# Small-amplitude envelope solitons in nonlinear lattices

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The general theory of small-amplitude envelope solitons in one-dimensional lattices with cubic and quartic nonlinearities is developed. It is shown for a wide diversity of interactions among particles that the dynamics of chain excitations is governed either by the nonlinear Schrödinger equation or by the system of coupled nonlinear Schrödinger equations. In particular, the theory allows the inclusion of lattices with long-range interactions and chains with a complex cell in the unique scheme, which is the envelope function approach. Classes of solitons in diatomic lattices and in chains with long-range interactions are described as particular examples.

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## I. INTRODUCTION

Properties of excitations in anharmonic lattices with nonlinear intersite interactions and on-site potentials were intensively investigated during the last few years. One of the most remarkable discoveries made in the lattice theory was the existence of intrinsic localized modes which are characterized by frequencies placed above the top of the harmonic chain spectrum [1]. The general theory of such stationary nonlinear localized modes has been developed by Takeno [2]. The approach of Takeno, being based on the linear-lattice Green's function expansion, has given a possibility to calculate both a frequency of the localized mode and its structure for any type of linear interactions in the lattice. Also, it has provided the justification of the so-called rotating wave approximation sometimes used for obtaining strongly localized excitations with frequencies located far enough from the top of the harmonic frequency band. In the opposit limit, when the carrier wave (CW) frequency is close to the top of the continuum spectrum, there are well established results in the nonlinear lattice theory, as well. In particular, it has been shown by many authors (see, e.g., [3–9], and references therein) that single-mode excitations of a chain with nearest-neighbor interactions and cubic or quartic nonlinearity are governed by the nonlinear Schrödinger (NLS) equation. The peculiarity of the lattice theory compared with other branches of physics (say, optics) is that the CW is taken to be discrete [3, 5]. For example, it is well known that in the case of the simplest monoatomic chain the CW is nothing more than $\cos[qan-\omega(q)t+\varphi]$ [here $q$ is a vector in the reciprocal space, $a$ is a lattice constant, $n$ is a number of a site, $\omega(q)$ is a frequency, and $\varphi$ is a real constant] and at the boundary of the Brillouin zone (BZ), $q=\frac{\pi}{a}$, it takes the form of the standing wave $(-1)^n\cos(-\omega_{\rm BZ}t+\varphi)$, where $\omega_{\rm BZ}=\omega(\pi/a)$ and the subindex "BZ" hereafter stands for values at the BZ edge. As in the theory of the stationary localized modes [2], the above mentioned approach allows natural generalization including lattices with *arbitrary* interparticle interactions and on-site potentials. Namely, one can develop the theory irrespective of types of interactions among particles (except some rather weak restrictions related to the convergence of the sets). Such a theory is the main goal of the present paper.

The consideration will be based on ideas similar [10] to those elaborated in the theory of optical gap solitons which can propagate in nonlinear periodic media. Indeed, the stationary gap soliton discovered numerically in [11] is the electric field localized inside a stop gap, i.e., at the frequency located above the cutoff frequency of the one of the allowed bands. The physical reason for existence of such an excitation consists of inducing the group velocity dispersion (GVD) by the periodicity [12]. The general theory of the gap solitons with frequencies lying about a stop gap edge [13], also called the envelope function approach, has at least three characteristic features important in the present context. First, it is based on the multiple scale expansion with respect to the only small parameter, which is the amplitude of the field. This gives a justified and self-consistent hierarchy of scales. Second, the CW is taken to be a formal solution of the underlying linear system, which makes the theory general and applicable to any kind of periodic structure. Third, the theory shows the prominent role of the second-order terms of the expansion. In the context of the lattice dynamics the last point has not been discussed in literature in full measure and this is also the purpose of the present paper. In particular, it will be demonstrated that sometimes the second order of the approach determines coupled mode dynamics and imposes rather robust restrictions on possible types of lattice excitations.

Since the discreteness itself originates GVD, which is particularly strong at the BZ edges, and therefore can be regarded as a counterpart of the continuum medium periodicity, it is natural to use a discrete version of the envelope function approach in order to work out the general theory of small-amplitude lattice excitations. Meantime, the existence of a gap itself in the chain spectrum

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is not a necessary condition for creation of envelope solitons and that is why the latter will not be referred to as gap solitons.

Development of the general theory seems to be important for the following reasons: (i) It allows one to relate soliton parameters directly with the spectrum of the respective harmonic lattice without referring to a CW structure. In this context it should be mentioned that lattices are widely used as models for the macromolecule dynamics [6]. From the viewpoint of the applications in biology the phenomena of localization and of energy transport are of much more importance than the lattice pattern itself. Also the general aspects of the theory seem to be especially prominent in view of the recent interest in lattices with long-range interactions [14–16]. (ii) The consideration below is provided for bounded systems and soliton parameters are expressed through the discrete spectrum of the linear chain. This may turn out to be important for quantization of nonlinear lattices. (iii) The general theory allows one to describe not only solitonic solutions but accompanying effects, as well. (iv) Finally, the theory allows description of the *coupled mode dynamics.*

The organization of the paper is as follows. In Sec. II the NLS equation for a single-mode envelope is derived on the basis of the multiscale expansion. Conditions for the envelope function approach to be applicable are studied. Section III is devoted to some examples, which are to illustrate the diversity of effects which can be obtained within the framework of the envelope function approach. We concentrate on the coupled mode dynamics in a diatomic lattice and in a lattice with long-range interactions. In fact Sec. III generalizes the theory for the case of multimode dynamics. The results are summarized in the Conclusion.

## II. THEORY OF ENVELOPE SOLITONS IN LATTICES

### A. Statement of the problem

In order to describe the effect of small perturbations we take into account that the method is based on the small-amplitude expansion and separate the principal Hamiltonian $H_{\rm latt}$ of an unperturbed lattice and an additional one $H_{\rm add}$ describing perturbations. First we consider an unperturbed lattice governed by the Hamiltonian

$$H_{\rm latt}=\frac{1}{2}\sum_{n,\alpha}M_\alpha(n)\left[\frac{d}{dt}u_\alpha(n)\right]^2+\frac{1}{2}\sum_{n_1,\alpha_1}\sum_{n_2,\alpha_2}K_2(n_1,\alpha_1;n_2,\alpha_2)u_{\alpha_1}(n_1)u_{\alpha_2}(n_2)$$
$$+\frac{1}{3}\sum_{n_1,\alpha_1}\cdots\sum_{n_3,\alpha_3}K_3(n_1,\alpha_1;\ldots;n_3,\alpha_3)u_{\alpha_1}(n_1)\cdots u_{\alpha_3}(n_3)$$
$$+\frac{1}{4}\sum_{n_1,\alpha_1}\cdots\sum_{n_4,\alpha_4}K_4(n_1,\alpha_1;\ldots;n_4,\alpha_4)u_{\alpha_1}(n_1)\cdots u_{\alpha_4}(n_4), \tag{1}$$

where $u_\alpha(n)$ is a small displacement from the equilibrium position associated with the $\alpha$th degree of freedom in the $n$th cell (here we use parametrization similar to [2]). The physical sense of the components $u_\alpha(n)$ may be different. If, for example, a monoatomic lattice is under consideration then $u_\alpha(n)$ is the $\alpha$th component of the displacement vector of the $n$th particle, and the positive quantity $M_\alpha(n)$ is a constant (i.e., does not depend on $n$ and $\alpha$) making a sense of a particle mass. Bearing in mind this interpretation of $u_\alpha(n)$ we use the names *scalar* lattice for the case $\alpha=1$ and *vector* lattice if $\alpha$ takes more than one value (but everywhere it will be assumed that the number of degrees of freedom is finite, say $\alpha\le N_0$, $N_0$ being an integer). Below in the case of a scalar lattice the index $\alpha$ is dropped. Meanwhile $u_\alpha(n)$ allows also another treatment (it is given in Sec. III) and in this sense the name "vector" is conditional. The real coefficients $K_m$ in (1) are force constants. They have properties

$$K_2(n_1,\alpha_1;n_2,\alpha_2)=K_2(n_2,\alpha_2;n_1,\alpha_1), \tag{2}$$

$$K_3(n_1,\alpha_1;n_2,\alpha_2;n_3,\alpha_3)=K_3(n_2,\alpha_2;n_1,\alpha_1;n_3,\alpha_3)=\cdots \tag{3}$$

(the same symmetry with respect to permutations of the arguments is valid for $K_4$, as well). Note, if the chain possesses the translational symmetry then there are additional properties

$$\sum_{n_1,\alpha_1}K_2(n_1,\alpha_1;n_2,\alpha_2)=\cdots=\sum_{n_1,\alpha_1}K_p(n_1,\alpha_1;\ldots;n_p,\alpha_p)=0 \tag{4}$$

[the summing over $\alpha_1$ can be dropped when $u_\alpha(n)$ is a coordinate of a conventional spatial displacement vector $\vec{u}(n)$]. Though the last relations simplify consideration, they are not imposed at the beginning.

Using new notations [2] $v(x)=\sqrt{M_\alpha(n)}u_\alpha(n)$ and

$$J_p(x_1;\ldots;x_p)=\frac{K_p(n_1,\alpha_1;\ldots;n_p,\alpha_p)}{[M_{\alpha_1}(n_1)\cdots M_{\alpha_p}(n_p)]^{1/2}}, \tag{5}$$

where $x_p$ stands for the pair of variables $(n_p,\alpha_p)$, the equations of lattice dynamics can be written as

$$\ddot{v}(x) = -\sum_{x_1} J_2(x;x_1)v(x_1) - \sum_{x_1}\sum_{x_2} J_3(x;x_1;x_2)v(x_1)v(x_2) - \sum_{x_1}\sum_{x_2}\sum_{x_3} J_4(x;x_1;x_2;x_3)v(x_1)v(x_2)v(x_3), \tag{6}$$

where an overdot stands for the derivative with respect to time. As follows from the properties of $K_p$ the coefficients $J_p$ are symmetrical with respect to permutations of the arguments $x_l$ and obey the relation (4) in the case of a translationally symmetrical chain.

Suppose now that the lattice is not perfect due to some reasons (it may be any external, say substrate, potential, defects of any kind, etc.) and that the respective additional influence on the particle dynamics is described by the Hamiltonian

$$H_{\text{add}} = \mu H^{(1)} + \mu^2 H^{(2)}, \tag{7}$$

where $H^{(j)}$ are of the same order as $H_{\text{latt}}$ and $\mu$ is a small parameter ($\mu \ll 1$). Since the small-amplitude limit is under consideration, one can approximate ($j = 1, 2$)

$$H^{(j)} = \frac{1}{2}\sum_{x_1}\sum_{x_2}\sqrt{M(x_1)M(x_2)}I_2^{(j)}(x_1;x_2)u(x_1)u(x_2) + \cdots \tag{8}$$

[here $M(x) \equiv M_\alpha(n)$ is introduced explicitly for the sake of convenience]. This general form implies the symmetry of the coefficients $I_p^{(j)}(x_1;\ldots;x_p)$ with respect to common permutations of the arguments $x_p$.

