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Influence of coupling on nonlinear waves localization

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ABSTRACT

Generation of bell-shaped localized wave solutions to nonlinear coupled equations is studied numerically. It is shown how predictions of the known exact traveling wave solutions may help in understanding and explanation of arising of localized wave solutions of permanent shape and velocity in numerical solution. It is found that just coupling gives rise to changing of the sign of the amplitude of the localized bell-shaped wave.

1. Introduction

It is known that propagation of localized nonlinear waves of permanent shape is supported by a balance between various factors described by the terms of the governing equation. In particular, bell-shaped or solitary wave usually exists thanks to a balance between nonlinearity and dispersion. Sometimes non-integrable nonlinear equations have exact traveling wave solutions accounting for bell-shaped localized waves. They are too restrictive and require specific initial conditions. However, an analysis of the parameters of these solutions allows us to define the conditions for the coefficients of the equation when such solutions may exist. This information turns out valuable for a numerical simulations since rather arbitrary initial condition may evolve into a sequence of solitary waves, and each of them is governed by an exact solution provided that the conditions for coefficients are satisfied. Direct numerical simulation (without use of exact solutions) may result in missing one or another possibility of the wave localization.

Considerable progress in such combined analytical and numerical study is achieved for single nonlinear equations. However, many problems are described by coupled equations. Coupling is another factor affecting wave localization what we are going to demonstrate further. The equation under study comes from the theory of microstructure where coupling between macro- and micro-strains happens. Thus, the rotatory molecular groups were added to the usual one in atomic chain in Refs. [1,2], and large rotations were considered. A more complicated internal motion was modeled in Refs. [3–5], where translational internal motion was studied.

The governing equations in both problems are similar. Here we consider the one-dimensional limit of equations from Refs. [3–5] accounted by the coupled equations of the form,

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

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

where $v = U_x$ describes macro strains, u accounts for non-dimensional relative micro-displacement [3–5]. Choice of the trigonometric function allows us to describe translational symmetry of the crystal lattice, however is choice is not unique,

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another one may be found in Ref. [6]. In our case at $S = 0$ there is no coupling, and Eq. (1) becomes usual linear wave equation. It will be seen later that for nonzero S the governing equation for v contains both dispersion and nonlinear terms that makes possible a balance between them yielding a bell-shaped or solitary wave solution.

The plan of the paper is as follows. In the first section we remind known exact traveling wave solutions of Eqs. (1) and (2). Then in Section 2 we perform numerical simulations to see how initial conditions affect the localization of the wave and how exact solutions may help to explain numerical results. The new effects caused by coupling will be revealed.

2. Exact localized bell-shaped solutions

To obtain exact traveling wave solutions to Eqs. (1) and (2) depending on the phase variable $\theta = x - Vt$ one has to resolve Eq. (1) for u by

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

where σ is a constant of integration. The Eq. (2) is integrated once, multiplied by u_θ and integrated again. Using Eq. (3) one obtains an ordinary differential equation (ODE) for the function $v(\theta)$,

$$v_\theta^2 = a_0 + a_1 v + a_2 v^2 + a_3 v^3 + a_4 v^4. \tag{4}$$

The relationships for the coefficients may be found in Ref. [5]. Hence v satisfies ODE with power nonlinearity. The well-known integrable Gardner equation [7–10],

$$v_t + q_1 v v_x + q_2 v^2 v_x + q_3 v_{xxx} = 0 \tag{5}$$

possesses the same ODE for its traveling wave solutions as well as the equation,

$$v_{tt} - a v_{xx} - c_1 (v^2)_{xx} - c_2 (v^3)_{xx} + b_1 v_{xxtt} - b_2 v_{xxxx} = 0 \tag{6}$$

obtained in Refs. [11–13] for longitudinal nonlinear strain waves. Dispersion terms $q_3 v_{xxx}$ in Eq. (5) and $b_1 v_{xxtt}$, $b_2 v_{xxxx}$ in Eq. (6) ensure the term v_θ^2 in ODE (4). In our case this dispersion term arises thanks to the coupling.

