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Nonlinear excitations of incommensurate surface structures

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Abstract. Nonlinear dynamics of the incommensurate surface layer with a spatially periodical structure is investigated analytically. In the framework of the Frenkel–Kontorova model the nonlinear excitations of the periodic soliton lattice, such as moving additional kinks and gap solitons, are discussed.

Key words: incommensurate structure, kink, gap soliton.

Nonlinear dynamics of real physical systems has always been the focus of attention in the theory of nonlinear waves and solitons, particularly periodic structures with physical parameters modulated in space ("modulated systems"), such as layered crystals. Spatial periodicity leads to a band–gap structure of the spectrum of linear waves and to the existence of the so-called gap solitons when the nonlinearity of the medium is taken into account [1–3]. In this paper, we discuss the existence of other "gap solitons" in systems with spatially homogeneous material parameters but spatially periodical ground state, which can be investigated exactly in the framework of integrable models. The periodic fluxon lattice in a long Josephson junction in an external field is one example of such a system [4,5]. The surface atomic layer in an incommensurate state (see, e.g., [6–8]) is another important example of similar "self-modulated" structures. In these cases the spectrum of linear excitations also has a gap structure, but solitons with frequencies within a gap differ from those in the modulated media. In the present paper one-parametric topological solitons ("kinks") [9] in the gap of the spectrum of incommensurate surface structures are investigated analytically using the Darboux transforms.

Let us consider, for example, an incommensurate structure of the surface layer of atoms. We take into account the interaction between surface atoms in the harmonic approximation and assume that, in the absence of substrate, the equilibrium distance between these atoms is equal to b and differs from the interatomic distance a in a bulk. The effect of a substrate on surface atoms can be simulated by a periodical potential landscape with period a. For simplicity, we approximate this by a trigonometric function and assume the substrate to be absolutely hard. Then the potential energy of the system is given by

$$U = \sum_n U_0 \left(1 - \cos\frac{2\pi y_n}{a}\right) + \sum_n \frac{\alpha}{2}(y_n - y_{n-1} - b)^2, \tag{1}$$

where y_n is the position of the nth atom with respect to the surface layer and α is the elastic constant in the layer. The dynamical equations for the atomic displacements $v_n = y_n - an$ in this model (Frenkel–Kontorova model [10]) have the following form:

$$mv_{tt} + \frac{2\pi U_0}{a}\sin\frac{2\pi v_n}{a} + \alpha(2v_n - v_{n+1} - v_{n-1}) = 0. \tag{2}$$

In the long-wave approximation for dimensionless variables $u = 2\pi v/a$, $x = n\,2\pi\sqrt{U_0/(\alpha a^2)}$, and $t = \tau\,2\pi\sqrt{U_0/(ma^2)}$ we obtain the well-known sine-Gordon equation (SGE) [9]:

$$u_{tt} - u_{xx} + \sin u = 0\,. \tag{3}$$

In the same approximation the total energy of the system (1) takes the form

$$E = E_0 \int dx[(u_t^2/2) + (u_x^2/2) + (1 - \cos u) + \xi u_x], \tag{4}$$

where $E_0 = (a/2\pi)\sqrt{U_0\alpha}$, and the incommensurability of the surface layer and substrate is characterized by the dimensionless parameter $\xi = \sqrt{\alpha/U_0}\,(a-b)$. The last term ξu_x in (4) is of divergent type and does not alter the form of Eq. (3) but changes the potential energy of the system and can change its ground state. In the case $b = a$, the ground state corresponds to the trivial solution of Eq. (3), $u \equiv 0$ with the energy $E = 0$. Under the condition $b \neq a$, the problem becomes more complicated.

Let us consider the case $b > a$ $(\xi < 0)$ where Eq. (3) allows additional nontrivial static solutions in the following form [4,5]:

$$u_0 = \pi + 2\,am(x/k, k), \tag{5}$$

where $am(z,k)$ is the elliptic amplitude with modulus k, and $z = x/k$. The solution (5) describes the "extended" system of a periodical chain of 2π-kinks (“one-dimensional dislocations” in a surface layer or fluxon lattice in a long Josephson junction) separated by the distance $L = 2kK(k)$, where $K(k)$ is the full elliptic integral of the first kind. The width of the kink expressed in terms of the initial dimensional variables is equal to $\Lambda = (a/2\pi)\sqrt{\alpha a^2/U_0}$. The energy density of such a periodical structure (per period) $\varepsilon = U/L$ depends on the parameter of incommensurability ξ. For small values of this parameter, the ground state of the system is homogeneous and the periodical solution (5) can exist only under pressure conditions applied at the infinity. But when the parameter ξ exceeds a critical value $\xi_c = 4/\pi$, where $b_c = a + (4/\pi)\sqrt{U_0/\alpha}$, the periodical state (5) with the modulus of elliptic function, derived from the equation $E(k)/k = \xi/\xi_c$, corresponds to the minimum of energy.

