Nonlinear Dynamics of Incommensurate Surface Layers

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We describe analytically the nonlinear dynamics of the incommensurate surface layer (“self-modulated” system) with a spatially periodical structure. 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 investigated.

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Investigation of the nonlinear dynamics of real physical systems, taking into account their discreteness, internal microstructure, and spatial inhomogeneity, 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, for example, 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 Letter, we notice the existence of other gap solitons in systems with spatially homogeneous material parameters but a spatially periodic 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 represents one example of such a system [4–6]. The surface atomic layer in an incommensurate state (see, for instance, [7–9]) is another important example of similar “self-modulated” structure. In all 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. We investigate analytically one-parametric topological solitons (“kinks”) [10] in the gap of the spectrum of incommensurate surface structure using the Darboux transform (see, for instance, [11]).

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 a substrate, the equilibrium distance between these atoms is equal to b and differs from the interatomic distance a in a bulk. The influence of a substrate on surface atoms can be simulated by a periodical potential relief with period a. For simplicity, we approximate this relief by a trigonometric function and assume the substrate to be absolutely hard. Then the potential energy of the system is given by

$$U = \sum_n U_0[1 - \cos(2\pi y_n/a)] + \sum_n \beta(y_n - y_{n-1} - b)^2/2, \quad (1)$$

where y_n is the position of nth atom with respect to the surface layer and β is the elastic constant in the layer. The dynamical equations for the atomic displacements $v_n = y_n - an$ in this Frenkel-Kontorova model [12] have the following form:

$$m v_{n\tau\tau} + (2\pi U_0/a)\sin(2\pi v_n/a) + \beta(2v_n - v_{n+1} - v_{n-1}) = 0, \quad (2)$$

where m is the mass of atom.

In the long-wave approximation for dimensionless variables $u = 2\pi v/a$, $x = n2\pi\sqrt{U_0/\beta}/a$, and $t = \tau 2\pi\sqrt{U_0/m}/a$, we come to the well-known sine-Gordon equation (SGE) [10]:

$$u_{tt} - u_{xx} + \sin u = 0. \quad (3)$$

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

$$U = E_0 \int dx[u_t^2/2 + u_x^2/2 + (1 - \cos u) + \xi u_x], \quad (4)$$

where $E_0 = a\sqrt{\beta U_0}/(2\pi)$, and the incommensurability of the surface layer and substrate is characterized by the dimensionless parameter $\xi = \sqrt{\beta/U_0}(a - b)$. The last term ξu_x in (4) has a divergent form and does not change 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 [4–6]:

$$u_0 = \pi + 2am(z, k), \quad (5)$$

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 first type full elliptic integral. The width of kink expressed in terms of the initial dimensional variables is equal to $\Lambda = a^2\sqrt{\beta/U_0}/(2\pi)$.

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 to the chain at the infinity. But when the parameter ξ exceeds a critical value $\xi_c = -4/\pi$, where $b_c = a + (4/\pi)\sqrt{U_0/\beta}$, 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 [$E(k)$ is the second type full elliptic integral].

Linear excitations on the background of the incommensurate structure (5) are well known [13]. They represent the high-frequency phonon mode in the layer (upper band) and the low-frequency Swihart mode of oscillations of a kink lattice (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 [11] which allows us to find more complicated solutions if an initial ("seed") solution is known [here, solution (5)]. Using the so-called "dressing" procedure for the initial solution $u_0(x)$ (5) and any arbitrary real parameter of the Darboux transform λ [11] we obtain the new real solution $u(x, t)$ describing the motion of an additional kink in the following final form:

$$u(x, t) = u_0(x) - 2i \ln\left\{\frac{\exp(i\kappa_+) - i\exp(\vartheta + i\kappa_-)}{\exp(-i\kappa_+) + i\exp(\vartheta - i\kappa_-)}\right\}, \tag{6}$$

where $\kappa_\pm = (\varphi \pm \rho)/2$, $\tan(\varphi) = dn(z, k)/(2k\mu)$, $\mu = \pm\sqrt{(\lambda + 1/\lambda)^2 - 4/k^2}/4$, $\tan(\rho) = 2sn(z, k)cn(z, k)/[2sn^2(z, k) - \lambda^2 - 1]$, and $\vartheta = 2\mu[t + f(x)]$, with

$$f(x) = (k^2/4)(\lambda^2 - 1/\lambda^2) \int_0^x dx[dn^2(z, k) + (2k\mu)^2]^{-1}. \tag{7}$$