When $a_0 = 0$, $a_1 = 0$, the ODE (4) possesses known exact bell-shaped localized solutions of two kinds that may be obtained by direct integration [7,8],

$$v_1 = \frac{A}{Q\cosh(k\theta) + 1}, \tag{7}$$

$$v_2 = -\frac{A}{Q\cosh(k\theta) - 1}. \tag{8}$$

The parameters are defined for two values of σ, $\sigma = 0$ and $\sigma = -2S$ [5]. Thus, for $\sigma = 0$ we obtain

$$A = \frac{4S}{\rho\left(c_0^2 + c_L^2 - V^2\right)}, \quad Q_\pm = \pm\frac{c_L^2 - V^2 - c_0^2}{c_L^2 - V^2 + c_0^2}, \quad k = 2\sqrt{\frac{p}{\mu\left(c_l^2 - V^2\right)}}, \tag{9}$$

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

The bounded solutions (7) and (8) may coexist for the Gardner equation and Eq. (6) [8,9]. Their amplitudes are always of either sign. However, an analysis of the reality of the parameters (9) gives rise to the conclusion that simultaneous existence of these bounded solutions is impossible [5], and bell-shaped or solitary wave for v may have only one sign for given velocity.

This is not true for the waves u as follows from Eq. (3). The shape of u depends upon the value of the first derivative at $\theta = 0$ in the r.h.s. of Eq. (3). Reversing the cos-function for derivation of the expression for u, one has to avoid the points where the first derivative does not exist. This breaking happens for $\theta = 0$ at $\sigma = 0$ and for $Q = Q_+$. Therefore, the solution for u obtained using both (7) and (8) should be written as

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \quad \text{for } \theta \leqslant 0, \tag{10}$$

$$u = \pm\pi \mp \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right) \quad \text{for } \theta > 0, \tag{11}$$

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

$$u = \pm \arccos\left(\frac{(\rho V^2 - E)U_x}{S} + 1\right). \tag{12}$$

The solution (10), (11) accounts for the kink-shaped profile of the wave, while solution (12) describes the bell-shaped localized wave. The velocity intervals when one or another profile exists as well as an analysis for $\sigma = -2S$ may be found in [5,14]. The sign ± in the above expressions means that one wave for v may be accompanied by two different waves for u.

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In the following we consider only the interval $(c_L^2 - c_0^2; c_L^2)$ for $\sigma = 0$ that corresponds to both bell-shaped localized waves for v and u [5,14]. A natural question arises: is the analysis based on the traveling wave solution sufficient to predict formation of the bell-shaped waves? Indeed, traveling wave solutions should satisfy specific initial conditions in the form these solutions at $t = 0$. One has to note that peaks of these initial conditions for v and u should coincide. What happens when these requirements are not satisfied? How deviations in the inputs for u and v affect generation and propagation of the localized bell-shaped waves and how they affect the sign of the amplitude of u? We address these questions in the next section.

3. Generation of localized bell-shaped waves

The dynamics of the solution differing from the single traveling one of the integrable Gardner Eq. (5), may be studied analytically, see, e.g., [8–10]. This is impossible for nonintegrable Eq. (6), and numerical simulations should be performed. In a series of papers [11–13] it was found that rather arbitrary initial input, motionless or with an initial velocity, splits into a sequence of solitary or bell-shaped waves. Each of them is described by exact traveling wave solution, either by (7) or by (8), and the sign of the amplitude of the wave is prescribed by the exact solution. Both solitary waves appear only when the conditions required for their simultaneous existence are satisfied in numerics.

Now we are going to check the validity of the similar predictions for behavior of the solutions to Eqs. (1) and (2). These equations were solved numerically by means of a standard ODE solver using the standard MATLAB routine *ode45* [15]. Also the calculations based on the numerical facilities of Mathematica 7 were performed. Both calculations were compared in order to avoid errors caused by the scheme. Numerical simulations with initial conditions coinciding with exact solutions (7) and (12) at $t = 0$ confirm propagation of the bell-shaped waves of permanent shape and velocity according to the exact solutions in the interval $(c_L^2 - c_0^2; c_L^2)$ for $\sigma = 0$. As predicted by Eq. (12), one and the same positive amplitude wave v accompany either wave u with positive amplitude shown in Fig. 1, or with negative amplitude shown in Fig. 2. In these cases the sign of u is defined by the sign of the initial condition for it. Horizontal lines in the figures illustrate permanent amplitudes of the waves, and both waves, v and u, propagate with the same velocity.

