Intrinsic localized modes as solitons of the discrete Hirota equation

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It is shown that intrinsic localized modes in a nonlinear lattice with a hard quartic nonlinearity are governed by the discrete Hirota equation. The requirement for the solution to be real results in a very restricted class of admissible soliton solutions corresponding to the localized excitations. In particular, it is shown that a single-soliton solution exists only at definite values of the amplitude and velocity. Two-soliton and multisoliton localized-mode solutions are reperesented. A small parameter of the problem is discussed. [S1063-651X(96)06507-5]

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I. INTRODUCTION

Since works [1] where the intrinsic localized modes were obtained a great number of papers devoted to the subject has been published. In spite of this, to the best of our knowledge, a consistent mathematical theory of the highly localized solutions on nonlinear lattices has not been elaborated, while in most previous investigations various analytical approximations were verified numerically. Speaking about the self-consistent theory we mean, first of all, a perturbative expansion of the solutions with respect to *only* small parameter at *all stages* of the so-called *rotating wave approximation*. Therefore the first aim of the present paper is to provide such an expansion.

The second purpose of the paper is to show that the intrinsic localized modes in the leading order are *solitons* in the narrow mathematical sense, i.e., that they are governed by an exactly integrable equation (and in this sense they can be considered as a counterpart of the envelope lattice solitons [2]). As a matter of fact, a deep relation of the intrinsic localized modes with solutions of the Ablowitz-Ladik (AL) model [3] has been realized in the papers [4,5]. However, no one has yet reported directly obtaining the AL model starting with a lattice Hamiltonian [see (1) below]. Here we fill the gap in the theory and show that the most convenient analytical treatment of the intrinsic localized modes can be given in terms of the discrete Hirota (DH) equation, which, meantime, is consistent with the AL model mentioned in [6,4]. This will give us an explanation of the stability of the localized modes observed in numerical experiments [7,8], will prove that they indeed are dynamical objects (this was noticed in [6,4]), and will allow us to represent multisoliton solutions for highly localized modes.

The paper is organized as follows. In Sec. II we provide the perturbative expansion, which corresponds to the method usually referred to as the rotating wave approximation. Section III is devoted to the discussion of various soliton solutions. The outcomes are summarized in the Conclusion.

II. ROTATING WAVE APPROXIMATION

We study a monoatomic lattice described by the Hamiltonian

$$H=\sum_n \left[\frac{M}{2}\dot{u}_n^2+\frac{K_2}{2}(u_{n+1}-u_n)^2+\frac{K_4}{4}(u_{n+1}-u_n)^4\right], \tag{1}$$

where $u_n=u_n(t)$ is a displacement of the nth atom having a mass M, K_2 and K_4 are harmonic and quartic anharmonic force constants, correspondingly, and a dot stands for the derivative with respect to time. Looking for a displacement field which allows representation [6,4]

$$u_{n+1}-u_n=2\phi_n(t)\cos(kna-\omega t), \tag{2}$$

$\phi_n(t)$ being an unknown function, k and ω being constant wave number and frequency, and a being a lattice constant, one obtains the following dynamical equation for $\phi_n(t)$:

$$\begin{aligned}&\{\ddot{\phi}_n-\omega^2\phi_n-J_2[(\phi_{n+1}+\phi_{n-1})\cos(ka)-2\phi_n]-3J_4[(\phi_{n+1}^3+\phi_{n-1}^3)\cos(ka)-2\phi_n^3]\}\cos(\psi_n)\\ &\quad+\{2\omega\dot{\phi}_n+J_2(\phi_{n+1}-\phi_{n-1})\sin(ka)+3J_4(\phi_{n+1}^3-\phi_{n-1}^3)\sin(ka)\}\sin(\psi_n)+J_4(\phi_{n+1}^3-\phi_{n-1}^3)\sin(3ka)\sin(3\psi_n)\\ &\quad-J_4[(\phi_{n+1}^3+\phi_{n-1}^3)\cos(3ka)-2\phi_n^3]\cos(3\psi_n)=0.\end{aligned} \tag{3}$$

Here $\psi_n=kna-\omega t$ is a ''rotating'' variable, and $J_{2,4}=K_{2,4}/M$.

