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PARAMETRIC SIMULTONS IN ONE-DIMENSIONAL NONLINEAR LATTICES*

Huang Guo-xiang(黄国翔)

Department of Physics and State Key Laboratory of Optical and Magnetic Resonance Spectroscopy, East China Normal University, Shanghai 200062, China

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Parametric simultaneous solitary wave (simulton) excitations are shown to be possible in nonlinear lattices. Taking a one-dimensional diatomic lattice with a cubic potential as an example, we consider the nonlinear coupling between the upper cut-off mode of acoustic branch (as a fundamental wave) and the upper cut-off mode of optical branch (as a second harmonic wave). Based on a quasi-discreteness approach the Karamzin–Sukhorukov equations for two slowly varying amplitudes of the fundamental and the second harmonic waves in the lattice are derived when the condition of second harmonic generation is satisfied. The lattice simulton solutions are given explicitly and the results show that these lattice simultons can be nonpropagating when the wave vectors of the fundamental wave and the second harmonic waves are exactly at π/a (where a is the lattice constant) and zero, respectively.

Keywords: nonlinear lattice waves, solitons, simultons
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I. INTRODUCTION

Since the pioneering work of Fermi, Pasta and Ulam[1] on the nonlinear dynamics in lattices, the understanding of the dynamical localization in ordered, spatially extended discrete systems have experienced considerable progress. In particular, the lattice solitons, which are localized nonlinear excitations due to the balance between nonlinearity and dispersion of the system, are shown to exist, and many important applications are found in transport of energy, proton contactivity, structural phase transition and associated central-peak phenomena, etc.[2,3] In recent years, the interest in localized excitations in nonlinear lattices has been renewed due to the identification of a new type of anharmonic localized modes.[4−6] These modes, called the intrinsic localized modes (ILM's),[4] or discrete breathers,[5,6] are the discrete analogue of the lattice envelope (or breather) solitons with their spatial extension only a few lattice spacings and the vibrating frequency above the upper cut-off of phonon spectrum band. The ILM's have been observed in a number of experiments.[7−13] Recently, much attention has been paid to the gap solitons in diatomic lattices.[14−25] In the linear case, a diatomic lattice allows two phonon bands. There is an upper cut-off for phonon frequency and a frequency gap (forbidden band) between acoustic and optical bands, induced by mass and/or force-constant difference of two different types of particles. No interaction occurs between phonons and the phonons cannot propagate in the system when their frequencies are in the gap or above the phonon bands. However, these properties of the phonons change drastically when nonlinearity is introduced into the system. New types of localized modes, especially the gap solitons, may appear as nonlinear localized excitations with their vibrating frequencies in the band gap. The gap solitons and ILM's as well as their chaotic motion have been observed in damped and parametrically excited one-dimensional (1D) diatomic pendulum lattices.[26−28]

On the other hand, in recent years, numerous achievements have been made for optical solitons in nonlinear optical media.[29−31] Besides the temporal optical solitons, which are promising for long-distance information transmission in fibre, spatial optical solitons also attract much attention. The spatial optical solitons are believed to be the candidates for all-optical devices, such as optical switches and logic gates, etc.[32] Recently, the study of optical parametric processes, in particular the second harmonic generation (SHG), which marked the birth of nonlinear optics, has generated a great deal of new interest.[33] It was suggested that it is possible to obtain large nonlinear phase shifts by using a cascaded second-

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order nonlinearity.[34] In 1974, Karamzin and Sukhorukov (KS) recognized that the cascaded second-order parametric processes may support solitons under general phase-matching conditions. They derived two coupled nonlinear equations for the envelopes of the fundamental and second harmonic waves.[35] The difference between the KS equations and the envelope equations for usual SHG is the inclusion of dispersion and/or diffraction, which are necessary for short pulses and/or narrow light beams. Simultaneous solitons (i.e. two components are solitons) are found for the KS equations and these solitons are later termed as the parametric simultons.[36] The concept of the simultons has been generalized to the nonlinear optical media with periodically varying refractive index.[37] Since the eigenspectrum of linear electromagnetic waves consists of many photonic bands and the vibrating frequencies of the simultons may be in the gaps between these bands, the name parametric band-gap simulton is given by Drummond *et al.*[37−39] Different from the self-trapping mechanism for Keer solitons, the formation of the simultons is due to the energy transfer and mutual self-trapping between the fundamental and the second harmonic waves.