The dynamical equation (6) is now generalized

$$\ddot{v}(x) + \sum_{x_1} J_2(x;x_1)v(x_1) + \sum_{x_1}\sum_{x_2} J_3(x;x_1;x_2)v(x_1)v(x_2) + \mu\sum_{x_1}\left[I_2^{(1)}(x;x_1) + \mu I_2^{(2)}(x;x_1)\right]v(x_1) + \sum_{x_1}\sum_{x_2}\sum_{x_3} J_4(x;x_1;x_2;x_3)v(x_1)v(x_2)v(x_3) = 0. \tag{9}$$

### B. Some properties of the linear lattice

For the next consideration it is convenient to recall some properties of the underlying linear lattice. First of all let us introduce a set of eigenfunctions $\phi_l(x)$ and eigenvalues $\omega_l^2$ (the latter can be interpreted as eigenfrequencies of the harmonic lattice) of the spectral problem

$$\omega_l^2\phi_l(x) = \sum_{x_1} J_2(x;x_1)\phi_l(x_1). \tag{10}$$

In what follows we consider a finite chain subject to the cyclic boundary conditions. Therefore the spectrum is discrete and the index $l$ refers to the quantum number of the mode. The eigenfunctions can be chosen to be normalized and mutually orthogonal,

$$\sum_x \bar{\phi}_l(x)\phi_p(x) = \delta_{l,p}. \tag{11}$$

Here $\delta_{l,p}$ is the Kronecker delta and the bar stands for the complex conjugation. They make up a complete set:

$$\sum_l \bar{\phi}_l(x)\phi_l(x_1) = \delta_{x,x_1}. \tag{12}$$

As it follows from (10) and (11) the eigenfrequencies are expressed through the eigenfunctions by the formula

$$\omega_l^2 = \sum_x\sum_{x_1} J_2(x;x_1)\bar{\phi}_l(x)\phi_l(x_1), \tag{13}$$

which determines the dispersion relation of the linear lattice.

### C. Multiscale expansion

In accordance with the envelope function approach the solution of (9) must be represented as

$$v = \mu v_1 + \mu^2 v_2 + \mu^3 v_3 + \cdots. \tag{14}$$

In the present paper we study lattice excitations characterized by the only small parameter which coincides with one parametrizing perturbation [see (7)]. Then $\mu$ defines also a set of "times" $t_\nu = \mu^\nu t$, which are regarded as independent variables, and therefore

$$\frac{d}{dt} = \sum_{\nu=0}^{\infty}\mu^\nu\frac{\partial}{\partial t_\nu}. \tag{15}$$

By analogy, a set of spatial coordinates $n_\nu = \mu^\nu n$ can be introduced. However, in order to deal with long-range interactions this step has to be justified, which naturally leads to some restrictions on the force coefficient $K_2(n,\alpha;n_1,\alpha_1)$ [or $J_2(x;x_1)$].

To this end, let us take into account that after all one needs the expansion of the first sum in (9) with respect to $\mu$. Let us also introduce a provisional designation $u_\alpha(n_0, \{n_\nu\})$ ($\nu$ being a positive integer, $\nu \geq 1$) explicitly indicating the dependence of the displacement on the slow spatial variables. Then the sum under consideration is rewritten as

$$\sum_{\alpha_1} \sum_{m=-\infty}^{\infty} K_2(n_0, \alpha; n_0 + m, \alpha_1) \times u_{\alpha_1}(n_0 + m, \{n_\nu + \mu^\nu m\}).$$

Now the displacement $u_\alpha(n_0 + m, \{n_\nu + \mu^\nu m\})$ can be formally expanded in the Taylor series with respect to $\mu^\nu m$,

$$\sum_{\alpha_1} \sum_{m=-\infty}^{\infty} K_2(n_0, \alpha; n_0 + m, \alpha_1) u_{\alpha_1}(n_0 + m, \{n_\nu\}) + \sum_{\alpha_1} \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{\nu_1=1}^{\infty} \cdots \sum_{\nu_p=1}^{\infty} \mu^{\nu_1+\cdots+\nu_p} \sum_{m=-\infty}^{\infty} m^p K_2(n_0, \alpha; n_0 + m, \alpha_1) \times \frac{\partial}{\partial n_{\nu_1}} \cdots \frac{\partial}{\partial n_{\nu_p}} u_{\alpha_1}(n_0 + m, \{n_\nu\}). \quad (16)$$

The expansion makes sense if an estimate of the rest of the last set starting with some item, say $p = p_0$, is much less than the preceding terms. As is shown in Appendix A, to this end it is enough to require the coefficients $K(n_0, \alpha; n_1, \alpha_1)$ to satisfy the inequality

$$\max_{\{\alpha_1, \alpha\}} \left| \sum_{m=-\infty}^{\infty} m^p K_2(n_0, \alpha; n_0 + m, \alpha_1) \right| \leq C p! G^p, \quad (17)$$

where $C$ and $G$ are constants.

Let us introduce new independent variables: $X_0$ for the pair $(n_0, \alpha)$ and $X_\nu = a n_\nu$ for $\nu \geq 1$ [whenever the multiscale variables are used the subindex stands for the scaling, while in all expressions written down in terms of the original coordinates $x_p = (n_p, \alpha_p)$, the subindex is to distinguish discrete variables]. In these terms $v_m$ in the expansion (9) are the functions of the set of variables $\{t_\nu, X_\nu\}$ ($\nu \geq 0$). Then taking into account (15) and (A4) and restricting calculations to the order $O(\mu^3)$ one can write down the dynamical equation (9) in the form

$$\left[\frac{\partial^2}{\partial t_0^2} + 2\mu \frac{\partial^2}{\partial t_0 \partial t_1} + \mu^2 \left(\frac{\partial^2}{\partial t_1^2} + 2\frac{\partial^2}{\partial t_0 \partial t_2}\right)\right] v(X_0, \ldots)$$

$$= -\sum_{X_0^{(1)}} \left[J_2(X_0; X_0^{(1)}) + \mu I_2^{(1)}(X_0; X_0^{(1)}) + \mu^2 I_2^{(2)}(X_0; X_0^{(1)})\right] v(X_0^{(1)}, \ldots)$$

$$-\mu \sum_{X_0^{(1)}} a(n_0^{(1)} - n_0) J_2(X_0; X_0^{(1)}) \frac{\partial}{\partial X_1} v(X_0^{(1)}, \ldots)$$

$$-\mu^2 \sum_{X_0^{(1)}} J_2(X_0; X_0^{(1)}) \left[a(n_0^{(1)} - n_0) \frac{\partial}{\partial X_2} + \frac{1}{2} a^2 (n_0^{(1)} - n_0)^2 \frac{\partial^2}{\partial X_1^2}\right] v(X_0^{(1)}, \ldots)$$

$$-\sum_{X_0^{(1)}} \sum_{X_0^{(2)}} J_3(X_0; X_0^{(1)}; X_0^{(2)}) v(X_0^{(1)}, \ldots) v(X_0^{(2)}, \ldots)$$

$$-\sum_{X_0^{(1)}} \sum_{X_0^{(2)}} \sum_{X_0^{(3)}} J_4(X_0; X_0^{(1)}; X_0^{(2)}; X_0^{(3)}) v(X_0^{(1)}, \ldots) v(X_0^{(2)}, \ldots) v(X_0^{(3)}, \ldots). \quad (18)$$

Hereafter the dependence on the times $\{t_\nu\}$ is not indicated explicitly if all the scales are presented (i.e., $\nu \geq 0$) and the index $(j)$ at $X_0^{(j)}$ is to distinguish independent discrete variables. If a function does not depend on all $t_\nu$, then the most "rapid" time is mentioned in the argument. As to the spatial variables, only the most rapid one is indicated.

As is customary, for the next step one has to gather all terms of the same order of $\mu$ after substituting (14) in (18). In the first order this leads to the equation

$$\frac{\partial^2 v_1(X_0, \ldots)}{\partial t_0^2} + \sum_{X_0^{(1)}} J_2(X_0; X_0^{(1)}) v_1(X_0^{(1)}, \ldots) = 0. \quad (19)$$

Comparing it with (10) one concludes that the general solution can be represented as a sum of different eigenmodes. In the present section the case of the *single-mode* dynamics will be considered in detail. This means that $v_1(x)$ must be chosen in the form

$$v_1 = A(t_1, ...; X_1, ...)e^{-i\omega_l t_0}\phi_l(X_0) + \text{c.c.}, \tag{20}$$

where $A(t_1, ...; X_1, ...)$ is a function of slow variables describing amplitude modulation of the discrete CW $e^{-i\omega_l t_0}\phi_l(X_0)$.

In the second order of $\mu$ (18) yields

$$\frac{\partial^2 v_2(X_0, ...)}{\partial t_0^2} + \sum_{X_0^{(1)}} J_2(X_0; X_0^{(1)}) v_2(X_0^{(1)}, ...)$$

$$= -2\frac{\partial^2}{\partial t_0 \partial t_1} v_1(X_0, ...) - \sum_{X_0^{(1)}} a(n_0^{(1)} - n_0) J_2(X_0; X_0^{(1)}) \frac{\partial}{\partial X_1} v_1(X_0^{(1)}, ...)$$

$$- \sum_{X_0^{(1)}} \sum_{X_0^{(2)}} J_3(X_0; X_0^{(1)}; X_0^{(3)}) v_1(X_0^{(1)}, ...) v_1(X_0^{(2)}, ...) - \sum_{X_0^{(1)}} I_2^{(1)}(X_0; X_0^{(1)}) v_1(X_0^{(1)}, ...). \tag{21}$$

In order to find an appropriate representation for $v_2$ one has to take into account the fact that the cubic nonlinearity leads to generation of the second harmonic $e^{-2i\omega_l t_0}$ and to a displacement independent of the rapid variables. Thus $v_2(x)$ has the form

$$\begin{aligned} v_2(X_0, ...) = \sum_m [&D_m(t_1, ...; X_1, ...) \\ &+ B_m(t_1, ...; X_1, ...)e^{-i\omega_l t_0} \\ &+ B_m^{(2)}(t_1, ...; X_1, ...)e^{-2i\omega_l t_0}] \\ &\times \phi_m(X_0) + \text{c.c.} \end{aligned} \tag{22}$$

Due to the prominent role of the components, in [13] $v_1(x)$ and $v_2(x)$ were called the principal term and the companion term.