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Let us define a small parameter, μ, of the problem through the relations

$$\phi_{n+1}+\phi_{n-1}-2\kappa\phi_n=\mu f_n, \quad \phi_{n+1}\phi_{n-1}-\phi_n^2=\mu g_n, \tag{4}$$

where $\kappa=\pm 1$, f_n and g_n are functions of the order of ϕ_n and ϕ_n^2, respectively: $f_n=O(\phi_n)$ and $g_n=O(\phi_n^2)$. Notice, *a priori*, ϕ_n is not assumed to be small. Formulas (4), which are assumed to be consistent, determine the basic approximation explored below.

If we concentrate on the points $ka=\pi/3$ and $ka=2\pi/3$, then the coefficient of $\sin(3\psi_n)$ in (3) describing the cubic harmonic becomes zero. By using (4) it is not difficult to show that the last term in (3) is of the order of $\mu\phi_n^3$ if κ is chosen such that it is 1 for $ka=2\pi/3$ and is -1 for $ka=\pi/3$. Hence taking into account that the respective term represents a cubic harmonic we can drop it [9].

Roughly speaking, after the above approximation the coefficients multiplied by the sine and cosine functions in (3), being simultaneously equated to zero, constitute a pair of equations determining both the space-time evolution of the localized intrinsic modes, i.e., ϕ_n, and the fundamental frequency ω, respectively [4,6]. (It is assumed, of course, that these equations are coordinated.) Then, the points $ka=\pi/3, 2\pi/3$ may be considered as corresponding to particular points in the Brillouin zone of the underlying harmonic lattice, at which mixing of the fundamental mode (or carrier wave, as it is sometimes called) with higher harmonics (with frequency 3ω) vanishes.

For the next step we introduce designations

$$\alpha_n=\ddot{\phi}_n-\Delta\phi_n-3J_4[(\phi_{n+1}+\phi_{n-1})(\phi_{n+1}^2+\phi_{n-1}^2-3\phi_n^2-\phi_{n+1}\phi_{n-1})\cos(ka)-2\phi_n^3], \tag{5}$$

$$\beta_n=3J_4[\phi_{n+1}^3-\phi_{n-1}^3-3(\phi_{n+1}-\phi_{n-1})\phi_n^2]\sin(ka), \tag{6}$$

$$\Delta=\omega^2-2(J_2+\mathcal{J}), \tag{7}$$

$\gamma^2=9J_4/J_2$, where Δ and $\mathcal{J}$ are real constants to be determined below. Then (3) is rewritten as

$$\{-2\mathcal{J}\phi_n-J_2\cos(ka)(\phi_{n+1}+\phi_{n-1})(1+\gamma^2\phi_n^2)+\alpha_n\}\cos\psi_n+\{2\omega\dot{\phi}_n+J_2\sin(ka)(\phi_{n+1}-\phi_{n-1})(1+\gamma^2\phi_n^2)+\beta_n\}\sin\psi_n=0. \tag{8}$$

Taking into account that all quantities in (8) are real, it is not difficult to conclude that the mentioned equation can be written down in the complex form

$$\{i2\mathcal{J}\phi_n+iJ_2\cos(ka)(\phi_{n+1}+\phi_{n-1})(1+\gamma^2\phi_n^2)-i\alpha_n+2\omega\dot{\phi}_n+J_2\sin(ka)(\phi_{n+1}-\phi_{n-1})(1+\gamma^2\phi_n^2)+\beta_n\}e^{i\psi_n}+\text{c.c.}=0. \tag{9}$$

The main advantage of the last equation comes from the fact that at $\alpha_n\equiv\beta_n\equiv 0$ it takes the form of the DH equation integrable by means of the inverse scattering technique [10]. This allows us to proceed in the following way. First, we show that under the assumption that in the leading order ϕ_n solves (9) with $\alpha_n\equiv\beta_n\equiv 0$ and subject to appropriate choice of the solution the terms α_n and β_n can be made small enough. Then we represent various solutions for the localized modes in the leading order as solitons of the DH equation and discuss the small parameter of the problem.