Linear excitations on the background of the incommensurate structure (5) are well known [11]. They represent the high-frequency phonon mode in the layer (upper band) and the low-frequency Swihart mode of oscillations of kink lattices (lower band). Let us consider nonlinear excitations on this background. The elementary nonlinear excitation corresponds to an additional kink (surface dislocation) which propagates through the kink lattice (5). To obtain the exact solution for this excitation, we use the Darboux transform which allows us to use the well-known “dressing” procedure for the initial solution (5) to find more complicated solutions. This transform is very simple in the case where the initial solution depends only on one variable as in our case with $u_0 = u_0(x)$, and does not depend on time. The Darboux transform for SGE (3) that we consider is well known [12]. To render compact this transform, it is convenient to change over from the initial field variable $u(x,t)$ to the new variables V and W, connected with the initial field u by the relations:

$$V = i(u_x + u_t), \qquad W = \exp(iu), \tag{6}$$

for which Eq. (3) reads:

$$V_x - V_t = (W - 1/W)/2, \qquad W_x + W_t = VW. \tag{7}$$

The associated linear problem for two complex functions $\Psi_1(x,t)$ and $\Psi_2(x,t)$ corresponds to the system (7). For the column function $\Psi = \{\Psi_1, \Psi_2\}$ and an arbitrary solution $u(x,t)$ (or $V(x,t)$ and $W(x,t)$) we have [12]:

$$4\Psi_x = \begin{vmatrix} V & \lambda + W/\lambda \\ \lambda + 1/(W\lambda) & -V \end{vmatrix} \cdot \Psi, \tag{8}$$

$$4\Psi_t = \begin{vmatrix} V & \lambda - W/\lambda \\ \lambda - 1/(W\lambda) & -V \end{vmatrix} \cdot \Psi, \tag{9}$$

where λ is the parameter of the Darboux transform. The initial Eq. (3) is the condition of consistency of the system (8), (9). The solution of this system with the given “seed” (initial) solution $u_0(x,t)$ (given functions $V_0(x,t)$ and

$W_0(x,t))$ and an arbitrary value of λ allows us to build up the new solution $u(x,t)$. Naturally, the parameter λ must be chosen in such a way that the real solution $u(x,t)$ can be obtained. The final relation between these two solutions $u_0(x,t)$ and $u(x,t)$ reads [12]

$$u(x,t) = u_0(x,t) - 2i \ln[\Psi_2(u_0,\lambda)/\Psi_1(u_0,\lambda)]. \tag{10}$$

The main task is to solve the system of linear equations with variable coefficients (8), (9). In our case the problem is simplified, as the initial solution $u = u_0(x)$ depends only on x, and Eq. (9) becomes an ordinary differential equation with constant coefficients. For the ground state (5), the functions V_0 and W_0 have the form

$$V_0 = (2i/k)\, dn(z,k), W_0 = [sn(z,k) - icn(z,k)]^2 \tag{11}$$

and the system of linear equations (9) can be easily solved. We can use any arbitrary real λ to obtain a new real solution. This parameter characterizes the average velocity of the additional moving kink. The solution of Eq. (9) reads

$$\begin{aligned} \Psi_1 &= a(x)\exp(\mu t) + b(x)\exp(-\mu t), \\ \Psi_2 &= a(x)A^{(-)}\exp(\mu t) - b(x)A^{(+)}\exp(-\mu t), \end{aligned} \tag{12}$$

with $A^{(\pm)} = \lambda(4\lambda \pm V_0)/(\lambda^2 - W_0)$ and $\mu = \pm\sqrt{(\lambda + 1/\lambda)^2 - 4/k^2}/4$. Positive μ corresponds to a $(0, 2\pi)$ additional kink, negative one to a $(2\pi, 0)$ kink.