Positive μ corresponds to a $(0, 2\pi)$ additional kink, negative one to a $(2\pi, 0)$ kink. The function $(\varphi \pm \rho)$ can be rewritten as $(\varphi \pm \rho) = \mp am(z, k) \pm am(z \pm \Delta/k, k)$, where the phase shift Δ of the solution 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 $\lambda_0 = (1 + k')/k$, $k' = (1 - k^2)^{1/2}$. This corresponds to a positive value of the function f, i.e., to the kink motion in the negative direction. The domain $0 < \lambda < \lambda_0$ corresponds to the opposite direction of kink motion. The function $f(x)$ in (7) can be expressed as $f(x) = x/v + \chi(x)$, 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 :

$$\langle v\rangle = 4K(k)\left\{k^2(\lambda^2 - 1/\lambda^2) \times \int_0^K dz[dn^2(z, k) + (2k\mu)^2]^{-1}\right\}^{-1}. \tag{8}$$

Consequently, the phase $\vartheta = 2\mu(x + vt)/v + 2\mu\chi(x)$ describes the kink motion in the negative direction with the average velocity v. Such a motion is accompanied by periodical oscillations at the moments when the kink propagates through each kink of the lattice.

In spite of the complexity of the obtained solution (6), it allows 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 additional 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 $s_0 = k'K(k)/E(k)$ which coincides with Swihart velocity, the width of the kink goes to infinity, and the phase shift tends to L: the perfect incommensurate structure rehabilitates itself. The solution (6) 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 the solution (6) describes the propagation of a moving kink through another standing kink: the last term in (6) transforms into the well-known expression for a moving soliton

$$\delta u(x, t) = \pm 4\,\mathrm{arctanexp}\{[x \pm vt - \gamma(x)]/\sqrt{1 - v^2}\}, \tag{9}$$

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 (6) 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 [10]:

$$u = u_0 + 4\arctan\left[\frac{\lambda_1 + \lambda_2}{\lambda_1 - \lambda_2}\tan\frac{u(\lambda_1) - u(\lambda_2)}{4}\right], \quad (10)$$

where the parameters of Backlund transform λ_1 and λ_2 are the same as the parameters λ in the previous Darboux transform.

In the simplest case of a trivial ground state $u_0 = 0$ we can choose in (10) the solutions for moving kink and antikink $u(\lambda_{1,2}) = \pm 4\,\mathrm{arctanexp}[(x - vt)/\sqrt{1 - v^2}]$ with $\lambda_1 = 1/\lambda_2 = -\sqrt{(1 - v)/(1 + v)}$ and opposite velocities as $u(\lambda_{1,2})$. Then formula (10) represents a two-soliton solution with an immobile center of masses. With $i\omega$ replacing v $[\lambda_1 = \lambda_2^* = -\exp(-i\omega)]$, the solution $u(x, t)$ from (10) 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 (10). Then the solution (6) with $\lambda = \lambda_1$ and $\mu = \mu_1$ may be taken as $u(\lambda_1)$ in (10). Another solution (6) 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 allows 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 $\omega_2 = 1/k$ corresponds to the lower boundary of the phonon band. At the lower boundary of the gap this excitation transforms into small-amplitude antiphase oscillations of the kinks, which form the incommensurate structure. In the vicinity of the frequency ω_1, the localized solitonlike 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 as 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 $L \gg 1$ ($k' \ll 1$) can be treated as a lattice of weakly interacting quasiparticles. The coordinates of these particles play the role of collective variables. From the well-known expression [10] for the energy of the moving SGE-kink $E = 8E_0/\sqrt{1 - v^2/c^2}$ (where $c = \sqrt{\beta a^2/m}$ is the limiting velocity of linear waves), it is easy to calculate the effective mass of a kink: $M = 4m\sqrt{U_0/\beta}/(\pi a)$. An effective potential energy of the interaction of two kinks with the same signs can be found from the exact two-kink solution. 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 reads as

$$E = \sum_N \{M(d\zeta_N/dt)^2/2 + 32E_0\exp(-L/\Lambda)\{\exp[-(\zeta_N - \zeta_{N-1})/\Lambda] + (\zeta_N - \zeta_{N-1})/\Lambda\}\}, \quad (11)$$