To this end we notice that it is a direct consequence of (4) that $\beta_n=O(\mu^{3/2}\phi_n^3)+O(\mu^2\phi_n^2)$. In order to estimate α_n we take into account that (4) implies $f_{n+1}+f_{n-1}-2\kappa f_n=O(\mu\phi_n)$. This allows us to obtain

$$\ddot{\phi}_n=\left[\frac{J_2}{2\omega}\cos(ka)\right]^2[2\kappa(\phi_{n+1}+\phi_{n-1})-8\phi_n]-\Delta\phi_n+O(\mu^2\phi_n). \tag{10}$$

By choosing

$$\Delta=-\kappa\frac{J_2^2}{\omega^2}\cos^2(ka) \tag{11}$$

we reduce (10) to

$$\ddot{\phi}_n=\mu\kappa\frac{J_2^2}{2\omega^2}\cos^2(ka)f_n+O(\mu^2\phi_n).$$

Hence the term under consideration is estimated as

$$\alpha_n=\mu\kappa\frac{J_2^2}{2\omega^2}\cos^2(ka)f_n+O(\mu^2\phi_n)+O(\mu\phi_n^3). \tag{12}$$

As will be shown below, $\phi_n^2=O(\mu)$ and that is why α_n is comparable with the nonlinear terms in (9) and cannot be dropped. Meantime, looking for the solution of (9) in the form

$$\phi_n=\phi_n^{(0)}+\mu\phi_n^{(1)}, \tag{13}$$

where $\phi_n^{(0)}$ and $\phi_n^{(1)}$ are of the order of ϕ_n and $\phi_n^{(1)}$ solves the equation

$$2\mathcal{J}\phi_n^{(1)}+J_2\cos(ka)(\phi_{n+1}^{(1)}+\phi_{n-1}^{(1)})=\kappa\frac{J_2}{2\omega^2}f_n, \tag{14}$$

we can eliminate the higher order contribution to α_n, without any change (in the leading order) of the term in (8) which is proportional to $\sin\psi_n$. The last statement is a consequence of the explicit form of $\phi_n^{(1)}$:

$$\phi_n^{(1)} = \frac{\kappa J_2}{2\sqrt{3}\omega^2} \sum_{m=-\infty}^{\infty} f_{n-m}[\kappa(\sqrt{3}-2)]^{|m|}, \tag{15}$$

of the representation for f_n, and of the fact that within the accuracy accepted

$$2\omega\dot{\phi}_n^{(0)} + J_2 \sin(ka)(\phi_{n+1}^{(0)} - \phi_{n-1}^{(0)}) = O(\phi_n^3).$$

One more important consequence of (15) to be mentioned here is the fact that if $\phi_n^{(0)}$ is bounded in time and localized in space, then $\phi_n^{(1)}$ possesses the same properties.

Now introducing a complex function

$$q_n = \gamma \exp\left(i \frac{\mathcal{J}}{\omega} t \right) \phi_n^{(0)} \tag{16}$$

we arrive at the conventional form of the DH equation, which in the case at hand describes the particle displacement field

$$\dot{q}_n + i \frac{J_2}{2\omega} \cos(ka)(q_{n+1} + q_{n-1})(1 + |q_n|^2) + \frac{J_2}{2\omega} \sin(ka) \times (q_{n+1} - q_{n-1})(1 + |q_n|^2) = 0. \tag{17}$$

III. SOLITON SOLUTIONS FOR THE LOCALIZED MODES

Let us analyze the ''unperturbed'' equation (17). First, it is interesting to mention that due to the special relation between the constant coefficients it is reduced to the AL model by the substitution $q_n = e^{ikna} Q_n$. However, in such a way the rotating phase ψ_n appears in the dynamical equation again and the function Q_n has an initial form different from that of ϕ_n. Due to this reason in what follows we prefer to deal with the DH equation rather than with the respective AL model. Next, we notice that in spite of the fact that the DH equation is integrable not all its solutions make physical sense. A very strong restriction comes from the requirement for ϕ_n to be real.

In order to explain the last statement let us consider some points of the inverse scattering scheme applied to the DH equation. A multisoliton solution can be written in the form (see [11] where a multisoliton solution for the AL model is represented)

$$q_n = \frac{2i}{\det D} \sum_{l=1}^{N} c_l z_l^{n+1} \det D^{(l)}. \tag{18}$$

Here D is an $N \times N$ matrix with the element $D_{kj} = \delta_{kj} + 4\sum_{l=1}^{N} \alpha_{lk}(n)\alpha_{lj}(n) c_k \overline{c_l}$ (δ_{kj} being the Kronecker delta and the bar standing for the complex conjugation), $D^{(l)}$ is obtained from D by substituting the lth column in D by $\mathrm{col}(z_1^{n-1}, \ldots, z_N^{n-1})$,