If we substitute the solution (12) into Eq. (8) and take the coefficients before $\exp(\pm\mu t)$ equal to zero, we obtain $a(x)$ and $b(x)$ in the form

$$a(x) = \sqrt{W - \lambda^2}\, \exp\left(\mu \int_0^x \frac{\lambda^2 + W}{\lambda^2 - W} dx\right) = -i(W - \lambda^2)/b.$$

Using (12) we can transform the expression for the ratio Ψ_2/Ψ_1 into the following form:

$$\frac{\psi_2}{\psi_1} = \exp(i\rho) \cdot \frac{\exp(i\varphi) - i \cdot \exp(\vartheta)}{1 + i \cdot \exp(i\varphi + \vartheta)}, \tag{13}$$

where $\tan\varphi = dn(z,k)/2k\mu$, $\tan\rho = 2sn(z,k)\,cn(z,k)/[2sn^2(z,k) - 1 - \lambda^2]$, and $\vartheta = 2\mu[t + f(x)]$ with

$$f(x) = \frac{k^2}{4}\left(\lambda^2 - \frac{1}{\lambda^2}\right)\int_0^x dx\,[dn^2(x/k,k) + (2k\mu)^2]^{-1}.$$

The function $(\varphi \pm \rho)$ may be rewritten as $\varphi \pm \rho = \mp am(z,k) \pm am(z \pm \Delta/k, k)$, where the phase shift of the solution Δ depends on the parameters k and λ in the following implicit form: $k\, sn(\Delta/k, k) = 2\lambda/(\lambda^2 + 1)$.

In all above formulas we considered $\lambda_0 < \lambda < \infty$, where $\lambda_0 = (1+k')/k$. This corresponds to a positive value of f, i.e. to the kink motion in the negative direction. The domain $0 < \lambda < 1/\lambda_0$ corresponds to the opposite direction of kink motion. The function $f(x)$ can be expressed as $f = x/v + \chi(x)$, where the average value of the periodical function $\chi(x)$ is equal to zero. The linear growing component of $f(x)$ determines the average velocity of a kink propagating through the incommensurate structure:

$$< v >= \frac{4K(k)}{k^2(\lambda^2 - 1/\lambda^2)} \left[\int_0^K \frac{dz}{dn^2(z,k) + (2k\mu)^2} \right]^{-1}. \tag{14}$$

Consequently, the phase ϑ in Eq. (13), $\vartheta = 2\mu/\upsilon\,(x + \upsilon t) + 2\mu\chi(x)$, describes the kink motion in the negative direction with the average velocity υ. Such a motion is accompanied by periodical oscillations at the moments when the kink propagates through each kink from the lattice. After substitution of (12) into the formula (10) we obtain the final solution for the motion of an additional kink:

$$u(x,t) = u_0(x) - 2i \ln \left[\frac{\exp(i\kappa_+) - i\exp(\vartheta + i\kappa_-)}{\exp(-i\kappa_+) + i\exp(\vartheta - i\kappa_-)} \right], \tag{15}$$

where $\kappa_\pm = \rho \pm \varphi$.

Although this solution is somewhat complicated, it admits a simple physical interpretation. The additional kink propagates through the incommensurate surface structure, and this propagation is accompanied by the total deformation with the phase shift 2Δ. In the limit $\lambda \to \infty$ the kink velocity tends to its maximum value $(v \to 1)$ and the phase shift tends to zero $(2\Delta \to 0)$: the singular extra-kink moves through the undeformed periodical structure. In the opposite limit $\lambda \to \lambda_0$ the velocity of a kink tends to its minimal value $s_0 = k'K(k)/E(k)$ coinciding with Swihard velocity, the width of the kink goes to infinity, and the phase shift tends to L: the perfect incommensurate structure rehabilitates itself. The solution (15) develops an evident form in the limit $k \to 1$. In this limit the period of the incommensurate structure tends to infinity $(L \to \infty)$ and Eq. (15) describes the propagation of a moving kink through another standing kink: the last term in (15) transforms into the well-known expression for a moving soliton

$$\delta u(x,t) = \pm 4 \arctan \exp\{[x - vt - \gamma(t)]/\sqrt{1-v^2}\}, \tag{16}$$

where $\gamma(x)$ is a localized function which describes the deformation of a kink during its propagation through the standing kink and depends on functions φ and ρ. (The polarity of the kink and the sign of its velocity depend on the sign of the parameter μ and the value of the parameter λ).

The knowledge of the one-soliton solution (15) allows us to find the exact solution for the envelope two-parametric gap soliton. In addition, we can use the Backlund transform for SGE (3). This dressing method establishes a link between different solutions of a nonlinear evolution equation. At the second step of the Backlund transform we can link four different solutions by the algebraic relation [9]:

$$u = u_0 + 4\arctan\left[\frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2}\tan\frac{u(\lambda_1) - u(\lambda_2)}{4}\right], \tag{17}$$

where the parameters of the Backlund transform λ_i are the same as the parameters λ_i in the previous Darboux transform in (8), (9).