For the next step the expression (22) must be substituted in (21). Then multiplying the result by $\bar{\phi}_l(X_0)$, singling out harmonics with the frequency $\omega_l$, summing over $X_0$, and using (11) one obtains the equation for $A$,

$$2i\omega_l \frac{\partial A}{\partial t_1} - \Gamma_{ll} \frac{\partial A}{\partial X_1} - \Gamma_{ll}^{(1)} A = 0. \tag{23}$$

Here the notations

$$\Gamma_{ml} = \sum_{x_0} \sum_{x_1} a(n_1 - n_0) J_2(x_0; x_1) \bar{\phi}_m(x_0) \phi_l(x_1) \tag{24}$$

and

$$\Gamma_{ml}^{(1)} = \sum_{x_0} \sum_{x_1} I_2^{(1)}(x_0; x_1) \bar{\phi}_m(x_0) \phi_l(x_1) \tag{25}$$

are introduced. As is shown in Appendix B, the diagonal element $\Gamma_{ll}$ is connected with the group velocity $v_l = \frac{d\omega_l}{dq}$ [see (B1)]. Equation (23) has a solution

$$A(t_1, ...; X_1, ...) = e^{-i\Delta\omega_l t_1} a(t_2, ...; \tilde{X}_1, ...), \tag{26}$$

where $\tilde{X}_1 = X_1 - v_l t_0$ and $\Delta\omega_l = \frac{\Gamma_{ll}^{(1)}}{2\omega_l}$ is the shift of the CW frequency originated by the perturbation $I_2^{(1)}$. The sign of $\Delta\omega_l$ determines whether the soliton mode lies above ($\Delta\omega_l > 0$) or below ($\Delta\omega_l < 0$) the CW frequency.

An important consequence of (26) is that the envelope soliton created at some point of the spectrum moves with a velocity equal to the group velocity of the linear excitations corresponding to that point. For various particular examples of chains with nearest-neighbor interactions and the quartic nonlinearity this result has been obtained by many authors (see, e.g., [4–7]).

In order to find the coefficients $B_m$ (at $m \neq l$) one has to single out in (21) the companion harmonics with the frequency $\omega_l$, to multiply both sides of the resulting equation by $\bar{\phi}_m(X_0)$, and to calculate the sum with respect to $X_0$. This yields

$$B_m = \frac{1}{\omega_l^2 - \omega_m^2} \left( \Gamma_{ml} \frac{\partial A}{\partial X_1} + \Gamma_{ml}^{(1)} A \right). \tag{27}$$

Proceeding by analogy and using the property (3) one finds the displacement term

$$D_m = -\frac{2}{\omega_m^2} \mathcal{J}_{llm} |A|^2, \tag{28}$$

where

$$\mathcal{J}_{klm} = \sum_{x_0} \sum_{x_1} \sum_{x_2} J_3(x_0; x_1; x_2) \bar{\phi}_k(x_0) \phi_l(x_1) \bar{\phi}_m(x_2), \tag{29}$$

and amplitudes of the second harmonic components

$$B_m^{(2)} = -\frac{1}{\omega_m^2 - 4\omega_l^2} \bar{\mathcal{J}}_{lml} A^2. \tag{30}$$

Formula (30) implies the condition $\omega_m^2 \neq 4\omega_l^2$ at $\mathcal{J}_{lml} \neq 0$. This requirement will hold whenever the cubic nonlinearity is under consideration (otherwise resonant generation of the second harmonic occurs, which will be considered in detail elsewhere).

Passing to the terms of the third order of $\mu$ one arrives at the dynamical equation

$$\frac{\partial^2 v_3(X_0,...)}{\partial t_0^2}+\sum_{X_0^{(1)}} J_2(X_0;X_0^{(1)})v_3(X_0^{(1)},...)$$

$$=-2\frac{\partial^2}{\partial t_0\partial t_1}v_2(X_0,...)-\left(\frac{\partial^2}{\partial t_1^2}+2\frac{\partial^2}{\partial t_0\partial t_2}\right)v_1(X_0,...)-\sum_{X_0^{(1)}} a(n_0^{(1)}-n_0)J_2(X_0;X_0^{(1)})\frac{\partial v_2(X_0^{(1)},...)}{\partial X_1}$$
$$-\sum_{X_0^{(1)}} J_2(X_0;X_0^{(1)})\left[a(n_0^{(1)}-n_0)\frac{\partial}{\partial X_2}+\frac{1}{2}a^2(n_0^{(1)}-n_0)^2\frac{\partial^2}{\partial X_1^2}\right]v_1(X_0,...)$$
$$-\sum_{X_0^{(1)}}\sum_{X_0^{(2)}} J_3(X_0;X_0^{(1)};X_0^{(2)})v_1(X_0^{(1)},...)v_2(X_0^{(2)},...)$$
$$-\sum_{X_0^{(1)}}\sum_{X_0^{(2)}}\sum_{X_0^{(3)}} J_4(X_0;X_0^{(1)};X_0^{(2)};X_0^{(3)})v_1(X_0^{(1)},...)v_1(X_0^{(2)},...)v_1(X_0^{(3)},...)$$
$$-\sum_{X_0^{(1)}} I_2^{(1)}(X_0;X_0^{(1)})v_2(X_0^{(1)},...)-\sum_{X_0^{(1)}} I_2^{(2)}(X_0;X_0^{(1)})v_1(X_0^{(1)},...). \tag{31}$$

For the last step we multiply this equation by $\bar{\phi}_l(X_0)$, sum over $X_0$, and take into account (20), (26)–(28), and (30). The outcome reads

$$2i\omega_l\frac{\partial a}{\partial t_2}+2i\omega_l v_l\frac{\partial a}{\partial X_2}+\left(-v_l^2+\sum_{m\neq l}\frac{|\Gamma_{ml}|^2}{\omega_l^2-\omega_m^2}-\Lambda_l\right)\frac{\partial^2 a}{\partial\tilde{X}_1^2}+\left[-2i\Delta\omega_l v_l+\sum_{m\neq l}\frac{\Gamma_{ml}^{(1)}\bar{\Gamma}_{ml}-\bar{\Gamma}_{ml}^{(1)}\Gamma_{ml}}{\omega_l^2-\omega_m^2}\right]\frac{\partial a}{\partial\tilde{X}_1}$$
$$-(\chi_3+\chi_{ll})|a|^2a-\left[(\Delta\omega_l)^2+\Gamma_l^{(2)}+\sum_{m\neq l}\frac{|\Gamma_{ml}^{(1)}|^2}{\omega_l^2-\omega_m^2}\right]a=0. \tag{32}$$

Here

$$\Lambda_l=\frac{a^2}{2}\sum_{x_0}\sum_{x_1} J_2(x_0;x_1)(n_1-n_0)^2\bar{\phi}_l(x_0)\phi_l(x_1), \tag{33}$$

the coefficients

$$\chi_{lm}=3\sum_{x_1}...\sum_{x_4} J_4(x_1;...;x_4)\bar{\phi}_l(x_1)\phi_l(x_2)\times\bar{\phi}_m(x_3)\phi_m(x_4) \tag{34}$$

and

$$\chi_3=2\sum_m\left(-\frac{4}{\omega_m^2}|\mathcal{J}_{llm}|^2+\frac{1}{4\omega_l^2-\omega_m^2}|\mathcal{J}_{lml}|^2\right) \tag{35}$$

play the part of the effective nonlinearity, and

$$\Gamma_l^{(2)}=\sum_{x_0}\sum_{x_1} I_2^{(2)}(x_0,x_1)\bar{\phi}_l(x_0)\phi_l(x_1). \tag{36}$$

Finally, looking for a solution independent of $X_2$, introducing new variables

$$\psi=\sqrt{\frac{|\chi_3+\chi_{ll}|}{2\omega_l}}e^{-i\tilde{\omega}_l T}a, \tag{37}$$

$$T=t_2,\qquad X=\sqrt{\frac{2}{|d^2\omega_l/dq^2|}}(\tilde{X}_1+vT), \tag{38}$$

$$v=\frac{1}{\omega_l}\sum_{m\neq l}\frac{\mathrm{Im}(\bar{\Gamma}_{ml}^{(1)}\Gamma_{ml})}{\omega_l^2-\omega_m^2}+\frac{\Delta\omega_l}{\omega_l}v_l, \tag{39}$$

and

$$\tilde{\omega}_l=\frac{1}{2\omega_l}\left[(\Delta\omega_l)^2+\Gamma_l^{(2)}+\sum_{m\neq l}\frac{|\Gamma_{ml}^{(1)}|^2}{\omega_l^2-\omega_m^2}\right], \tag{40}$$

where (B2) has been used, Eq. (32) is reduced to the classical NLS equation

$$i\frac{\partial\psi}{\partial T}+\kappa_\omega\frac{\partial^2\psi}{\partial X^2}+2\kappa_\chi|\psi|^2\psi=0, \tag{41}$$

with $\kappa_\omega=\mathrm{sgn}(d^2\omega_l/dq^2)$ and $\kappa_\chi=-\mathrm{sgn}(\chi_3+\chi_{ll})$.

## III. EXAMPLES OF ENVELOPE SOLITONS IN LATTICES. COUPLED SOLITONS

In this section we consider different examples of the small-amplitude solitons in lattices [17]. Though the above theory allows one to treat a quite general situation each time a model is simplified to emphasize only the main effect.

### A. Solitons in the simplest monoatomic lattice

Let us start with some properties of the simplest lattice possessing only nearest-neighbor interactions. This is the

case of

$$J(x;x_1) \equiv \frac{K}{M}(2\delta_{n_1,n} - \delta_{n_1,n-1} - \delta_{n_1,n+1}), \tag{42}$$

where $K$ is a linear force constant and $M$ is a mass of a particle. The normalized eigenmodes are given by

$$\phi_l(x) = \mathcal{N}^{-1/2} e^{iq_l na}. \tag{43}$$

Hereafter $\mathcal{N}$ stands for the number of cells in the chain (in the case at hand it coincides with a number of atoms). Direct algebra allows one to ensure that $\Gamma_{lm} = -2ia(K/M)\sin(q_l a)\delta_{lm}$. Then it follows from (27) that the companion modes are not excited in the unperturbed monoatomic lattice with quartic nonlinearity. Notice that in the case of existence of more than one branch of the spectrum, i.e., in the case of a complex cell, there is a coefficient $B_m$ which is not zero (it corresponds to the wave vector of the CW but to the different branch) and this is a principle difference between monoatomic and multiatomic lattices. The additional Hamiltonian $H^{(1)}$ originates companion modes which have the shape of the principal mode. Also $H^{(1)}$ effects on the velocity of a soliton, but the respective addendum is of the order of $\mu^2$ [see (39)]. The perturbation $H^{(2)}$ gives only a $\mu^2$-order contribution to the frequency shift.

As follows from (41) the type of a soliton solution depends on the product $\kappa_\omega \kappa_\chi$: if it is 1, bright solitons can be excited, if it equals $-1$ there can exist dark solitons against a nonzero background. For the scalar lattice with nearest-neighbor interactions in the vicinity of the BZ edge one has $d^2\omega_l/dq^2 < 0$. Then only bright (dark) solitons are available at $\chi_{ll} + \chi_3 > 0$ ($\chi_{ll} + \chi_3 < 0$).