The initial positions of the inputs for v and u are the same in both Figs. 1 and 2 and equal to 58 units. Keeping the shape of the input for u in the form of the exact solution (12) but moving its position ahead of that of v one obtains another evolution of the waves. Thus, when the difference in initial positions is small, the initial profile of u suffers considerable deviations but finally evolves to the localized traveling wave similar to the exact solution (12) whose peak coincides with that of the wave v. This example is shown in Fig. 3 when initial position of the peak of u is equal to 59.6. Again the dotted lines in the figure illustrate variations in the amplitude of both waves. Further slight increase in the distance between initial positions gives rise to drastic variations in the behavior of the waves. Shown in Fig. 4 is the case when the position of the peak of u is chosen equal to 59.7. In the initial stage the amplitude of u rapidly decreases to zero since the wave delocalizes as seen in Fig. 5 where the initial stage is shown in detail. Then a negative amplitude localized wave emerges with an amplitude equal to the positive amplitude wave in Fig. 3 and finally propagates according to the exact solution (12). Therefore positive amplitude input for u evolves nevertheless to the negative amplitude solitary wave. Such behavior is observed in some interval of the reference initial distance. Then a propagation of positive amplitude wave u recovers. The higher is the reference initial distance the more perturbed initial stage for u is observed. Shown in Fig. 6 is the case of the large distance when an initial

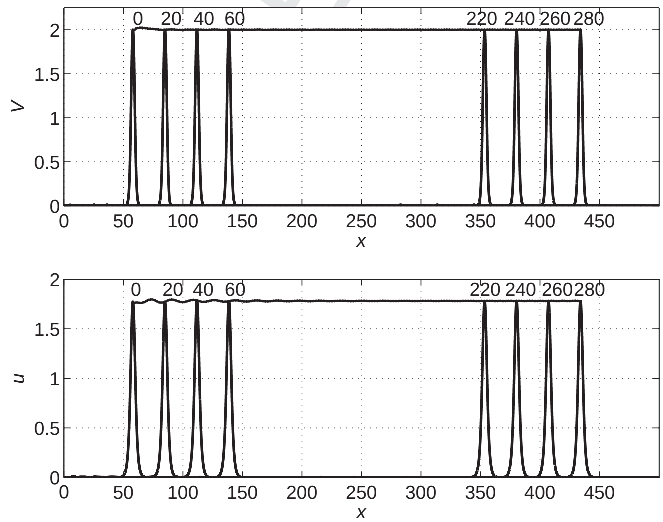

Fig. 1. Simultaneous propagation of positive amplitude bell-shaped waves v and u according to the exact solutions. Points of time are marked at the corresponding peaks. Horizontal lines mark permanency of the amplitude of the waves.

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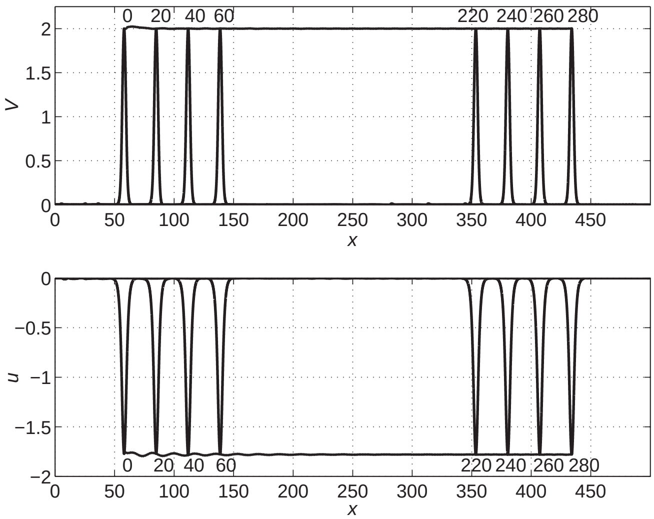

Fig. 2. Simultaneous propagation of positive amplitude bell-shaped waves v and negative amplitude wave for u according to the exact solutions. Points of time are marked at the corresponding peaks and holes (negative peaks). Horizontal lines mark permanency of the amplitude of the waves.