$$z_m = \exp(-w_m + i\theta_m), \tag{19}$$

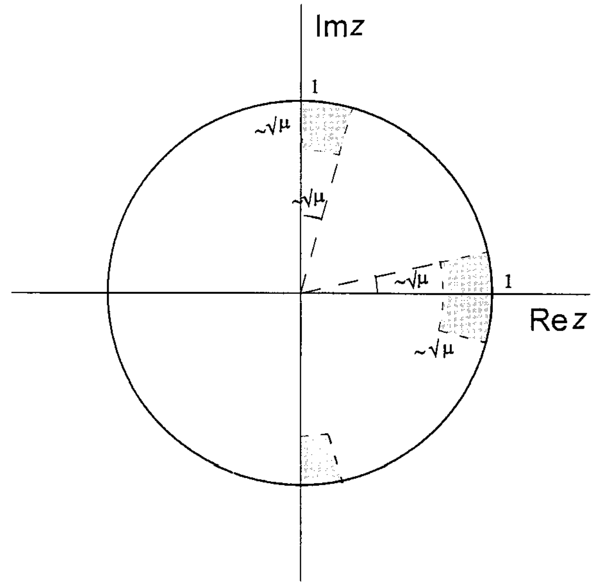

FIG. 1. The polygons painted over correspond to regions where the complex conjugate pairs $(z_m, \overline{z_m})$ can be chosen in order to fulfill all the requirements imposed in the derivation of the DH equation. The regions near the imaginary and real axes correspond to the carrier wave numbers $\pi/3$ and $2\pi/3$. By $\sim\sqrt{\mu}$ we emphasize the characteristic scale of the respective regions.

$m = 1, \ldots, N$, are eigenvalues of the problem

$$\Phi_{n+1} = \begin{pmatrix} z & i\overline{q_n} \\ iq_n & z^{-1} \end{pmatrix} \Phi_n \tag{20}$$

placed inside the unit circle on the right half plane of the complex z (respectively, w_m and θ_m are real, $w_m > 0$ and $-\pi/2 < \theta_m \leqslant \pi/2$, see Fig. 1),

$$\alpha_{lm}(n) = \frac{(\overline{z_m} z_l)^{n+1}}{1 - (\overline{z_m} z_l)^2}, \tag{21}$$

and the coefficients c_m depend on time according to the formula

$$c_m(t) = c_m(0) \exp\left[it \frac{J_2}{\omega} \cos(2\theta_m + ka) \cosh(2w_m) \right] \times \exp\left[t \frac{J_2}{\omega} \sin(2\theta_m + ka) \sinh(2w_m) \right]. \tag{22}$$

In (18) N is a number of eigenvalues of (20) in the right half plane.

We are interested in solutions of the Cauchy problem (17) subject to real initial conditions $\mathrm{Im} q_n(0) = 0$. The complexity is allowed to appear with time only through the harmonic exponent $\exp[i(\mathcal{J}/\omega)t]$ [this gives a real $\phi_n^{(0)}$, see (16)]. The mentioned initial condition implies that (i) the eigenvalues either appear only in complex conjugate pairs, say $\theta_m = -\theta_{m+1}$ and $w_m = w_{m+1}$, or are placed on the real, $\theta_m = 0$, or imaginary $\theta_m = \pi/2$, axes, and correspondingly (ii) the respective coefficients $c_m(0)$ either satisfy the relation $c_m(0) = -\overline{c_{m+1}}(0)$ or $c_m(0)$ is pure imaginary. Taking into account that z_m does not depend on time, from the explicit form (18) one concludes that the above requirements for the solution of the DH equation are fulfilled if $c_m(t)=\tilde{c}_m(t)\exp[i(\mathcal{J}/\omega)t]$, where in the case of complex conjugate pairs $\tilde{c}_m(t)$ holds the property $\tilde{c}_m(t)=-\tilde{c}_{m+1}(t)$ at any moment of time. It follows from (22) that the last relation takes place if

$$J_2\cos(ka+2\theta_m)\cosh(2w_m)=-\mathcal{J}. \tag{23}$$

Below we will see that in fact the last formula gives a relation between the soliton parameters and the frequency of the carrier wave.