In the simplest case of a trivial ground state $u_0 = 0$ we can choose the solutions for a moving kink and anti-kink $u(\lambda_i) = \pm 4\arctan\exp[(x \mp vt)/\sqrt{1-v^2}\,]$ with $\lambda_1 = 1/\lambda_2 = -\sqrt{(1-v)/(1+v)}$ and opposite velocities as $u(\lambda_i)$ in (17). Then it represents a two-soliton solution with an immobile centre of masses. With $i\omega$ replacing v ($\lambda_1 = \lambda_2^* = -\exp(-i\omega)$), the solution $u(x,t)$ from (17) transforms into a breather solution with the frequency ω. In our problem we can carry out the same procedure taking the incommensurate structure (5) as the initial solution u_0 in (17). Then the solution (15), with $\lambda = \lambda_1$ and $\mu = \mu_1$, may be taken as $u(\lambda_1)$ in (17). Another solution (15), with $\lambda_2 = 1/\lambda_1$ and $\mu_2 = -\mu_1$, may be taken as $u(\lambda_2)$. After the substitution $v \to i\omega$ (when $\lambda_1 = \lambda_2^* = \exp(i\eta)$ and the parameter μ is purely imaginary) we can obtain the final real solution for nonlinear excitations of the incommensurate surface structure. This solution has a very complicated form, but admits a simple physical interpretation. The frequencies of localized nonlinear excitations of the incommensurate structure lie in the gap of the spectrum $\omega_1 < \omega < \omega_2$, where the frequency $\omega_1 = k'/k$ corresponds to the upper boundary of the Swihart band and the frequency $\omega_2 = 1/k$ to the lower boundary of the phonon band. At the lower boundary of the gap this excitation transforms into small-amplitude anti-phase oscillations of the kinks, which form the incommensurate structure. In the vicinity of the frequency ω_1, the localized soliton-like small-amplitude excitations have the typical form of gap solitons in modulated systems [1], and kinks play the role of point defects in such a system. But transformation of this gap soliton in the opposite limit $\omega \to \omega_2$ is unusual. In modulated systems in this limit the domains between defects oscillate in opposite directions and a gap soliton transforms into an algebraic soliton with nonzero amplitude. In our case of the "self-modulated" structure in the limit $\omega \to \omega_2$ the gap soliton transforms into a small-amplitude soliton with infinitely increasing spatial size. But like in modulated systems, in this limit kinks are unmovable and domains between them oscillate in opposite directions. It also followed from the exact solution that, in contrast to usual gap solitons in modulated systems as discussed above, solitons are accompanied by nonzero shift of the kink structure at infinity.

The dynamics of gap solitons in the small-amplitude limit $\omega \to \omega_1$ allows a simple analysis in the approach of a collective-variable method. In this approach the isolated kinks of the incommensurate structure with a large period $L >> 1\,(k' << 1)$ may be treated as a lattice of weakly interacting quasi-particles. The coordinates of these particles play the role of collective variables. From the well-known expression [9] for the energy of the moving SGE-kink

$E = 8E_0 \big/ \sqrt{1 - v^2/c^2}$ (where $c = \sqrt{\alpha a^2/m}$ is the limiting velocity of linear waves), it is easy to calculate the effective mass of a kink:

$$M = m\sqrt{16U_0/\alpha a^2 \pi^2}.$$

An effective potential energy of the interaction of two kinks with the same signs can be found from the exact two-kink solution and was calculated in [13]. Two kinks repel each other and the energy of this repulsion is $U(\tilde{L}) \approx 32E_0 \exp(-\tilde{L}/\Lambda)$, where $\tilde{L}$ is the distance between the kinks and Λ is their width. If we define the coordinate of the Nth kink as $y_N = LN + \zeta_N$, where L is the equilibrium distance between the kinks and ζ_N are their small displacements from the equilibrium positions, the total energy of the system approximately reads as

$$E = \sum_N \left\{ \frac{1}{2} M \left(\frac{d\zeta_N}{dt} \right)^2 + 32E_0 \exp\left(-\frac{L}{\Lambda} \right) \left[\exp\left(-\frac{\zeta_N - \zeta_{N-1}}{\Lambda} \right) + \frac{\zeta_N - \zeta_{N-1}}{\Lambda} \right] \right\}, \tag{18}$$

