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Oscillatory motions of solitons in finite inhomogeneous structures

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Abstract. The soliton scattering by one single and two point impurities in a finite domain of an infinite ϕ^4 chain is analytically discussed. It is shown, for the single-point-impurity configuration, that the impurity causes the soliton to oscillate about the host site, whereas for the two-point-impurities configuration the soliton oscillates from one impurity wall to the other of the finite domain delimited by the two host sites. The oscillation frequency in each configuration has been estimated. We have also shown that in the second configuration the soliton falls into the finite domain with an exponentially increasing velocity and escapes at the transmitting wall with a velocity that decreases exponentially as the domain thickness increases.

1. Introduction

Recently, understanding of the combined effects of disorder and non-linearity and the important role that they play in condensed-matter systems has been a subject of particular interest. In this framework, the starting point has been the determination of whether or not non-linearity modifies qualitatively the effects of disorder on transport properties, and vice versa, i.e. of whether or not disorder affects the remarkable solitonic properties of non-linear systems. To provide insights into the subject, several analytical as well as numerical studies have been carried out (Li *et al* 1988, Mistriotic *et al* 1988, Bishop *et al* 1989, Fraggis *et al* 1989, Kivshar and Malomed 1989, Braun and Kivshar 1990, 1991, Kivshar *et al* 1992, Woafo and Kofané 1993a, b). Most of these studies model the non-linear disordered system by an infinite chain of particles interconnected by linear springs and subjected to a non-linear substrate potential, with a few (one or two) point impurities at some sites of the lattice, owing either to mass defects or excess at these sites (Abdullaev *et al* 1990, Kivshar and Malomed 1989, Kivshar *et al* 1992, Woafo and Kofané 1993b). Indeed, the model of a Klein–Gordon lattice with inhomogeneities provides a better method of investigating the scattering properties of solitons in disordered systems. More explicitly, this model allows for the use of standard methods, among which are the Hamiltonian perturbation theories (Fogel *et al* 1977, McLaughlin and Scott 1978, Kaup and El-Sayed 1986) which have already been exploited at length in similar contexts (Pascual and Vazquez 1985, Kivshar and Malomed 1989, Rodriguez-Plazza and Vazquez 1990) and have led to quite interesting results on the subject. Thus, it has been proved that the main effect of the impurities was the modulation of the soliton's dynamical parameters, so that the soliton may be captured, reflected or transmitted by the impurities with possibly more or less distortion of its structure and the excitation of new degrees of freedom, among which is the impurity mode (Fraggis *et al* 1989, Kivshar *et al* 1992).

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If we restrict ourselves to the consideration of only topological solitons, these solitons are precisely self-localized waves which describe large-amplitude non-linear excitations in many physical systems. From the physical point of view, the 'large-amplitude' feature of these self-localized excitations just traduces the fact that they are insensitive to end effects as they propagate along the infinite Klein–Gordon chain. Really, such consideration seems purely theoretical since it is unlikely that any condensed-matter system has infinite length. Indeed, molecular, biomolecular and in general hydrogen-bonded compounds, to name only a few cases, provide typical examples of physical systems in which the chain backbone consists of a precise number of molecular or ionic units and therefore has finite length.

In this paper, we analyse the influence of one single point impurity and two point impurities on the motion of a solitary wave in a finite ϕ^4 system. For this purpose, we consider a finite domain on an infinite ϕ^4 lattice, delimited by two walls at a finite distance from each other. First, we discuss the configuration in which a given site inside the finite domain lodges a mass defect or excess, and next we treat the case where each wall of the domain frontiers is the host of a local impurity. As an instructive remark, the finiteness of our scattering domain renders inadequate the existence and the stability of the usually assumed ϕ^4 kink, but rather of an appropriate type of soliton excitation which will be derived in terms of a snoidal ϕ^4 kink. However, the role of a large-amplitude ϕ^4 kink will be of particular importance when analysing the continuity of the soliton at the domain boundaries.

The paper is outlined as follows. In section 2, we seek the appropriate soliton solutions for the system dynamics on the one hand and for the finite domain and in the domain as well, in the absence of impurities, on the other hand. In section 3, with the help of the perturbation methods we estimate the main dynamical parameters of the soliton in the presence of a single point impurity, and in section 4 the case of two point impurities is considered. Section 5 is devoted to a conclusion.