Let us now discuss physical aspects of the above findings. Starting with a one-soliton solution we note that $\theta_m=0$ or $\theta_m=\pi/2$. Then taking $N=1$ we obtain

$$\phi_n^{(0)}=\frac{\kappa^n}{\gamma}\frac{\sinh(2w_1)}{\cosh[2w_1(n-n_0)-\kappa(J_2/\omega)\sinh(2w_1)\sin(ka)t]}, \tag{24}$$

where n_0 is a constant defined by $n_0=(1/2w_1)\ln[|c_1(0)|/\sinh(2w_1)]$. Thus the space-time evolution of the ''discrete envelope'' $\phi_n^{(0)}$ of the one-soliton solution is characterized by the wave number $K=2w_1/a$ and the frequency $\Omega=(J_2/\omega)\sinh(Ka)\sin(ka)$. Then, calculating the soliton velocity $V=\kappa(\Omega/K)$ with the accuracy $O(\mu)$ we arrive at the result $V=\kappa(d\omega/dk)$. Hence the soliton moves with the group velocity of the linear carrier wave, but the direction of its propagation depends on κ.

Recalling the requirement (4) we conclude that the choice of θ_1 must depend on κ. Namely, there is a relation $\theta_1=[(1-\kappa)/2]\pi$.

Now we are at the point to discuss the small parameter μ. To this end we substitute (24) in (4) and obtain that the right hand side of both expressions in (4) is small provided

$$\mu=\sinh^2(2w_1)\ll 1. \tag{25}$$

As is seen from this formula, the soliton amplitude is not necessarily very small: it is proportional to $\sqrt{\mu}$. It is important to note that the last fact coordinates with all the steps of the perturbative scheme developed above.

In the case at hand the frequency $2(J_2+\mathcal{J})$ coincides with the frequency of the linear spectrum and hence Δ gives the shift of the localized-mode frequency with respect to the spectrum of the linear chain. Formula (24) recovers the solutions found in [6,4].

Passing to the two-soliton solution, first of all we notice that as follows from (23) there are no multisoliton solutions corresponding to different eigenvalues z_m located on the positive real axis (see also the discussion below). Hence in order to calculate the two-soliton solution one has to consider a pair of complex conjugate eigenvalues, say z_1 and $z_2=\bar{z}_1$. For the sake of definiteness $\theta_1\in[0,\pi/2]$ will be taken. Then, it is straightforward to show that in this case the solution (18) takes the form

$$\begin{aligned}\phi_n^{(0)}(t)=\frac{1}{\gamma}(2\sin^2\theta_1 e^{\zeta_n(t)}\{&2\sinh^2(2w_1)\sqrt{\sinh^2(2w_1)+\sin^2(2\theta_1)}\sin(2\theta_1 n+\varphi+\delta_1)\\&-\sinh(2w_1)[\cosh(4w_1)+\cos(2\theta_1)]\sin(2\theta_1 n+\varphi+\delta_2)\}\\&+\sinh(2w_1)\sin(2\theta_1 n+\varphi)[\sinh^2(2w_1)+\sin^2(2\theta_1)]e^{-\zeta_n(t)})\\&\times\{\sin^2(2\theta_1)\cosh^2[\zeta_n(t)+\zeta]+\sinh^2(2w_1)\sin^2(2\theta_1 n+\varphi+\delta_1)\}^{-1}.\end{aligned} \tag{26}$$

Here

$$\zeta_n(t)=-2w_1(n-n_0)+t\frac{J_2}{\omega}\sin(2\theta_1+ka)\sinh(2w_1), \tag{27}$$

$$\delta_1=\arg\sinh(2w_1-2i\theta_1), \tag{28}$$

$$\tan\frac{\delta_2}{2}=2\tan(\theta_1)\frac{\cosh^2(2w_1)+\cos(2\theta_1)}{\sinh(4w_1)}, \tag{29}$$

$$\zeta=\ln\frac{\sin(2\theta_1)}{2\sqrt{\sinh^2(2w_1)+\sin^2(2\theta_1)}}, \tag{30}$$

$\varphi=\arg c_1(0)$ is a real constant, and n_0 has been defined above.

We start the discussion of the two-soliton solution with the fact that (26) reduces to the one-soliton solution (24) in the limits $\theta_1\to 0$, $\pi/2$. The respective solitons have been interpreted in [4] as different branches of the localized modes. Now we can generalize that interpretaion by considering (24) as different limits of the family of the two-soliton solutions parametrized by θ_1.