The principal difference between the cases of the cubic and quartic nonlinearities is that in the former case the displacement and the companion mode with the frequency $2\omega_l$ can be excited together with the principal harmonic [see (28)–(30)]. These modes are localized about the soliton.

Presence of a linear eigenfrequency $\Omega_0$ of an uncoupled oscillator leads to change of the sign of the GVD in some intermediate point of the BZ. Indeed, in this case the dispersion relation (13) takes the form

$$\omega^2 = \Omega_0^2 + 4\frac{K}{M}\sin^2\frac{qa}{2} \tag{44}$$

and hence in the region of small wave numbers $d^2\omega/dq^2 > 0$. This means that creation of solitons of different types in the vicinity of the BZ edge and in the center of the BZ is possible. So, for example, in the lattice with quartic nonlinearity $\chi_{ll} > 0$ at the edge and at the center of the BZ there can be excited bright and dark solitons, respectively. Also, in the case at hand there is a point $\tilde{q}$ defined by

$$\cos(\tilde{q}a) = 1 + \Omega_0^2\frac{M}{2K}\left(1 - \sqrt{1 + \frac{4K}{\Omega_0^2 M}}\right)$$

at which the GVD is zero, which means that in the vicinity of $\tilde{q}$ conventional small-amplitude envelope solitons of the NLS type cannot exist and higher dispersion and nonlinearity have to be taken into account.

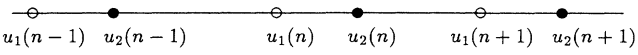


FIG. 1. The example of the terminology for the diatomic lattice. The atoms designated by circles and disks have masses $M_1$ and $M_2$, correspondingly.

### B. Multiatomic lattices. Coupled solitons in a diatomic lattice with quartic nonlinearity

In the present subsection a class of *coupled solitons* in multiatomic lattices is obtained. These solutions are different from the localized modes reported earlier [18]. Mathematically, the distinction comes from the method of analysis of a lattice: here the envelope function approach rather than the rotating wave approximation is used. Physically, the differences consist of a nonzero velocity of the forward motion of coupled solitons, of their sizes, and of their behavior when the gap width tends to zero. The solitons presented below are analogous to the optical coupled gap solitons discovered numerically in [19] and later found analytically [20].

Let us start with a brief discussion about possible ways to generalize the theory developed in the preceding section. Suppose that a lattice with a complex cell having $N_0$ different atoms is under consideration. It can be treated as a vector lattice if one identifies the index $\alpha$ with a number of an atom in a cell (say, from the left to the right $\alpha = 1, 2, ..., N_0$) and the index $n$ with a cell number (see the example in Fig. 1). Then $M(x) \equiv M_\alpha$ (i.e., is independent on $n$). Restricting consideration to the case of a lattice with nearest-neighbor interactions and without linear on-site potential the kernel $K(n,\alpha;n_1,\alpha_1)$ can be written as

$$\begin{aligned} K(n,\alpha;n_1,\alpha_1) = {} & V_{\alpha+1}\delta_{n,n_1}(1-\delta_{\alpha,N_0})(\delta_{\alpha_1,\alpha}-\delta_{\alpha_1,\alpha+1}) + V_\alpha\delta_{n,n_1}(1-\delta_{\alpha,1})(\delta_{\alpha_1,\alpha}-\delta_{\alpha_1,\alpha-1}) \\ & + V_1\delta_{n_1,n}(\delta_{\alpha,N_0}\delta_{\alpha_1,N_0} + \delta_{\alpha,1}\delta_{\alpha_1,1}) - V_1(\delta_{n_1,n-1}\delta_{\alpha,1}\delta_{\alpha_1,N_0} + \delta_{n_1,n+1}\delta_{\alpha,N_0}\delta_{\alpha_1,1}). \end{aligned} \tag{45}$$

Here $V_\alpha$ (at $\alpha = 2, 3, ..., N_0$) is a harmonic constant of interaction between $(\alpha-1)$th and $\alpha$th atoms in the same cell and $V_1$ is a force constant between the first atom in the $n$th cell and the $N_0$th atom in the $(n-1)$th cell.

The case which can be treated analytically is that of the small dispersion of both the atom masses and the force constants from their average values $M$ and $V$, or in other words, the case where $|M_\alpha - M| = o(M)$;

$|V_\alpha - V| = o(V)$. Then, introducing new variables, say $m_\alpha = M - M_\alpha$ and $w_\alpha = V - V_\alpha$, one can interpret the differences among the masses and the force constants as perturbations, include them in $H^{(j)}$ [see (8)], and employ the above results for the monoatomic lattice with the potential $H_{\rm add}$ given by (7). The important fact now is that in the limit when $M_\alpha \to M$ and $V_\alpha \to V$ one arrives at the monoatomic lattice with a lattice constant $a$ which is $N_0$ times less than the lattice constant $a_{N_0}$ of the multiatomic lattice: $a_{N_0} = N_0 a$ (we use a natural assumption that in this limit the distances between neighbors become equal). Therefore if one is interested in the behavior of solitons near the edge of the BZ of the multiatomic lattice, the associated limiting monoatomic model has to be investigated at the point $q_{N_0} = \frac{\pi}{a_{N_0}} = \frac{\pi}{N_0 a}$ (see the illustration in Fig. 2). It is this point in which the eigenmode $\phi_l(x)$ must be chosen. The qualitative result immediately follows from (26): respective *solitons* (if any) *move with the group velocity of a CW in the limiting monoatomic lattice at the point* $q_{N_0}$. Below this result is obtained on the basis of the perturbation expansion.

As follows from these arguments in the limit $m_\alpha \to 0$, $w_\alpha \to 0$ a soliton of the complex lattice transforms to a soliton of the monoatomic lattice (if of course the GVD at the point $q_{N_0}$ is not negligibly small, i.e., is of the order of the frequency itself).

The behavior just described seems to be interesting and not too trivial if one looks at the problem from another viewpoint. Indeed, the curvatures of the acoustic and optical branches of the spectrum in the vicinity of the BZ edge have different signs. This means that if the acoustic mode at the BZ edge supports propagation of bright solitons, then the optical mode is a CW for dark solitons subject to the same nonlinearity (this statement is a direct consequence of the analysis provided in the preceding subsection). Then in the presence of interaction the question about the possibility of simultaneous excitation of these modes arises. Here we consider treatment of the problem different from that outlined above and close to the method applicable to optical gap solitons [20].

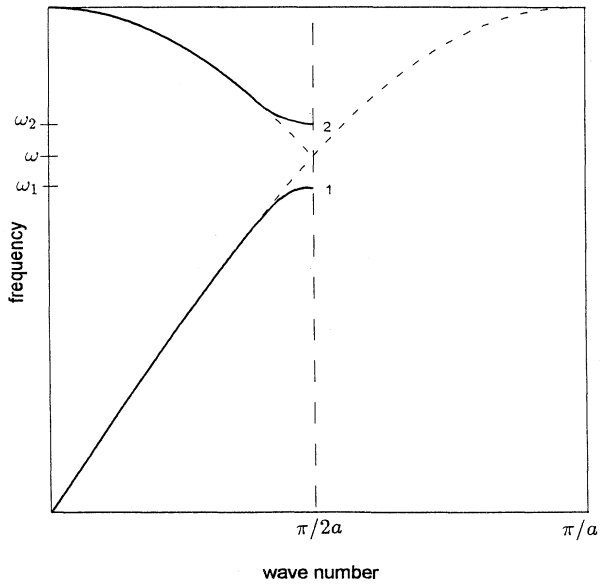


FIG. 2. The spectrum of the diatomic lattice with the small gap (solid line) and the associated spectrum of the monoatomic lattice (dashed line).

We investigate an unperturbed diatomic ($\alpha = 1, 2$) lattice with nearest-neighbor interactions and quartic nonlinearity. Then $J_3 \equiv 0$ and $H_{\rm add} = 0$. It is well known that if $M_{1,2} = M \pm \mu^j m$ and $V_{1,2} = V \pm \mu^j w$ ($j$ being a positive integer, it is discussed below) then in the leading order of the small parameter $\mu$ the gap between the optical and acoustic branches of the spectrum is given by

$$\delta\omega = \omega^{(\rm op)} - \omega^{(\rm ac)} = 2\mu^j \Delta\omega = \mu^j \sqrt{2\frac{V}{M}\left(\frac{w^2}{V^2} + \frac{m^2}{M^2}\right)}, \tag{46}$$

where $\omega^{(\rm op)}$ and $\omega^{(\rm ac)}$ are frequencies of the respective branches at the BZ edge and a normalized half-width $\Delta\omega$ of the gap is introduced [note that $\Delta\omega = O(\omega^{(\rm op,ac)})$].

Let us consider solutions of the evolution equation (6) which correspond to a CW frequency located inside the gap. Since now $\delta\omega = O(\mu^j\omega)$, where $\omega = \frac{1}{2}(\omega^{(\rm op)} + \omega^{(\rm ac)})$ is a frequency of the middle of the gap (see Fig. 2), the modes associated with the gap edges are coupled and one has to represent a CW solution as a superposition of two modes: optical $\phi^{(\rm op)}_{\rm BZ}(X_0)$ and acoustic $\phi^{(\rm ac)}_{\rm BZ}(X_0)$ ones:

$$v_1 = [A_{\rm op}(t_1, ...; X_1, ...)\phi^{(\rm op)}_{\rm BZ}(X_0) + A_{\rm ac}(t_1, ...; X_1, ...)\phi^{(\rm ac)}_{\rm BZ}(X_0)]e^{-i\omega t_0} + \text{c.c.} \tag{47}$$

There are some general comments to be made here. First, the consistent expansion requires the use of only one frequency (say $\omega$) in (47) instead of $\omega^{(\rm op)}$ and $\omega^{(\rm ac)}$ since $(\omega^{(\rm op)} - \omega^{(\rm ac)})t = 2\Delta\omega t_j$ [this is in accordance with the above qualitative arguments and with the outcomes (26), (37), and (40): indeed, $\delta\omega$ can be taken into account by the perturbation $H^{(j)}$]. Second, the subindex of the eigenfunctions $\phi_m(X_0)$ should refer to *two* quantum numbers indicating a branch of the spectrum and the wave number in the reduced BZ. We avoid this by introducing direct reference to the branch of the spectrum by means of the abbreviations "op" and "ac." Third, a technical feature of the expansion which will be done below is that due to the differences between $\omega$ and the eigenvalues $\omega^{(\rm op)}$ and $\omega^{(\rm ac)}$ new (compared with the development of the preceding section) perturbative terms appear. For example, now one has

$$\mu^{-j}\left\{\left(\omega^2 - [\omega^{(\rm op)}]^2\right) A_{\rm op}\phi^{(\rm op)}_{\rm BZ}(X_0) + \left(\omega^2 - [\omega^{(\rm ac)}]^2\right) A_{\rm ac}\phi^{(\rm ac)}_{\rm BZ}(X_0)\right\}e^{i\omega t_0}$$

in the right hand side of (21) and/or (31).