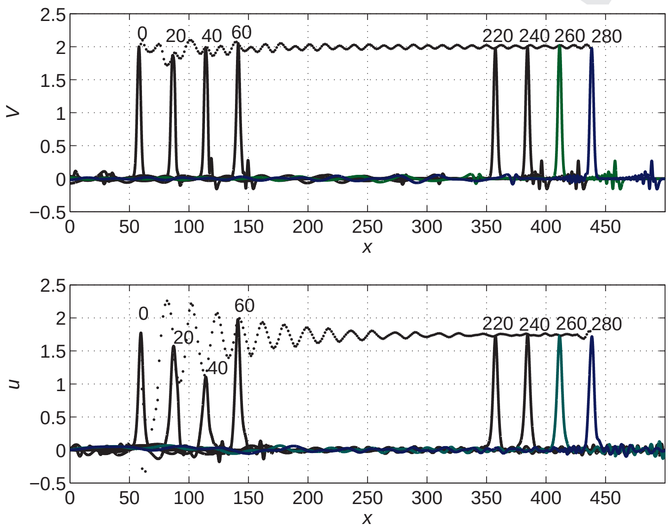

Fig. 3. Evolution of positive amplitude bell-shaped waves v and u when initial position of u equal to 59.6 units is slightly ahead of that of v equal to 58 units. Points of time are marked at the corresponding peaks. Dotted curved lines mark variations in the amplitude of the waves.

peak of u precedes that of v by 17 units. One can see that now initial stage delocalization transforms into the localized wave of permanent shape whose peak coincides with that of v at each time. The amplitude of the wave is slightly lower than that shown in Fig. 3 due to radiation. In all above mentioned cases the positions of peaks and holes (negative peaks) of u and v finally coincide, the waves propagate with one and the same velocity. Displacement of an initial peak of u behind a peak of v gives rise to similar scenarios of evolution of the bell-shaped wave u including change of a sign of the amplitude. However, now the wave amplitude changes its sign in much smaller interval of relative initial distances while there exists wider intermediate intervals where the wave u propagates changing the sign of the amplitude almost periodically. In all cases the wave u catches up with the wave v and then propagate altogether with it similar to the cases shown in Figs. 3, 4 and 6.

Variation of the relative position of the initial peaks is not the only factor affecting localization of the wave u. Similar scenarios are observed when an amplitude of an initial pulse for v varies, namely, when the initial conditions are chosen in the form of the exact solutions for both functions v and u but the first one is multiplied by an amplitude factor. The factor less than unity corresponds to a decrease in the initial amplitude of v. Slight decrease gives rise only to oscillating variations of the amplitude of u with subsequent propagation of the localized wave according to the exact solution. Further decrease in the amplitude of the input for v yields temporal change of the sign of the amplitude of u but the resulting wave evolves to the

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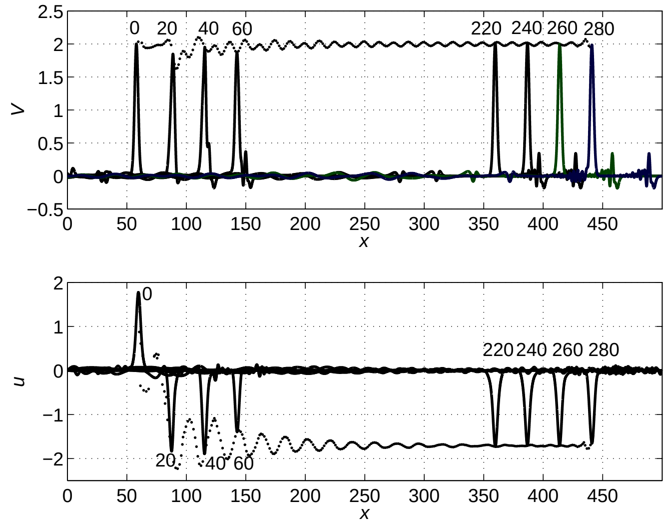