2. Model and explicit soliton solutions

Consider a ϕ^4 chain, in which ϕ is the displacement field. In the presence of inhomogeneities, the system dynamics are governed by the perturbed equation

$$\phi_{tt} - \phi_{xx} + (1/l^2)(\partial/\partial\phi)U(\phi) = P(\phi, \phi_t, x, t) \tag{1}$$

where the subscripts t and x refer to time and space derivatives, respectively, and $U(\phi)$ is the ϕ^4 substrate potential given by

$$U(\phi) = \tfrac{1}{4}(\phi^2 - 1)^2. \tag{2}$$

In (1), $1/l$ defines the scale of non-linearity, and the function P is the inhomogeneous term, for which two particular forms will be considered:

$$P = \varepsilon\delta(x)\phi_{tt} \tag{3a}$$

$$P = \varepsilon[\delta(x - d) + \delta(x + d)]\phi_{tt}. \tag{3b}$$

Equation (1) with P given by (3a) describes a ϕ^4 system with one single point impurity (Kivshar and Malomed 1989), whereas equation (1) with P given by (3b) corresponds to a ϕ^4 system with two point impurities at the distance $2d$ from each other (Kivshar *et al*

1992, Woafo and Kofané 1993a). ε in (3) is a weak parameter which plays the role of the impurity rate at the host site(s). When $\varepsilon > 0$, we are faced with heavy mass impurities, whereas $\varepsilon < 0$ will refer to light mass impurities (Woafo and Kofané 1993b). When $\varepsilon = 0$, (1) is non-integrable. Nevertheless, it leads to the following set of solitary wave (kink) solutions, in the non-relativistic limit:

$$\phi(x,t) = \begin{cases} \tanh\{[x - x_1 - X(t)]/\sqrt{2}l\} & x \leqslant -d \\ [2m/(1+m)]^{1/2}\mathrm{sn}[\![\{[x - X(t)]/l\sqrt{1+m}\}/m]\!] & -d \leqslant x \leqslant d\,. \\ \tanh\{[x - x_2 - X(t)]/\sqrt{2}l\} & x \geqslant d \end{cases} \tag{4}$$

$X(t)$ is the kink centre of mass, which in the present case reads $X(t) = vt$ (v is the kink translation velocity). sn appearing in the second solution of the set (4) is a Jacobi elliptic function of modulus m (appendix 1). In this context, this solution will be called a snoidal ϕ^4 kink, of characteristic length l. The first and the third solutions in the same set (4) are the well known large-amplitude kink solutions of the unperturbed ϕ^4 equation. It is easily verified that, in the limit $m \to 1$, the snoidal kink turns into a large-amplitude kink, with the same characteristic length l.

The quantities x_1 and x_2 measure the characteristic positions of kinks in the two semi-infinite media with respect to position of the finite domain on the chain. They result from the continuity of solutions at the frontiers $-d$ and d, which yields

$$x_1 = -x_2. \tag{5a}$$

In turn, setting $x_1 = x_0$, we derive

$$x_0 = -d + \sqrt{2}l\ln\left(\frac{1 + [2m/(1+m)]^{1/2}\mathrm{sn}(d/l\sqrt{1+m})/m}{1 - [2m/(1+m)]^{1/2}\mathrm{sn}(d/l\sqrt{1+m})/m}\right) \tag{5b}$$

which displays a strong dependence upon the two relevant physical parameters d and m.

3. Scattering of the kinks by a single point impurity

Let $\varepsilon \neq 0$, and P be given as in (3a). On the assumption that the point impurity is at a site inside the scattering domain or, in other words, in the interval $-d \leqslant x \leqslant d$, then the relevant dynamic equation is that governing the time evolution of the kink centre of mass, i.e.

$$X_{tt} = -\varepsilon\int \delta(x)\phi_{tt}\phi_x\,\mathrm{d}x. \tag{6}$$

Inserting the second explicit solution of (4) in (6) and using the series expansions of Jacobi elliptic functions (appendix 2), we arrive at the following second-order differential equation:

$$X_{tt} = -A_0\sin[\pi/2Kl\sqrt{1+m}]X \tag{7a}$$

$$A_0 = [\varepsilon m^2\pi^3/K^5l^3(1+m)^{5/2}]\,\mathrm{cosech}^2(\pi K'/K). \tag{7b}$$

Equation (7) may be interpreted as the equation of an effective particle with mass unity, moving into the field of the effective potential:

$$U(X) = U_0\cos[\pi/2Kl\sqrt{1+m}]X. \tag{8a}$$

This effective potential is a periodic function of the kink centre of mass coordinate X, and its barrier height U_0 is obtained as

$$U_0 = 2Kl\sqrt{1+m}A_0/\pi. \tag{8b}$$

In equations (7) and (8), K and K' are complete elliptic integrals of the first kinds.