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 [10]. It is well known that the Toda lattice allows 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 $(\zeta_N - \zeta_{N-1}) \ll \Lambda$. It is then possible to expand the exponential function in (11) up to a nonlinear term of the fourth power in its argument. In this approach the dynamical equations for the effective chain of kinks have the form

$$G(d^2\zeta_N/dt^2) + (2\zeta_N - \zeta_{N+1} - \zeta_{N-1}) \times [1 - (\zeta_{N+1} - \zeta_{N-1})/(2\Lambda) + (\zeta_N^2 + \zeta_{N+1}^2 + \zeta_{N-1}^2 - \zeta_N\zeta_{N+1} - \zeta_N\zeta_{N-1} - \zeta_{N+1}\zeta_{N-1})/(6\Lambda^2)] = 0, \quad (12)$$

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 neighboring kinks oscillate in opposite phases, and it is convenient to introduce the new variables $\zeta_N = \phi_N$ for even sites $N = 2n$ and $\zeta_N = \sigma_N$ for $N = 2n + 1$. In the long-wave approximation in terms of relative displacements of neighboring kinks $P = \phi - \sigma$, displacements of their centers of masses $Q = \phi + \sigma$ and continuous coordinate $Z = NL$, Eq. (12) can be reduced to the following system of equations:

$$GP_{tt} + 4P + L^2 P_{ZZ} + 2P^3/(3\Lambda^2) - 2LPQ_Z/\Lambda = 0, \tag{13}$$

$$GQ_{tt} - L^2 Q_{ZZ} + 2LPP_Z/\Lambda = 0. \tag{14}$$

Near the lower boundary of the gap where the value of parameter $(G\omega^2 - 4) \sim \varepsilon^2$ is small ($\varepsilon \ll 1$), we have in the main approximation $P \sim \varepsilon$, $Q \sim \varepsilon$. In the "rotating phase approximation" $P \approx p(Z)\sin(\omega t)$ it follows from Eq. (14) that $Q_Z \approx p^2(Z)/(2L\Lambda)$ and the equation for $p(Z)$ reads

$$L^2 p_{ZZ} = 4p[(\omega/\omega_1)^2 - 1] + p^3/(2\Lambda^2). \tag{15}$$

Under the gap, nonlinear excitations have the form of "dark antiphase solitons"

$$P \approx 2\sqrt{2}\Lambda\sqrt{(\omega/\omega_1)^2 - 1} \times \tanh[\sqrt{2}\sqrt{(\omega/\omega_1)^2 - Z/L}]\sin(\omega t), \tag{16}$$

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

In the gap, the soliton solution has another form:

$$P \approx 4\Lambda\varepsilon \sinh^{-1}(2\varepsilon Z/L)\sin(\omega t), \quad Q \approx -4\Lambda\varepsilon \coth(2\varepsilon Z/L), \tag{17}$$

where $\varepsilon = \sqrt{(\omega/\omega_1)^2 - 1}$. As predicted by the exact solution of the problem, the solitonlike 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. (12) and the initial problem for the kink lattice, we must take $Z/L = N + 1/2$ to avoid a singularity in the center of this gap soliton.

In conclusion, we note that the investigation of the problem was performed within the continuum approximation. The discreteness of the system and the existence of the Pierls relief can essentially change the dynamics of the system. But the gap character of the spectrum of linear waves of the "self-modulated" system and the unusual properties of gap solitons in such system shall be kept.

Finally, we studied analytically the nonlinear dynamics of the incommensurate structure of a surface atomic layer with a spatially periodic ground state. The nonlinear excitations of the periodic soliton lattice (moving additional kinks and gap solitons) were investigated in the framework of the Frenkel-Kontorova model. The results can be of importance for the description of a fluxon lattice in a long Josephson junction in an external magnetic field (essentially continuous system). We think that the nonlinear excitations of incommensurate surface structure discussed above may be detected experimentally if the wave with frequency in the gap of the spectrum will be excited near the surface.

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