Fig. 4. Transition from positive to negative amplitude bell-shaped wave u when initial position of u is equal to 59.7 units ahead of that of v equal to 58 units. Points of time are marked at the corresponding peaks and holes. Dotted curved lines mark variations in the amplitude of the waves.

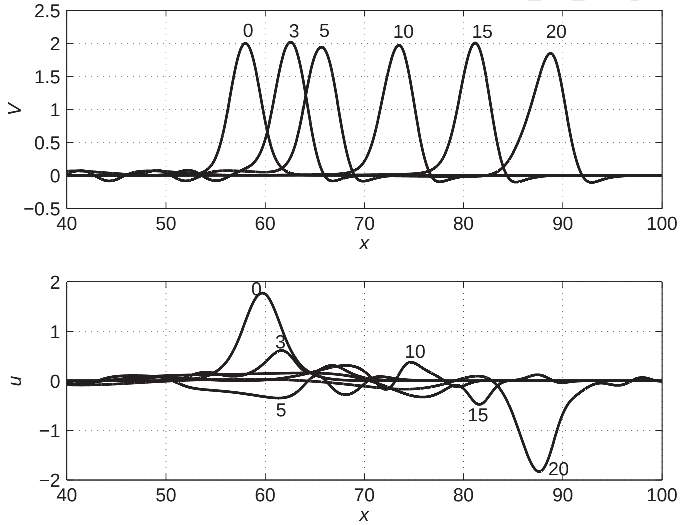

Fig. 5. Initial stage of the transition from positive to negative amplitude bell-shaped wave u when initial position of u is slightly ahead of that of v. Points of time are marked at the corresponding peaks and holes. Dotted curved lines mark variations in the amplitude of the waves.

positive amplitude localized wave of permanent shape. At smaller initial amplitude of v a more complicated evolution of u happens similar to that shown in Figs. 4, 5 where changing of the sign of the amplitude of the wave u is seen. Decreasing the initial amplitude of v we finally obtain a delocalization of the initial profile of u. Contrary to variations in the relative initial distance, now slight increase in the amplitude of v does not provide changing of the sign of u, while further increase in the initial amplitude of v yields a delocalization of the wave for u.

Another important factor is variation in the initial velocity. Changing of the initial velocity for u relative to that of the exact solution, does not result in significant variations in the wave behavior shown in Figs. 1,2. This is not the case of variations in the initial velocity for v. Keeping again the shapes of the inputs in the form of the exact solutions and decreasing or increasing initial velocity for v, we obtain changing in the sign of the amplitude for u but this process occurs almost periodically as shown in Fig. 7. One can see that part of the input moves to the left, then the resulted amplitude of the wave moving to the right turns out less than before. Therefore, there exist localized wave u of permanent velocity but either sign of amplitude, hence it does not keep its shape.

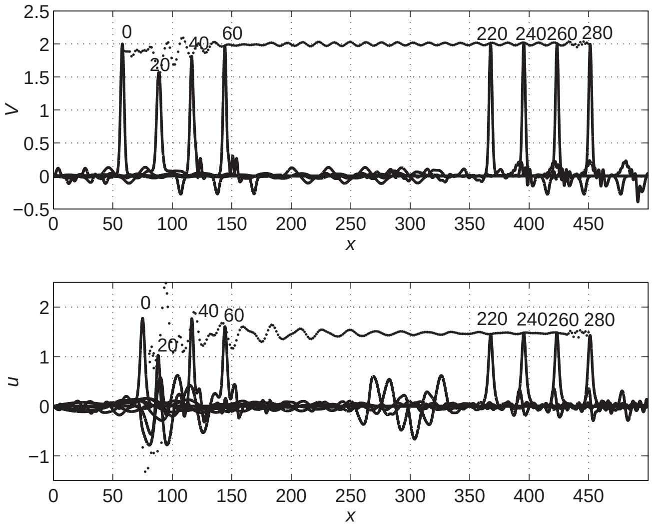

Fig. 6. Generation of positive amplitude bell-shaped wave u when initial position of the peak of u equal to 75 units is considerably ahead of that of v equal to 58 units. Points of time are marked at the corresponding peaks. Dotted curved lines mark variations in the amplitude of the waves.