Actually, the periodic feature of the trapping potential $U(X)$ has the following meaning: near the impurity, the snoidal kink oscillates, being pinned to a potential barrier whose height varies as a function of its characteristic width l, the impurity rate ε and the parameter m which, precisely, is characteristic of the finiteness of the scattering domain. In the limit of small-amplitude motions, the pinning frequency will obey the relation

$$\Omega^2 = A_0\pi/2Kl\sqrt{1+m}. \tag{9}$$

In figure 1, we draw Ω^2 as a function of m. One sees that it increases as m is increased. Traducing this variation, Ω^2 becomes larger as the snoidal kink behaves more like a large-amplitude excitation. Therefore, the frequency itself will increase with increasing m, such that the maximum frequency is reached when $m = 1$.

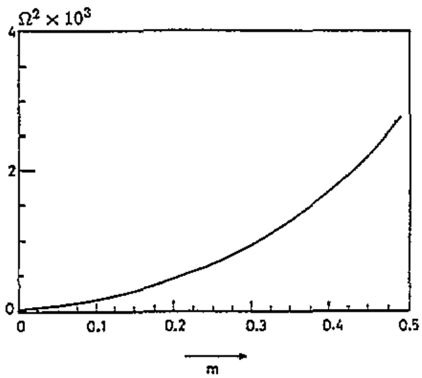

Figure 1. Variation in the square of the kink oscillation frequency as a function of the parameter m, in the configuration of a single point impurity.

4. Kink scattering by two point impurities

Next, consider (1) and (3b). In that case the evolution equation derived from equation (6) will be of the form

$$X_{tt} = -A_0[\sin(\pi/2Kl\sqrt{1+m})(d-X) - \sin(\pi/2Kl\sqrt{1+m})(d+X)]. \tag{10}$$

Equation (10) is subjected to two continuity relations at the frontiers. These relations are in fact the kink evolution equations at the domain boundaries:

$$X_{tt} = (3\varepsilon/4l^2)\text{sech}^4[(d+X+x_1)/\sqrt{2}l]\tanh[(d+X+x_1)/\sqrt{2}l] \qquad x=-d \tag{11a}$$

$$X_{tt} = (3\varepsilon/4l^2)\text{sech}^4[(d-X-x_2)/\sqrt{2}l]\tanh[(d-X-x_2)/\sqrt{2}l] \qquad x=d. \tag{11b}$$

As in the previous case, (10) can be interpreted as the equation of an effective particle with unit mass, moving into the field of the effective potential:

$$U'(X) = U_0[\cos[\pi/2Kl\sqrt{1+m}](d-X) + \cos[\pi/2Kl\sqrt{1+m}](d+X)]. \tag{12}$$

However, in contrast with (7), $U'(X)$ is somewhat an almost doubly periodic potential, but with the same amplitude as calculated in (8). The frequency of kink oscillations in this doubly periodic potential is derived from the relation

$$\Omega_m^2 = A_0\pi/Kl\sqrt{1+m}. \tag{13}$$

Then, this frequency is greater than that found in the previous configuration.

In fact, Ω_m is the frequency with which the snoidal kink oscillates from one wall to the other of the domain boundaries. The continuity relation (11*a*) provides us with the local potential that perturbs the kink motion about the incident wall, i.e.

$$U_i(X) = (\varepsilon/8l^2)\mathrm{sech}^4[(d+X+x_1)/\sqrt{2}l]. \tag{14a}$$

On the other hand, let us consider a kink approaching towards the transmission wall, inside the finite domain. For this latter case the local impurity potential will be given by

$$U_t(X) = (\varepsilon/8l^2)\mathrm{sech}^4[(d-X-x_2)/\sqrt{2}l]. \tag{14b}$$

Since, in both cases, the kink centre of mass coordinate must obey the energy equation (Kivshar and Malomed 1989)

$$X_t^2 = 2[E - U(X)] \tag{15}$$

where E is the total energy conserved about the impurity after the interaction with kink, then the considerations $\varepsilon > 0$ and $\varepsilon < 0$, respectively, allows us to distinguish between two different classes of behaviours for each of these configurations.