For the next step one has to represent [cf. (22)]

$$v_2(X_0,...)=\sum_m B_m^{(\mathrm{op})}(t_1,...;X_1,...)\phi_m^{(\mathrm{op})}(X_0)e^{-i\omega t_0} + \sum_m B_m^{(\mathrm{ac})}(t_1,...;X_1,...)\phi_m^{(\mathrm{ac})}(X_0)e^{-i\omega t_0}+\mathrm{c.c.} \tag{48}$$

Further development of the theory depends on the value $j$ which determines the scaling of the problem. There are three interesting cases: $j=1$, 2, and 3.

Let us start with the case $j=3$ which exactly corresponds to a negligibly small gap, i.e., to the situation qualitatively described at the beginning of the present subsection.

Substituting (48) in (21), multiplying the result subsequently by $\phi_{\mathrm{BZ}}^{(\mathrm{op})}$ and by $\phi_{\mathrm{BZ}}^{(\mathrm{ac})}$, and summing over $X_0$ one obtains two equations for the amplitudes,

$$i\frac{\partial A_{\mathrm{op}}}{\partial t_1}-v\frac{\partial A_{\mathrm{ac}}}{\partial X_1}=0,\quad i\frac{\partial A_{\mathrm{ac}}}{\partial t_1}+v\frac{\partial A_{\mathrm{op}}}{\partial X_1}=0, \tag{49}$$

where a real quantity

$$v=\frac{1}{2\omega}\sum_{x_0}\sum_{x_1}a_2(n_1-n_0)J_2(x_0;x_1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_0)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1) \tag{50}$$

can be interpreted as a velocity (see Appendix B) and it is taken into account that now the lattice constant is $a_2$.

The first important consequence of the system (49) is that it possesses a solution characterized by the relation

$$A_{\mathrm{op}}=\pm iA_{\mathrm{ac}}, \tag{51}$$

which means that the modes are coupled. The so determined amplitudes $A_{\mathrm{op}}$ and $A_{\mathrm{ac}}$ depend on $t_1$ and $X_1$ only through the combinations $X_1\mp vt_1$. In other words, the pair $A_{\mathrm{op}}$, $A_{\mathrm{ac}}$ describes a wave packet traveling with the velocity $v$ either in positive or in negative directions.

For the sake of definiteness further consideration is provided for the "polarization"

$$A_{\mathrm{op}}=iA_{\mathrm{ac}}=iA(z),\qquad z=X_1-vt_1. \tag{52}$$

For the next step one has to determine the coefficients $B_m^{(\mathrm{op,ac})}$ which can be done by multiplying (21) subsequently by $\bar\phi_l^{(\mathrm{op})}$ and by $\bar\phi_l^{(\mathrm{ac})}$ after substituting the expansion (48). The result reads

$$B_m^{(\mathrm{op})}=\frac{1}{\omega^2-\omega_m^2}\left(\Gamma_m^{(11)}\frac{\partial A_{\mathrm{op}}}{\partial X_1}+\Gamma_m^{(12)}\frac{\partial A_{\mathrm{ac}}}{\partial X_1}\right), \tag{53a}$$

$$B_m^{(\mathrm{ac})}=\frac{1}{\omega^2-\omega_m^2}\left(\Gamma_m^{(21)}\frac{\partial A_{\mathrm{op}}}{\partial X_1}+\Gamma_m^{(22)}\frac{\partial A_{\mathrm{ac}}}{\partial X_1}\right), \tag{53b}$$

where $\Gamma_m^{(ij)}$ stands for the element at $i$th row and $j$th column of the matrix

$$\sum_{x_0}\sum_{x_1}a_2(n_1-n_0)J_2(x_0;x_1)\times\begin{pmatrix}\bar\phi_m^{(\mathrm{op})}(x_0)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_1) & \bar\phi_m^{(\mathrm{op})}(x_0)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1)\\ \bar\phi_m^{(\mathrm{ac})}(x_0)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_1) & \bar\phi_m^{(\mathrm{ac})}(x_0)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1)\end{pmatrix}. \tag{54}$$

By the direct algebra one can ensure that in the case of an unperturbed diatomic lattice $\Gamma_m^{(ij)}=0$ and, hence, $B_m^{(\mathrm{ac,op})}=0$.

The formulas (53a), (53b), however, do not give $B_{\mathrm{BZ}}^{(\mathrm{op})}$ and $B_{\mathrm{BZ}}^{(\mathrm{ac})}$ which are not zero. Moreover, sometimes the companion term imposes special conditions on the principal mode. The reason for this is that the principal states bordering the BZ can be considered as doubly degenerate (see Appendix B) and the companion term has a component which is orthogonal to the principal mode (in the space of the eigenfunctions of the linear operator) and has the CW frequency. In order to find this component one has to consider the equations appearing in the third order.

Multiplying (31) by $\phi_{\mathrm{BZ}}^{(\mathrm{op})}(X_0)$ and by $\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(X_0)$ and summing over $X_0$ one arrives at the system for $A_{\mathrm{op}}$ and $A_{\mathrm{ac}}$. Changing variables $(X_1,t_1)$ to $(z,t_1)$, introducing new composite states

$$b_\pm=B_{\mathrm{BZ}}^{(\mathrm{op})}\pm iB_{\mathrm{BZ}}^{(\mathrm{ac})}, \tag{55}$$

and using the properties of the kernel $J_4(x_1;...;x_4)$ and relations (52), (B16), and (B17) one can obtain the equations of the third order in the form

$$2i\left(\frac{\partial A}{\partial t_2}-v\frac{\partial A}{\partial X_2}\right)+\Omega''\frac{\partial^2 A}{\partial z^2}+\chi_+|A|^2A+\frac{\partial b_+}{\partial t_1}=0, \tag{56}$$

$$(i\tilde\Lambda+\tilde\Gamma)\frac{\partial^2 A}{\partial z^2}+(\chi_--i\chi)|A|^2A+\frac{\partial b_-}{\partial t_1}-2v_{st}\frac{\partial b_-}{\partial z}=0. \tag{57}$$

Here

$$\chi_\pm=-\frac{1}{2\omega}\sum_{x_1}...\sum_{x_4}J_4(x_1;...;x_4)\{\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_2)+\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_2)\}\times\{\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_3)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_4)\pm\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_3)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_4)\}, \tag{58}$$

$$\chi=\frac{1}{\omega}\sum_{x_1}...\sum_{x_4}J_4(x_1;...;x_4)[\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_2)+\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_2)]\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_3)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_4), \tag{59}$$

$$\tilde\Lambda=\frac{a_2^2}{2\omega}\sum_x\sum_{x_1}(n_1-n)^2J_2(x;x_1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_1), \tag{60}$$

$$\tilde\Gamma=\frac{1}{2\omega}(\Lambda_{\mathrm{ac}}-\Lambda_{\mathrm{op}}). \tag{61}$$

$\Omega''$ is the GVD induced by the coupling [it is given by (B12)], $\Lambda_{\mathrm{ac}}$ and $\Lambda_{\mathrm{op}}$ are defined by the direct analogy with $\Lambda_l$ [see (33)] where $\phi_l(x)$ must be replaced by $\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x)$ and $\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x)$, respectively, and for the definition of $\sum'$ see Appendix B.

In terms of the variables $(z,t_1)$ the amplitude $A$ does not depend on $t_1$. Hence, it follows from (56), (57)

that $b_\pm = b_\pm(z)$, i.e., they do not depend on $t_1$, as well. Then $b_+(z)$ is excluded from the evolution equations, which means that the component of the companion term with the frequency $\omega$ is characterized by the link $B_{\rm BZ}^{\rm (op)} = -iB_{\rm BZ}^{\rm (ac)}$, and this corresponds to the polarization determined by the lower sign in (B12). Comparing this outcome with (52) one concludes that the excited companion term has a component with the CW frequency and its polarization is orthogonal to the polarization of the principal mode.

Now considering solutions independent of $X_2$, one obtains the NLS equation for the envelope amplitude

$$2i\frac{\partial A}{\partial t_2} + \Omega''\frac{\partial^2 A}{\partial z^2} + \chi_+|A|^2A = 0. \tag{62}$$

In the generic case not all solutions of this equation make physical sense. The condition determining available types of solutions comes from the requirement for the companion term to be localized in space, i.e., to decay with $|z|$. However, there appear to be no restrictions if

$$\chi_- = \chi = 0. \tag{63}$$

This requirement is fulfilled at least in the cases of nonlinear nearest-neighbor interactions and a homogeneous nonlinear on-site potential (see Appendix C).

In this last case the general form of the Bloch functions bordering the gap is given by (C1) and, for example, the one-soliton lattice pattern at $\chi_+ < 0$ is described by

$$v_1(x) = \mathcal{A}\,\mathrm{sech}(z/z_0)(-1)^n \sin\left(\tilde\omega t + \vartheta_{\rm op} - \frac{\pi}{2}(\alpha-1)\right), \tag{64}$$

where $\mathcal{A} = \sqrt{\frac{2}{\chi_+}\Omega''}\frac{2}{z_0\mathcal{N}}$ is the soliton amplitude, $\tilde\omega = \omega - \frac{\mu^2}{2z_0^2}\Omega''$ is the frequency of internal oscillations, $z_0$ is a constant, and $\vartheta_{\rm op}$ is introduced in Appendix C. It is to be emphasized that in spite of similar forms of a soliton in a monoatomic lattice and the solution (64) the essential difference of these cases is that in a diatomic lattice the companion term defined by (57) is not zero.

Let us show that the obtained result coordinates with the qualitative arguments given in the beginning of this section. To this end consider the limit $m = 0$ and without restriction of generality $V_2 > V_1$. Then $a_1^{\rm (ac)}/a_2^{\rm (ac)} = -a_1^{\rm (op)}/a_2^{\rm (op)} = 1$ and one can take $\vartheta_{\rm op} = -\pi/4$. Now let $w \to 0$. Then the polarization (52) means that the respective composite state (B12) is nothing but $\mathcal{N}^{-1/2}(-1)^n \exp\left[i\frac{\pi}{4} + i\frac{\pi}{2}(\alpha-1)\right]$. Taking into account that the limit of equivalent particles is under consideration, introduce new numbering of the atoms $\tilde n$, such that an atom characterized by the pair $(n,\alpha)$ is indicated by the single index $\tilde n = 2(n-1)+\alpha$. Then the first term in the representation (47) is proportional to $\exp\left(\frac{i\pi}{2}\tilde n\right)$. Recalling the definition of $q_{N_0}$ one can note that $\frac{\pi}{2} = q_2 a$. Comparing this with the expression (20), one finds that we are in the point $q_{\rm BZ}/2$ of the spectrum of the monoatomic lattice. This is the reason the solution obtained has the form of the envelope soliton in a monoatomic lattice. Thus one concludes that for the chosen branch $v > 0$ and $\Omega'' < 0$. As is evident, the orthogonal polarization is characterized by $v < 0$ and $\Omega'' < 0$.