The small parameter in the case at hand is determined by (25). This is a general result which follows directly from the explicit expression for the multisoliton solution (18). Thus one can say that the *intrinsic localized modes are small amplitude solitons of the DH equation* which correspond to zeros of the Jost coefficient $a(z)$ placed in the vicinity of the unit circle. Moreover, returning once more to the basic requirement (4) we found that the two-soliton solution is coordinated with all suppositions made above only if $\theta_1\sim\sqrt{\mu}$ or $\pi/2-\theta_1\sim\sqrt{\mu}$. Bearing in mind the two-soliton solution, in Fig. 1 we schematically represent regions in the complex z

plane, where the pair of the eigenvalues $(z_1,\overline{z_1})$ must be chosen.

The fundamental frequency ω of the localized-mode solution is obtained from the system of equations (7), (11), and (23). Considering the branch which lies above the spectrum of the linearized lattice (17) we calculate

$$\omega^2 = J_2\left[\left(1+\frac{\kappa}{2}\right)+\sqrt{3}\vartheta_\kappa+\sqrt{\frac{5+3\kappa}{4}+\sqrt{3}(2+\kappa)\vartheta_\kappa}\right] + O(\mu J_2). \tag{31}$$

Here $\vartheta_{-1}=\pi/2-\theta_1$ and $\vartheta_1=\theta_1$. As has been mentioned in [7] in the case of $\kappa=1$, $\theta_1=0$, the frequency of the localized mode is less than the frequency of the linear chain, $\omega_{\rm lin}^2=3J_2$. In the case of the two-soliton solution the situation is changed. At $\kappa=1$ the frequency increases with θ_1 and the critical value at which ω^2 turns out to be greater than $\omega_{\rm lin}^2$ is estimated to be $\theta_c\approx 0.024$. Thus almost in the whole admissible region of the parameters of the two-soliton solution (excluding a narrow neighborhood of the real axis) $\omega^2>\omega_{\rm lin}^2$.

In the case of N-soliton solution $(N=2p,\ p=2,3,\dots)$ the relation (23) results in new restrictions of the choice of the eigenvalues z_m. Besides belonging to the region painted over in Fig. 1, they must be placed on the curve in the z plane determined by $\mathcal{J}$. In particular, one can say that the eigenvalues z_m must be placed in the neighborhood of a radius $\theta_m=$const (the size of the neighborhood is estimated to be of order μ). In this context returning to the above conclusion about the two eigenvalues belonging to the real axis we can consider respective solutions as approximations to a four-soliton solution in the ''near degenerate'' case.

IV. CONCLUSION

To conclude we have shown that the intrinsic localized modes are governed (in the leading order) by the DH equation. This gives an explanation of the remarkable stability of the modes in various numerical experiments, on the one hand, and, on the other hand, provides us with analytical tools of the detail and self-consistent study of the localized-mode dynamics. The latter can be done within the framework of the perturbation theory for solitons. Also, as far as the model is reducible to exactly integrable [see (17)] we were able to represent a multisoliton localized-mode solution. In solitonic terms a localized-mode solution is parametrized by a complex eigenvalue, the phase of which determines the fundamental frequency while its absolute value determines the amplitude of the mode.

We have defined the small parameter of the theory and have shown that the evolution of a nonlinear localized mode is accompanied by excitation of a linear harmonic [see (15)]. The DH equation obtained in this paper is intrinsically related to the AL model which in the continuum limit is nothing but a nonlinear Schrödinger equation, appearing in the theory of envelope solitons. Meantime, it follows from the above results that any approach based on the envelope function approximation cannot take into account all features of the dynamics, especially in the ''highly discrete limit'' (when $\mu\approx 0.01$–0.1) since the width of a localized mode is of the order of the square root of the small parameter. The solutions obtained here are basically different from the conventional pulselike solitons having the form of $\mathrm{sech}(kx-\omega t)$, known to exist for $v_n=u_{n+1}-u_n$ in the continuum limit.

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[9] Strictly speaking, representation (2) must be written down in the form of a sum including all higher harmonics. Subject to the conditions imposed in the present paper, they have amplitudes much smaller than the amplitude of the fundamental harmonic. In this sense the cubic harmonic in (3) is taken into account by the respective terms in the expansion mentioned above rather than dropped. Since, however, we are interested only in the leading order effects it is enough to show that the cubic harmonic is small.

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