where the last term appears due to the incommensurability of the structure and is connected with the last term in (4). This energy corresponds to the exactly-integrable Toda model [9]. It is well known that the Toda lattice admits exact solutions only for one-parameter nonlinear excitations which correspond to the above-discussed kinks propagating through the kink lattice. But it is possible to find approximate solutions for small-amplitude periodical (in time) nonlinear excitations using an asymptotical procedure. We restrict ourselves to the small-amplitude approximation in which $\zeta_N - \zeta_{N-1} << \Lambda$. It is then possible to expand the exponential function in (18) up to nonlinear term of the fourth power in its argument. In this approach the dynamical equations for the effective chain of kinks have the form

$$G(d^2\zeta_N/dt^2) + (2\zeta_N - \zeta_{N+1} - \zeta_{N-1})[1 - (\zeta_{N+1} - \zeta_{N-1})/2\Lambda + (\zeta_N^2 + \zeta_{N+1}^2 + \zeta_{N-1}^2 - \zeta_N\zeta_{N+1} - \zeta_N\zeta_{N-1} - \zeta_{N+1}\zeta_{N-1})/6\Lambda^2] = 0, \tag{19}$$

where $G = (M\Lambda^2/32E_0)\exp(L/\Lambda) \approx 4/\omega_1^2$. Near the lower boundary of the gap $(\omega \approx \omega_1)$ the neighbouring kinks oscillate in opposite phases, and it is convenient to introduce the new variables $\zeta_N = \phi_N$ for even sites $N = 2n$ and $\zeta_N = \chi_N$ for $N = 2n+1$. In the long-wave approximation in terms of relative displacements of neighbouring kinks $P = \phi - \chi$, displacements of their centres of masses $Q = \phi + \chi$ and continuous coordinate $Z = NL$, Eq. (19) may be reduced to the following system of equations:

$$GP_{tt} + 4P + L^2 P_{ZZ} + (2/3\Lambda^2)P^3 - (2L/\Lambda)PQ_Z = 0, \tag{20}$$

$$GQ_{tt} - L^2 Q_{ZZ} + (2L/\Lambda)PP_Z = 0. \tag{21}$$

Near the lower boundary of the gap where the value of parameter $G\omega^2 - 4$ is small $(\propto \varepsilon^2, \varepsilon << 1)$, we have in the main approximation $P \sim \varepsilon$, $Q \sim \varepsilon$, and $L\partial/\partial Z \sim \varepsilon$. So, in "the rotating phase approximation" $P \approx p(Z)\sin(\omega t)$ it follows from Eq. (21) that $Q_Z \approx p^2(Z)/(2L\Lambda)$ and the equation for $p(Z)$ reads

$$L^2 p_{ZZ} = 4[(\omega/\omega_1)^2 - 1]p + p^3/2\Lambda^2. \tag{22}$$

Under the gap, nonlinear excitations have the form of "dark anti-phase solitons"

$$P \approx 2\sqrt{2}\Lambda\sqrt{\omega^2/\omega_1^2 - 1}\tanh(\sqrt{2}\sqrt{\omega^2/\omega_1^2 - 1Z/L})\sin(\omega t), \tag{23}$$

which is accompanied with an extension of the kink lattice: $Q(\pm\infty) \to 4\Lambda(\omega^2/\omega_1^2 - 1)Z/L$. These "near-gap solitons" have a structure different from that for near-gap solitons in modulated structures.

In the gap, the soliton solution has another form:

$$P \approx 4\Lambda\varepsilon\sinh^{-1}(2\varepsilon Z/L), \qquad Q \approx -4\Lambda\varepsilon\coth(2\varepsilon Z/L), \tag{24}$$

where $\varepsilon = \sqrt{1 - \omega^2/\omega_1^2}$. As predicted by the exact solution of the problem, the soliton-like excitations in the gap of the spectrum are accompanied by the total shift of the kinks displacements at infinity. Taking into account the discreteness of Eq. (19) and the initial problem for the kink lattice, we must take $Z/L = N + 1/2$ to avoid a singularity in the centre of this gap soliton.

We hope that the above-discussed nonlinear excitations of incommensurate surface structures may be detected experimentally if the wave with frequency in the gap of the spectrum is excited near the surface.

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Ühismõõduta pinnastruktuuride mittelineaarsed häiritused

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Analüütiliselt on uuritud ruumiliselt perioodilise struktuuriga ühismõõduta pinnakihi dünaamikat. Frenkeli–Kontorova mudeli raamides on kirjeldatud üleminekusolitonidest ja vahesolitonidest koosneva solitonvõre mittelineaarseid häiritusi.