The GVD $\Omega''$ can be directly expressed through $v$. To this end insert the composite state (B12) in the dispersion relation (13), differentiate it twice with respect to $q$, and take into account that $\omega^{\rm (op)}(d^2\omega^{\rm (op)}/dq^2) = -\omega^{\rm (ac)}(d^2\omega^{\rm (ac)}/dq^2)$. As a result we find

$$\Omega'' = -\frac{v^2}{\Omega}. \tag{65}$$

This is nothing more than the GVD of the limiting monoatomic lattice in the point $qa = \pi/2$.

In a more general situation the condition (63) may be not satisfied. Meantime, at $j = 2$, Eq. (57) for the companion term is modified. It takes the form

$$(i\tilde\Lambda + \tilde\Gamma)\frac{\partial^2 A}{\partial z^2} + (\chi_- - i\chi)|A|^2A + \frac{\partial b_-}{\partial t_1} - 2v\frac{\partial b_-}{\partial z} = 2\Delta\omega A \tag{66}$$

and has a solution decaying with $|z|$ if

$$\chi = 0 \tag{67}$$

and

$$\int_{-\infty}^{\infty}(\chi_-|A|^2 - 2\Delta\omega)A\,dz = 0. \tag{68}$$

The requirement (67) turns out to be crucial for existence of the coupled solitons, while (68) results in restrictions on the soliton amplitude. So, for instance, $\mathcal{A}$ (and hence $z_0$) in (64) cannot be arbitrary anymore. Instead one calculates from (68)

$$\mathcal{A} = 2\sqrt{\frac{\Delta\omega}{\chi_-}}, \tag{69}$$

where there must be $\Delta\omega\chi_- > 0$. Thus the intensity of the soliton is directly proportional to the gap width.

In contrast to the cases $j = 2,3$ the gap of the order of $\mu\omega$ changes the situation drastically. The gap being of the order of the pulse amplitude leads to the coupling of the harmonics in the second order of the perturbation theory, which results in the strong linear dispersion. To illustrate this, by analogy with (49) deduce the system for the amplitudes in the second order for the case $j = 1$,

$$\begin{aligned}\Delta\omega A_{\rm op} &= i\frac{\partial A_{\rm op}}{\partial t_1} - v\frac{\partial A_{\rm ac}}{\partial X_1},\\ -\Delta\omega A_{\rm ac} &= i\frac{\partial A_{\rm ac}}{\partial t_1} + v\frac{\partial A_{\rm op}}{\partial X_1}.\end{aligned} \tag{70}$$

The dispersion relation $\Omega(K)$ associated with this system reads $\Omega^2 = v^2K^2 + (\Delta\omega)^2$ and hence in the present scaling the GVD cannot be compensated by the weak nonlinearity.

All the cases considered above allow interpretation from another viewpoint. First one can say that cou-

pled gap solitons can be excited only if $\chi = 0$. If also $\chi_- = 0$ then their intensity must be much bigger than the gap width (in dimensionless units). Otherwise, i.e., when $\chi_- \neq 0$, the intensity of the pulse is determined by the gap width. Finally, the localized solitonic pulses of the NLS type cannot be excited with the amplitude comparable with the gap width.

### C. Envelope solitons in Kac-Baker model

The preceding studies of the nonlinear lattices with long-range interactions within the framework of the Kac-Baker model have displayed a number of interesting effects, including novel solitonic states [16]. Those investigations were carried out in the long wavelength approximation. The aim of the present section is to examine influence of long-range interactions on envelope solitons in a monoatomic lattice at the wave numbers of $\pi/a$ order. We also deal with the Kac-Baker model [21], which is characterized by the harmonic coefficient

$$K(n;n_1) = K(2\delta_{n,n_1} - \delta_{n_1,n-1} - \delta_{n_1,n+1}) + \frac{J(1-r)}{r}\left[\delta_{n_1,n}\frac{1+r}{1-r} - r^{|n_1-n|}\right]. \quad (71)$$

Here $K$ and $J$ are positive constants; $r = e^{-\gamma}$, $\gamma$ ($\gamma > 0$) determines the effective range of interactions, and the index $\alpha$ is dropped. In accordance with the theory developed above, the value $J$ is considered to be of the order of $K$, otherwise (if $J \sim \mu^j K$ where $j = 1, 2$) it must be included in the Hamiltonian $H^{(j)}$ and in the case $\mu^3 K \ll J \ll \mu^2 K$ long-range interactions have to be treated as a perturbation of the NLS equation (41).

The dispersion relation of the model at hand is

$$\omega^2(q) = 4\frac{K}{M}\sin^2\left(\frac{aq}{2}\right)\left[1 + \frac{(J/K)\,(e^\gamma + 1)}{8\sin^2\left(\frac{aq}{2}\right) + 8\sinh^2\left(\frac{\gamma}{2}\right)}\right]. \quad (72)$$

In investigating the lattice with long-range interactions we address the question how does the nonlocality change properties of the chain compared with the lattice possessing only nearest-neighbor interactions and the same type of the nonlinearity? In such a statement all peculiarities of the model are concentrated in the dispersion relation (72).

More precisely, as follows from the above theory it is necessary to study the group velocity and GVD associated with $\omega(q)$ given by (72). Starting with the single-mode dynamics and recalling that the effective soliton width can be characterized by the parameter $l_s = \sqrt{\frac{1}{2\omega}\left|\frac{d^2\omega}{dq^2}\right|}$ one finds nonmonotonic dependence of $l_s$ on the parameter $\gamma$ (for the BZ edge it is represented in Fig. 3). Thus there is a relation among the parameters of the nonlocal potential at which an effective width of a soliton is smallest. In general, if $\gamma$ is not much smaller than one, long-range interactions lead to stronger localization of the modes, which is expressed by the fact that $l_s(\gamma) < l_s(\infty)$ (however, in the limit $\gamma \ll 1$ the effective soliton width is defined by $l_s/\gamma$).

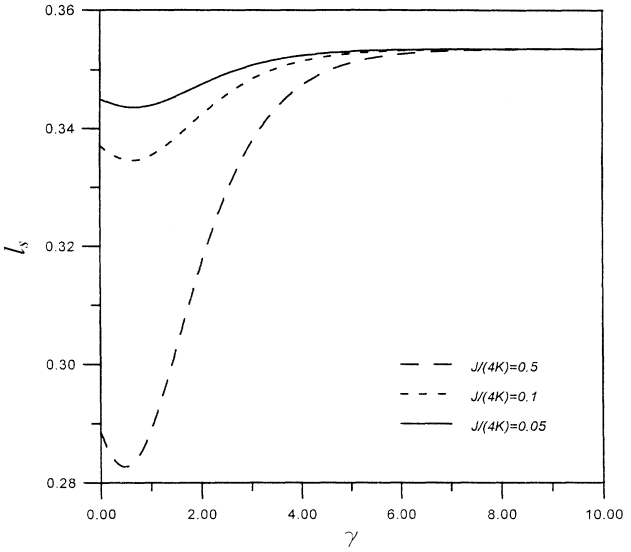


FIG. 3. Dependence of the effective soliton width at the BZ edge on the parameters of the Kac-Baker potential.

The basic qualitative effects come from the analysis of the group velocity in the whole BZ (except the center which corresponds to the long wavelength excitations). It is sketched in Fig. 4. At $\gamma$ small enough (less than some critical value) the curves take $N$-shape form (the solid line in Fig. 4), which means existence of points where GVD changes the sign (in Fig. 4 they are indicated by $q_{\min}$ and $q_{\max}$). In those points there occurs alteration of a type of an available solution. If, for exam-

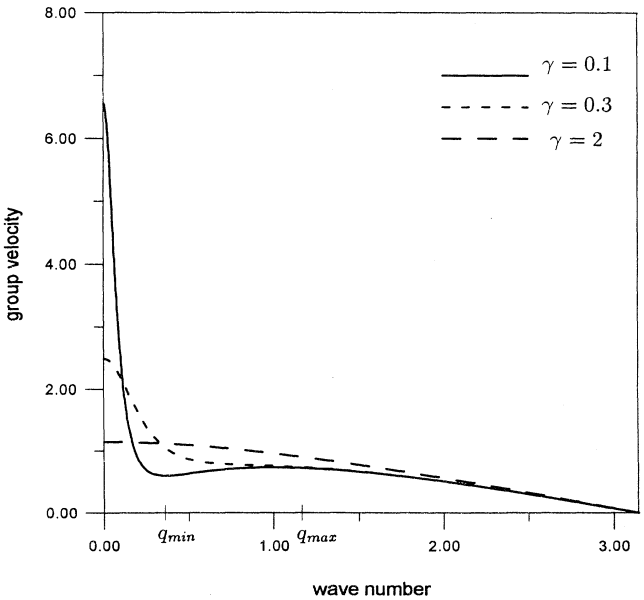


FIG. 4. The group velocity vs the wave number for the lattice with the parameters $K = 1$, $M = 1$, $J = 0.4$, $a = 1$, and different $\gamma$.

ple, the respective "local" lattice supports propagation of bright solitons then in the spectral region between $q_{\min}$ and $q_{\max}$ the lattice with long-range interactions supports propagation of dark solitons. For the first time the effect of coexistence of bright and dark solitons due to the nonlocal interactions has been discovered by Remoissenet and Flytzanis [14] in the long wavelength approximation. Here that result is generalized for the whole BZ including essentially discrete limit.

Another peculiarity of the model at hand is that there exist modes with different frequencies, say $\omega_1$ and $\omega_2$, and equal group velocities. Such modes being excited simultaneously display coupled dynamics. In order to illustrate the phenomenon let us consider the CW of the form

$$v_1 = A_1(t_1,...;X_1,...)\phi_1(X_0)e^{-i\omega_1 t_0} + A_2(t_1,...;X_1,...)\phi_2(X_0)e^{-i\omega_2 t_0} + \text{c.c.}, \quad (73)$$

where the difference between the frequencies is of the order of the frequencies themselves: $\omega_2 - \omega_1 = O(\omega_{1,2})$.

Next consideration is provided for the case when cubic nonlinearity is absent ($J_3 \equiv 0$). Then straightforward algebra leads to the relations

$$i\frac{\partial A_1}{\partial t_1} + v_1\frac{\partial A_1}{\partial X_1} = 0, \quad i\frac{\partial A_2}{\partial t_1} + v_2\frac{\partial A_2}{\partial X_1} = 0, \quad (74)$$

where $v_j = d\omega_j/dq$. As has been mentioned above in the case of the chain with long-range interactions there are points at which $v_1 = v_2$. Assuming that $\omega_{1,2}$ are chosen respectively one has $A_j = A_j(z)$, where $z = X_1 - v_1 t_1$.