(1) $\varepsilon > 0$. A kink in the field of the local impurity potential (14*a*) could not cross the incident wall as long as the incident velocity exceeds the threshold:

$$v_1 \simeq \frac{2\sqrt{\varepsilon}}{l}\exp\left(\frac{2d}{\sqrt{2}}\right)\left[1 - \pi^2 d[Kl^2\sqrt{m(1+m)}]\,\mathrm{cosech}\left(\frac{\pi K'}{K}\right)\right]. \tag{16a}$$

A kink inside the finite domain will permanently oscillate from the incident to the transmitting wall (i.e. the kink could remain trapped inside the scattering domain of length $2d$) until it acquires a velocity which is higher than the threshold:

$$v_2 \simeq \frac{2\sqrt{\varepsilon}}{l}\exp\left(-\frac{2d}{\sqrt{2}}\right)\left[1 + \pi^2 d[Kl^2\sqrt{m(1+m)}]\,\mathrm{cosech}\left(\frac{\pi K'}{K}\right)\right]. \tag{16b}$$

(2) When $\varepsilon < 0$, v_1 turns into the threshold velocity below which the soliton remains trapped into the potential well at the incident impurity site, while v_2 is the threshold velocity above which the soliton could overcome the trapping of the transmitting impurity site (where ε is replaced by $-\varepsilon$).

Figures 2(*a*) and 2(*b*) are plots of v_1 and v_2 as functions of the domain thickness d, for a few values of m. Figure 2(*a*) shows that the reflection velocity v_1 increases as d increases,

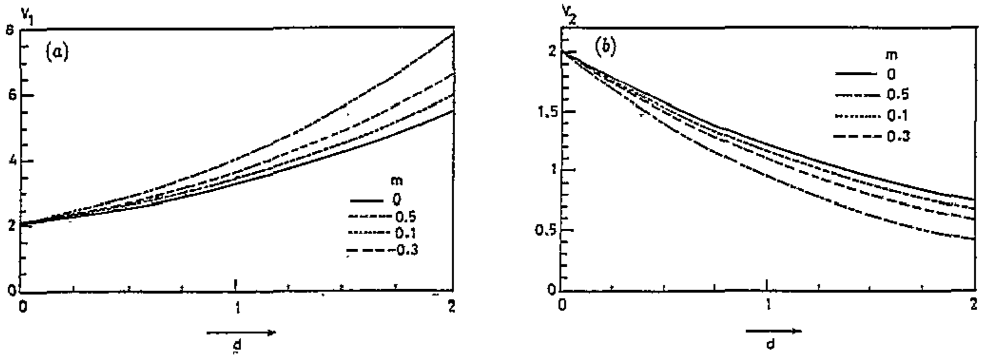

Figure 2. (a) Increase in the threshold velocity at the incident impurity wall, for increasing values of the domain thickness d. It is seen that the exponential growth of v_1 becomes more marked as m is increased. (b) Decrease in the threshold velocity at the transmitting impurity wall, for increasing values of the domain thickness d. In the present case, the exponential fall-off decreases as m is increased.

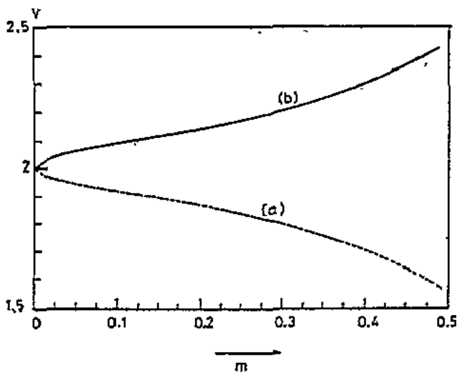

Figure 3. Variations in v_1 (curve a) and v_2 (curve b) as a function of the modulus m of the Jacobi elliptic function.

and this increase becomes more marked as m is increased. On the contrary, figure 2(b) shows that v_2 is lowered with increasing d and m. More suggestively, it is seen in figure 3 that $v_1(a)$ decreases whereas $v_2(b)$ increases with increase in m.

