systems can provide an additional information on their behavior under various loading conditions, thus, forming the basis for new methods of damage examination which – after their experimental validation – can be used in new procedures for analysis of structural integrity, safety and reliability.

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