The equations of the third order are derived to be (as above, the dependence on $X_2$ is not considered)

$$2i\omega_1\frac{\partial A_1}{\partial t_2} + \omega_1\frac{d^2\omega_1}{dq^2}\frac{\partial^2 A_1}{\partial z^2} - (\chi_{11}|A_1|^2 + 2\chi_{12}|A_2|^2)A_1 = 0, \quad (75a)$$

$$2i\omega_2\frac{\partial A_2}{\partial t_2} + \omega_2\frac{d^2\omega_2}{dq^2}\frac{\partial^2 A_2}{\partial z^2} - (2\chi_{21}|A_1|^2 + \chi_{22}|A_2|^2)A_2 = 0 \quad (75b)$$

[the coefficients $\chi_{lm}$ have been introduced in (34)].

The system (75a), (75b) is well known in nonlinear optics [23]. In particular, it has been studied in the context of the coupled mode dynamics [24]: however, it is to be emphasized here that the case at hand is essentially different since the frequency shift between modes in [24] was a small parameter.

Let us mention two interesting particular situations: when one of $q_j$ corresponds to one of the extrema of the group velocity. Suppose, for example, that $q_2 > q_{\max}$ and $q_1 = q_{\min}$. Then $\frac{d^2\omega_1}{dq^2} = 0$, $\frac{d^2\omega_2}{dq^2} < 0$ and depending on the sign of the nonlinearity the system (75a), (75b) possesses either the bright soliton solution ($\chi_{22} + 2\chi_{21} < 0$)

$$A_1 = \frac{A}{\cosh(z/z_0)}\exp\left(i\frac{\chi_{11}+2\chi_{12}}{2\omega_1}\frac{A^2}{\cosh^2(z/z_0)}t_2\right), \quad (76a)$$

$$A_2 = \frac{A}{\cosh(z/z_0)}\exp\left(i\frac{2\chi_{21}+\chi_{22}}{4\omega_2}A^2 t_2\right), \quad (76b)$$

where

$$z_0^{-1} = \sqrt{\left|\frac{2\chi_{21}+\chi_{22}}{2\omega_2(d^2\omega_2/dq^2)}\right|}A \quad (77)$$

and $A$ is a constant, or the dark soliton solution ($\chi_{22} + 2\chi_{21} > 0$)

$$A_1 = A\tanh\left(\frac{z}{z_0}\right)\exp\left[i\frac{\chi_{11}+2\chi_{12}}{2\omega_1}A^2\tanh^2\left(\frac{z}{z_0}\right)t_2\right], \quad (78a)$$

$$A_2 = A\tanh\left(\frac{z}{z_0}\right)\exp\left[i\frac{2\chi_{21}+\chi_{22}}{2\omega_2}A^2 t_2\right] \quad (78b)$$

[the characteristic scale $z_0$ being given by (77)].

The peculiarity of the obtained solutions consists of the difference between the frequencies of envelope oscillations which means that their superposition, giving the lattice pattern, is characterized by *two* internal frequencies. Also, the frequency of the first mode is not a constant but depends on the "spatial" coordinate $\zeta$.

## IV. CONCLUSION

To conclude, the general theory of the small-amplitude envelope solitons in lattices has been developed. It is based on the multiscale expansion and allows one to obtain moving localized excitations in monoatomic and multiatomic chains with nearest-neighbor and long-range interactions. A type of a soliton solution is determined by the sign of the product of the GVD and the effective nonlinearity. The theory allows the description of the coupled mode dynamics resulting in tied solitonic states. Propagation of such pulses is accompanied by excitation of companion modes, which represent states orthogonal to the principal harmonic. The coupled solitons in the diatomic lattice link optical and accoustic branches of the spectrum, which gives a possibility for the energy transfer between the modes. In the case of a lattice with long-range interactions the solitons due to coupling of two modes having different wave numbers but the same group velocities are characterized by two oscillating degrees of freedom. The additional internal frequencies can serve as sources for various resonant phenomena. The coupled solitonic states are movable and hence may play a remarkable role in the energy transfer along chains.

The necessary condition for the coupled envelope solitons to be created is the dispersionless character of equations of the second order of the expansion.

As a matter of fact the theory provides us with the possibility to predict a type of a soliton even on the basis of numerical analysis of the spectrum (the last of course is not enough for detail description of the lattice pattern). Finally, the consistent multiscale expansion allows one to

analyze perturbations which are classified on the basis of their amplitudes.


## ACKNOWLEDGMENT

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## APPENDIX A: INEQUALITY (17)

In order to show that the requirement (17) is enough for validity of the multiscale expansion, let us estimate the rest $R$ of the set in the last sum in (16) starting with the term $p = p_0$. We have

$$|R| = \left| \sum_{\alpha_1} \sum_{p=p_0}^{\infty} \frac{1}{p!} \sum_{\nu_1=1}^{\infty} \cdots \sum_{\nu_p=1}^{\infty} \mu^{\nu_1+\cdots+\nu_p} \sum_{m=-\infty}^{\infty} m^p K_2(n_0, \alpha; n_0+m, \alpha_1) \frac{\partial}{\partial n_{\nu_1}} \cdots \frac{\partial}{\partial n_{\nu_p}} u_{\alpha_1}(n_0+m, \{n_\nu\}) \right|$$

$$\leq \tilde{C} \sum_{\alpha_1} \sum_{p=p_0}^{\infty} \frac{1}{p!} \left( \sum_{\nu=1}^{\infty} \mu^\nu \right)^p \left| \sum_{m=-\infty}^{\infty} m^p K_2(n_0, \alpha; n_0+m, \alpha_1) \right| \tag{A1}$$

($\tilde{C}$ =const). Here it is taken into account that in accordance with the multiscale method all derivatives $\partial^p u_\alpha / \partial n_\nu^p$ are of the order of one, i.e., $|\partial^p u_\alpha / \partial n_\nu^p| \leq \tilde{C}$ for arbitrary $\nu$ and $p$ (otherwise the method itself fails). Now the sum over $\nu$ is calculated explicitly to give $\mu^p (1-\mu)^{-p}$. Assuming that (17) takes place and supposing that the sum over $\alpha_1$ has no more than $N_0$ terms one obtains

$$|R| \leq N_0 \tilde{C} C \sum_{p=p_0}^{\infty} \left( \frac{G\mu}{1-\mu} \right)^p . \tag{A2}$$

Since we are interested in the limit $\mu \to 0$ (or $\frac{G\mu}{1-\mu} \ll 1$) the last estimation can be rewritten as $|R| = O(G^{p_0} \mu^{p_0})$. Hence under the condition (17) the expression (16) takes the form

$$\sum_{\alpha_1} \sum_{m=-\infty}^{\infty} K_2(n_0, \alpha; n_0+m, \alpha_1) u_{\alpha_1}(n_0+m, \{n_\nu\}) + \sum_{\nu=1}^{\infty} \mu^\nu \sum_{\alpha_1} \sum_{m=-\infty}^{\infty} m K_2(n_0, \alpha; n_0+m, \alpha_1) \frac{\partial}{\partial n_\nu} u_{\alpha_1}(n_0+m, \{n_\nu\})$$

$$+ \frac{1}{2} \sum_{\nu_1=1}^{\infty} \sum_{\nu_2=1}^{\infty} \mu^{\nu_1+\nu_2} \sum_{\alpha_1} \sum_{m=-\infty}^{\infty} m^2 K_2(n_0, \alpha; n_0+m, \alpha_1) \frac{\partial}{\partial n_{\nu_1}} \frac{\partial}{\partial n_{\nu_2}} u_{\alpha_1}(n_0+m, \{n_\nu\}) + \cdots . \tag{A3}$$

Our aim is to describe the effect of the nonlinearity, and that is why all the terms in the above formula must be calculated with accuracy $O(\mu^3)$. This gives the final expression for the sum under consideration,

$$\sum_{\alpha_1} \sum_{m=-\infty}^{\infty} K_2(n_0, \alpha; n_0+m, \alpha_1) \left[ u_{\alpha_1}(n_0+m, \{n_\nu\}) + \mu m \frac{\partial}{\partial n_1} u_{\alpha_1}(n_0+m, \{n_\nu\}) \right.$$

$$\left. + \mu^2 m \frac{\partial}{\partial n_2} u_{\alpha_1}(n_0+m, \{n_\nu\}) + \frac{1}{2} \mu^2 m^2 \frac{\partial^2}{\partial n_1^2} u_\alpha(n_0+m, \{n_\nu\}) \right] + O(G^3 \mu^3). \tag{A4}$$

Let us ensure that the condition (17) is satisfied by the Kac-Baker [21] potential (71). To this end it is enough to note that

$$\left| \sum_{m=1}^{\infty} m^p e^{-\gamma m} \right| = \left| \left( (\xi - 1) \frac{d}{d\xi} \right)^p \frac{1}{\xi} \right| \leq 2^p p! \xi^{-(p+1)},$$

where $\xi = 1 - e^{-\gamma}$ and $p > 1$. Thus the constant $G$ in (17) can be taken equal to $2/\xi$. If, however, $\gamma \ll 1$ the multiscale expansion requires modification, which can be done by defining $n_\nu = (\gamma\mu)^\nu n$.

## APPENDIX B: GROUP VELOCITY AND ITS DISPERSION

First we can use a discrete analog of the elegant arguments of de Sterke and Sipe [13] to show that in the case of a scalar lattice there are relations

$$2\omega_l \frac{d\omega_l}{dq} = i\Gamma_{ll} \tag{B1}$$

and

$$\omega_l \frac{d^2\omega_l}{dq^2} + \left( \frac{d\omega_l}{dq} \right)^2 = \sum_{m \neq l} \frac{1}{\omega_l^2 - \omega_m^2} |\Gamma_{ml}|^2 - \Lambda_l, \tag{B2}$$

where the coefficients $\Gamma_{ml}$ and $\Lambda_l$ are introduced by (24) and (33). The idea of the method consists of the following: the shift of the frequency caused by an infinitesimal variation of the wave number is calculated by means of the perturbation theory on the one hand and on the other hand by means of the simple expansion in the Taylor series. Comparison of both sets allows one to express the derivatives of the frequency with respect to the wave number through the eigenfunctions.