Equations (16a) and (16b) also demonstrate that, at the asymptotic limit $d \to 0$, the threshold values of the reflection and the transmission velocities coincide whereas, in the limit $d \to \infty$, v_1 tends to infinity and v_2 to zero. Thus, when the domain thickness becomes sufficiently large, the soliton will always be totally reflected by the incident impurity wall. Nonetheless, as pointed out in recent developments (Fei *et al* 1991), the soliton may overcome this local effect of the incident impurity wall if its velocity is above some well defined resonance window.

5. Conclusion

We have investigated the scattering properties of solitary waves in a finite domain of an infinite ϕ^4 chain. As a first step, we studied the case of a single point impurity inside the finite domain. Thus we found that the impurity traps the snoidal kink and promotes it to an oscillating particle. The frequency of these oscillations has been calculated and is shown to depend upon the impurity rate, the kink width and a characteristic parameter related to the finiteness of the scattering domain.

As a second step, we treated the case where the two point impurities are sited at the two limiting walls. This configuration, described in terms of a two-point-impurities model, has led to behaviours which can be summarized as follows: a soliton inside the finite region (i.e. a snoidal kink) should oscillate from one impurity wall to the other at a frequency which is higher than that of the single-point-impurity configuration. However, provided that its velocity is at least equal to a threshold, the kink can be transmitted and thus escapes from the trapping caused by a doubly periodic potential. Otherwise, as long as the kink velocity about the incident impurity wall does not exceed a threshold, it will be permanently reflected and therefore could never get into the finite domain.

We have estimated the threshold velocities for the kink reflection and transmission. We found that these threshold velocities are dominated by an exponential dependence with the domain thickness d, increasing and decreasing, respectively, as d is increased. We have also noted that these threshold velocities vary as a function of the modulus m of the Jacobi elliptic functions. More precisely, the increase in m enhances the threshold value of the reflection velocity but lowers that of the transmission velocity. Finally, it is pertinent to draw attention to the fact that, when the scattering domain becomes too large (i.e. $d \to \infty$), the kink can always be totally reflected, since in that limit the threshold value of the reflection velocity tends to infinity. On the other hand, in the limit $d \to 0$, both the reflection and the transmission velocities coincide, consistently with the physical expectations. Moreover, these latter behaviours are in accordance with the results (Kivshar and Malomed 1989) obtained for the scattering of large-amplitude kinks by inhomogeneities in an infinite lattice.

Appendix 1. The Jacobi elliptic snoidal function sn

Let $F(\varphi/\alpha)$ be a functional, given in terms of the integral:

$$F(\varphi, \alpha) = \int_0^x \frac{\mathrm{d}t}{[(a^2 - t^2)(b^2 - t^2)]^{1/2}} \qquad \text{(A1.1)}$$

where

$$\sin\alpha = \frac{b}{a} \qquad \sin\varphi = \frac{x}{b} \qquad a > b. \qquad \text{(A1.2)}$$

Setting $m = b^2/a^2$, then the functional (A1.1) will be defined using the substitution

$$t = b\,\mathrm{sn}(x/m). \qquad \text{(A1.3)}$$

sn is called the 'Jacobi elliptic snoidal function', of argument x and modulus m (Abramowitz and Stegun 1968).

Appendix 2. Series expansions of Jacobi elliptic functions in terms of a nome $q = \exp(-\pi K'/K)$ and argument $v = \pi x/2K$

The Jacobi elliptic functions sn, cn and dn may, in some cases, be expanded in power series of a nome q and a renormalized variable v (v need not be small, as usually assumed in the perturbation theory). Thus we can write

$$\mathrm{sn}(x/m) = \frac{2\pi}{\sqrt{m}K} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1-q^{2n+1}} \sin[(2n+1)v] \tag{A2.1}$$

$$\mathrm{cn}(x/m) = \frac{2\pi}{\sqrt{m}K} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1+q^{2n+1}} \cos[(2n+1)v] \tag{A2.2}$$

$$\mathrm{dn}(x/m) = \frac{\pi}{2K} + \frac{2\pi}{K} \sum_{n=1}^{\infty} \frac{q^{n}}{1+q^{2n}} \cos[(2n)v]. \tag{A2.3}$$

Otherwise, the first derivative of the snoidal function sn is obtained as

$$[\mathrm{sn}(u)]' = \mathrm{cn}(u)\,\mathrm{dn}(u). \tag{A2.4}$$

Therefore, inserting (A2.2) and (A2.3) in (A2.4), one finds the formula of the series expansion of this last relation, and straightforwardly equations (7) and (10).

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