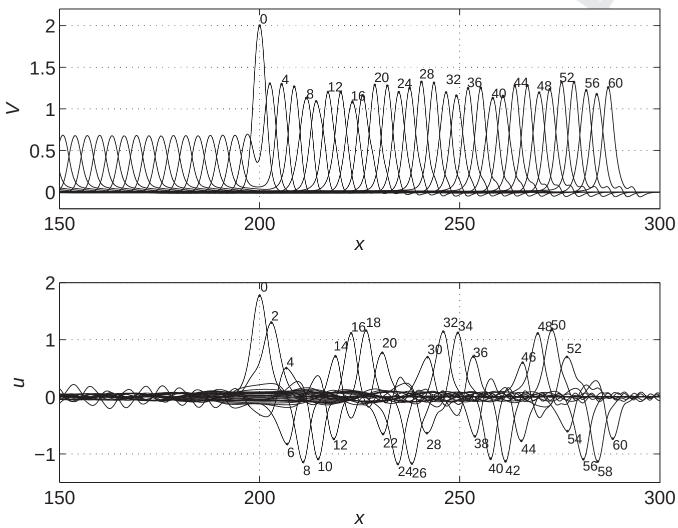

Fig. 7. Variation in the shape of u when the initial velocity for v is less than that of the exact solution. Points of time are marked at the corresponding peaks and holes.

4. Conclusions

The balance between nonlinearity and dispersion yields the localized bell-shaped or solitary wave solution of permanent shape and velocity. Only particular solutions accounting for stable propagation of coupled waves v and u, are possible to obtain analytically. However, their predictions about simultaneous existence of positive or negative amplitude solitary wave u for one and the same wave v, coincidence of the velocities of the coupled waves as well as relative positions of their peaks and holes – all these are realized in numerical study when the initial conditions differ from those of the exact solution. Also predicted strong dependence of the existence of localized waves on velocity is observed. Therefore even particular solutions may help to understand and explain numerical results.

However, some new effects are revealed in numerics such as an influence of the relative initial peaks distance on the wave localization and change of the sign of its amplitude. Despite stable propagation of the wave with either amplitude is described by the exact solution (12), the reason of changing the sign of the amplitude shown in Fig. 5, is still unclear. Certainly the coupling is responsible for it since single Eq. (6) obeying the same exact solution for v, does not undergo such variations in the solution in numerics [11–13].

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In Refs. [3,4] exact traveling localized solutions have been used to describe localized defects in bi-atomic lattices since u accounts for relative distance between atoms in a lattice. Our results show how localized moving defects may arise or decay in a lattice due to propagation of a macro-strain wave v. Change of the sign of the amplitude of u due to an influence of v describes transition from decrease to increase in the interatomic distance. It may help in description of re-arrangement of the crystalline structure caused by an external loading.

Another application may be suggested for a deformable monoatomic chain endowed with rotatory molecular group where Eqs. (1) and (2) are also valid. As noted in Refs. [1,2] the soliton solutions can be interpreted as the motion of a domain wall in a ferroelectric crystal or as a motion of a twist defect in a long deformable chain of macromolecules for polymer materials. Details may be found in Ref. [2].

There is a lack in estimations of the values of the parameters of the model (1) and (2), and knowledge of a relation between the amplitude of strain solitary waves and these parameters (9) might help in obtaining their values provided that measurements of the amplitude of solitary wave is available. Strain localized bell-shaped or solitary waves were already generated and observed in some crystals [16].

Acknowledgement

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