The classical formula of the perturbation theory,

$$\omega^2 = \omega_l^2 + V_{ll} + \sum_{m\neq l} \frac{|V_{ml}|^2}{\omega_l^2 - \omega_m^2}, \tag{B3}$$

where

$$V_{ml} = \sum_x \sum_{x_1} j(x;x_1)\bar{\phi}_m(x)\phi_l(x_1)$$

describes change of the frequency of the state $l$ affected by a perturbation $j(x;x_1)$ [i.e., when $J_2(x;x_1)$ in the equation of motion is replaced by $J_2(x;x_1) + j(x;x_1)$]. As follows from (43) a small variation $q_l \to q_l + dq$ results in the change

$$\phi_l(x) \to \phi_l(x) + \left[iandq - \frac{1}{2}a^2n^2(dq)^2\right]\phi_l(x) + O((dq)^3).$$

This is equivalent to the peturbation

$$j(x;x_1) = \left[ia(n_1-n)dq - \frac{1}{2}a^2(n_1-n)^2(dq)^2\right] \times J(x;x_1). \tag{B4}$$

Thus on the one hand

$$\omega^2(q+dq) = \omega^2(q) + \frac{d(\omega^2)}{dq}dq + \frac{1}{2}\frac{d^2(\omega^2)}{dq^2}(dq)^2 + O((dq)^3) \tag{B5}$$

and on the other hand (B3) yields

$$\omega^2(q+dq) = \omega_l^2 + ia(dq)\sum_x\sum_{x_1}(n_1-n)J_2(x;x_1)\bar{\phi}_l(x)\phi_l(x_1) - \frac{1}{2}a^2(dq)^2\sum_x\sum_{x_1}(n_1-n)^2J_2(x;x_1)\bar{\phi}_l(x)\phi_l(x_1)$$
$$+a^2(dq)^2\sum_{m\neq l}\frac{1}{\omega_l^2-\omega_m^2}\left|\sum_x\sum_{x_1}(n_1-n)J_2(x;x_1)\bar{\phi}_m(x)\phi_l(x_1)\right|^2 + O((dq)^3). \tag{B6}$$

Comparison of (B5) and (B6) yields (B1), (B2).

Let us now consider a diatomic lattice when $m \to 0$ and $w \to 0$. Then at the edge of the BZ the two branches of the spectrum tend to each other and at the point $q = \pi/a_2 = \pi/2a$ the spectrum becomes degenerate (Fig. 2). Corresponding point of the spectrum requires the well-known modification of the perturbation theory [22] and can be described by two subsequent steps. First, the normalized basis diagonalizing $j(x;x_1)$ can be determined. Second, the matrix element for the expansion of the frequency can be obtained. Since the purpose of these actions is the expression of the group velocity and its dispersion in the degeneration point through the set of the eigenfunctions, all the calculations must be done with the accuracy $O((dq)^3)$ [cf. (B5)].

Introduce the basis

$$\psi_j(x) = c_{j1}\varphi_1(x) + c_{j2}\varphi_2(x) \quad (j=1,2). \tag{B7}$$

Here, temporarily the Bloch functions $\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x)$ and $\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x)$ are designated by $\varphi_1(x)$ and $\varphi_2(x)$, correspondingly. The coefficients $c_{jk}$ are determined from the requirements $\sum_{x,x_1} j(x;x_1)\bar{\psi}_1(x)\psi_2(x_1) = 0$ and $\sum_x |\psi_j(x)|^2 = 1$. They have the form

$$c_{j1} = \left\{\frac{w_{12}}{2|w_{12}|}\left[1 + (-1)^{j-1}\frac{w_{11}-w_{22}}{\Delta}\right]\right\}^{1/2},$$

$$c_{j2} = (-1)^{j-1}\left\{\frac{w_{21}}{2|w_{12}|}\left[1 + (-1)^{j}\frac{w_{11}-w_{22}}{\Delta}\right]\right\}^{1/2},$$

where $w_{ij} = \sum_{x,x_1} j(x;x_1)\varphi_1(x)\varphi_2(x_1)$ [remember the Bloch functions $\varphi_k(x)$ are real] and $\Delta = \sqrt{(w_{11}-w_{22})^2 + 4|w_{12}|^2}$. Using (B4) it is straightforward to show that

$$w_{11} = -\Lambda_{\mathrm{ac}}(dq)^2 + O((dq)^3),$$
$$w_{22} = -\Lambda_{op}(dq)^2 + O((dq)^3); \tag{B8}$$

$$w_{12} = -2i\omega v dq + O((dq)^2),$$
$$w_{21} = 2i\omega v dq + O((dq)^2); \tag{B9}$$

and $\Delta = 4\omega v(dq)^2 + O((dq)^3)$, where $v$ is given by (50). Hence

$$c_{j1} = e^{-i\pi/4}\sqrt{\frac{s}{2}}\left[1 + (-1)^{j-1}\frac{\Lambda_{\mathrm{op}}-\Lambda_{\mathrm{ac}}}{2\omega|v|}dq\right] + O((dq)^2), \tag{B10}$$

$$c_{j2} = (-1)^{j-1}e^{i\pi/4}\sqrt{\frac{s}{2}}\left[1 + (-1)^{j}\frac{\Lambda_{\mathrm{op}}-\Lambda_{\mathrm{ac}}}{2\omega|v|}dq\right] + O((dq)^2), \tag{B11}$$

where $s = \mathrm{sgn} v$.

The last formulas lead to the important conclusion that the states

$$\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x) \pm i\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x) \tag{B12}$$

are orthogonal and diagonalize $j(x;x_1)$. But they are exactly the states determined by (51). Hence one can say that the soliton obtained in Sec. III B is an envelope of the composite state (B12).

Now, for the chosen branch (52) one must use the formula

$$\Omega^2 = \omega^2 + \tilde{V} + \sum_m{}' \frac{|V_m^{(1)}|^2 + |V_m^{(2)}|^2}{\omega^2 - \omega_m^2}, \tag{B13}$$

where $\Omega$ is the eigenvalue corresponding to the perturbed eigenstate $\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x) + i\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x)$,

$$\begin{aligned}\tilde{V} &= \sum_x \sum_{x_1} j(x;x_1)\bar{\psi}_1(x)\psi_1(x) \\ &= 2\omega v dq - \frac{1}{2}(\Lambda_{\mathrm{op}} + \Lambda_{\mathrm{ac}})(dq)^2,\end{aligned} \tag{B14}$$

$$\begin{aligned}|V_m^{(1)}|^2 &= \frac{1}{2}|\Gamma_m^{(11)} - i\Gamma_m^{(12)}|^2(dq)^2\ , \\ |V_m^{(2)}|^2 &= \frac{1}{2}|\Gamma_m^{(22)} - i\Gamma_m^{(21)}|^2(dq)^2\end{aligned} \tag{B15}$$

[the coefficients $\Gamma_m^{(ij)}$ being given by (54)] and $\sum'$ means that the sum does not include the harmonics with the frequencies $\omega^{(\mathrm{op})}$ and $\omega^{(\mathrm{ac})}$.

Comparing (B13) and (B5) one immediately finds the group velocity

$$\Omega' = v \tag{B16}$$

and its dispersion

$$\begin{aligned}\Omega'' = &-\frac{v^2}{\omega} - \frac{1}{2\omega}(\Lambda_{\mathrm{op}} + \Lambda_{\mathrm{ac}}) \\ &+ \frac{1}{2\omega}\sum_m{}' \frac{1}{\omega^2 - \omega_m^2} \\ &\times \left(|\Gamma_m^{(11)} - i\Gamma_m^{(12)}|^2 + |\Gamma_m^{(22)} + i\Gamma_m^{(21)}|^2\right).\end{aligned} \tag{B17}$$

## APPENDIX C: THE CONSTANTS $\chi$ AND $\chi_-$ IN THE CASES OF HOMOGENEOUS ON-SITE AND NEAREST-NEIGHBOR INTERACTION NONLINEARITIES

Here it is shown that under one of the following assumptions: (i) The nonlinearity is originated by an on-site potential equal for the both types of particles; (ii) the nonlinear interactions exist only between nearest neighbors and are the same for particles belonging to one cell and to adjacent cells; the relations (63) are fulfilled.

To this end note that in the case of a diatomic lattice the eigenfunction $\phi_m(x)$ at the BZ edge allows representation

$$\phi_{\mathrm{BZ}}^{(\mathrm{op,ac})}(x) = \frac{1}{\sqrt{\mathcal{N}}} a_\alpha^{(\mathrm{op,ac})}(-1)^n \tag{C1}$$

[here $a_\alpha^{(\mathrm{op,ac})}$ $(\alpha = 1,2)$ play the role of the normalized amplitudes of the atoms inside a cell]. Then it follows from (11) that

$$[a_1^{(\mathrm{op,ac})}]^2 + [a_2^{(\mathrm{op,ac})}]^2 = 1, \qquad a_1^{(\mathrm{op})}a_1^{(\mathrm{ac})} + a_2^{(\mathrm{op})}a_2^{(\mathrm{ac})} = 0. \tag{C2}$$

Equations (C2) allow one to introduce convenient parametrization

$$a_1^{(\mathrm{op,ac})} = \cos\vartheta_{\mathrm{op,ac}}, \quad a_2^{(\mathrm{op,ac})} = \sin\vartheta_{\mathrm{op,ac}}, \tag{C3}$$

where $\vartheta_{\mathrm{op}} = \vartheta_{\mathrm{ac}} + \frac{\pi}{2} = \vartheta$. Now simple algebra yields the relations

$$\begin{aligned}&\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n',2) - \phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n',2) \\ &\qquad = \frac{(-1)^{n+n'}}{\mathcal{N}}\sin 2\vartheta,\end{aligned} \tag{C4}$$

$$\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n',2) + \phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n',2) = 0, \tag{C5}$$

$$[\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,\alpha)]^2 + [\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,\alpha)]^2 = \frac{1}{\mathcal{N}}, \tag{C6}$$

$$[\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,\alpha)]^2 - [\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,\alpha)]^2 = \frac{(-1)^{\alpha+1}}{\mathcal{N}}\cos 2\vartheta, \tag{C7}$$

$$\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,1) + \phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,2)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,2) = 0, \tag{C8}$$

$$\phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n,2) + \phi_{\mathrm{BZ}}^{(\mathrm{op})}(n,1)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(n-1,2) = 0 \tag{C9}$$

[for the sake of convenience in the above formulas $x$ is replaced by the pair $(n,\alpha)$].

For the next step one must take into account that in $J_4(x_1;\ldots;x_4)$ only elements corresponding to nearest neighbors may differ from zero and they are equal for both neighbors of a given atom. Then it follows from (C5), and (C6) that the term in the square brackets in (59) is equal to zero unless the eigenfunctions correspond to the same atom and hence

$$\chi = \frac{1}{\omega\mathcal{N}}\sum_x \sum_{x_3} \sum_{x_4} J_4(x;x;x_3;x_4)\phi_{\mathrm{BZ}}^{(\mathrm{op})}(x_3)\phi_{\mathrm{BZ}}^{(\mathrm{ac})}(x_4).$$

The equivalence of the last sum to zero is a consequence of (C8), (C9).

Passing to the constant $\chi_-$ one notes that due to (C7) terms with $\alpha_3 = \alpha_4$ (and, respectively, $n_3 = n_4$, since only nearest-neighbor interactions are taken into account) give zero contribution after summing over one cell. As a consequence of (C4) terms corresponding to different atoms in one cell (i.e., with $\alpha_3 \neq \alpha_4$) are cancelled with each other. Thus $\chi_- = 0$.

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