In contrast, the SHG in lattices is much less investigated. Although in the standard textbook of solid-state physics[40] there exists a simple experimental description for three phonon processes in solids, it seems that there is no detailed theoretical approach to the SHG in nonlinear lattices until recently. In a recent paper, Konotop considered theoretically the SHG in a nonlinear diatomic lattice and obtained some interesting results.[41]

In many aspects, a nonlinear lattice is similar to a nonlinear, periodic optical media. The discreteness of the lattice results in the symmetry breaking for continuous translation and makes the property of the system periodic, in particular the frequency spectrum of corresponding linear wave splits into many bands. It should be stressed that the SHG does not occur in one-dimensional monatomic lattices (see the next section). However, a SHG can be realized if we consider nonlinear multi-atomic lattices. The reason is that in the monatomic lattices, an efficient energy transfer (resonance) between any two modes in the system does not occur. But the situation is different for the multi-atomic lattices. A multi-atomic lattice allows many branches of linear dispersion relation, and the dispersion relation is periodic with respect to lattice wave vector. It is just the multiple-value and periodic property of the dispersion relation makes it possible that the phase-matching condition for the SHG, i.e. the condition by which the resonance between the fundamental and second harmonic waves may occur, can be satisfied by selecting the wave vectors and the corresponding frequencies from different spectrum branches.

Motivated by the study of the optical simultons, in this paper we show that lattice simultons are possible in the multi-atomic lattices with cubic nonlinearity (different from the case in nonlinear optics, here the order of nonlinearity means the order in the Hamiltonian of the system). The paper is organized as follows. The next section presents our model and an asymptotic expansion based on a quasi-discreteness approach. In section III we solve the KS equations derived in section II and provide some lattice simulton solutions. A discussion and summary is given in the last section.

II. MODEL AND ASYMPTOTIC EXPANSION

A. The model

As mentioned in the last section, principally the SHG may occur in many multi-atomic lattice systems, but for definiteness and for the sake of simplicity we consider here a one-dimensional diatomic lattice with a cubic interaction potential. Such potential can be obtained by Taylor expanding some realistic atomic potentials in a power series of atomic displacements from equilibrium configuration. We focus on the displacements with smaller amplitude thus the higher-order nonlinear terms that give no contribution to underlying nonlinear processes in the power series can be disregarded. In fact, as in nonlinear optics, the second harmonic resonance in lattice systems is a second-order nonlinear process, thus only the cubic nonlinearity in the Hamiltonian is needed. Therefore, we neglect the higher-order nonlinear terms and consider a lattice Hamiltonian with the form

$$H=\sum_n\Big[\frac{1}{2}m\left(\frac{\mathrm{d}v_n}{\mathrm{d}t}\right)^2+\frac{1}{2}M\left(\frac{\mathrm{d}w_n}{\mathrm{d}t}\right)^2 +\frac{1}{2}K_2(w_n-v_n)^2+\frac{1}{2}K_2'(v_{n+1}-w_n)^2 +\frac{1}{3}K_3(w_n-v_n)^3+\frac{1}{3}K_3'(v_{n+1}-w_n)^3 +\frac{1}{3}V_3v_n^3+\frac{1}{3}V_3'w_n^3\Big], \quad (1)$$

where $v_n=v_n(t)$ $(w_n = w_n(t))$ is the displacement from its equilibrium position of the nth particle with mass $m\,(M)$. n is the index of the nth unit cell with a lattice constant $a = 2a_0$, a_0 is the equilibrium lattice spacing between two adjacent particles. Here for generality we assume that the nearest-neighbour force constants $K_j (j = 2, 3)$ in the same cell are different from the nearest-neighbour force constants $K_j' (j = 2, 3)$ in different cells. V_3 and V_3' are the force constants related to the on-site cubic potential for two types of particles. Without loss of generality we assume $m < M$, $K_j' \le K_j (j = 2, 3)$, and $V_3' \le V_3$. The equations of motion for describing the lattice read

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} v_n = I_2(w_n - v_n) + I_2'(w_{n-1} - v_n) + I_3(w_n - v_n)^2 - I_3'(w_{n-1} - v_n)^2 - \alpha_m v_n^2, \tag{2}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} w_n = J_2(v_n - w_n) + J_2'(v_{n+1} - w_n) - J_3(v_n - w_n)^2 + J_3'(v_{n+1} - w_n)^2 - \alpha_M w_n^2, \tag{3}$$

where $I_j = K_j/m$, $I_j' = K_j'/m$, $J_j = K_j/M$, $J_j' = K_j'/M\,(j = 2, 3), \alpha_m = V_3/m$ and $\alpha_M = V_3'/M$. The linear dispersion relation of Eqs. (2) and (3) is given by

$$\omega_\pm(q) = \frac{1}{\sqrt{2}} \Big\{ (I_2 + I_2' + J_2 + J_2') \pm [(I_2 + I_2' + J_2 + J_2')^2 - 16 I_2 J_2' \sin^2(qa/2)]^{1/2} \Big\}^{1/2}, \tag{4}$$

where the minus (plus) sign corresponds to acoustic (optical) mode. Thus we have two phonon bands $\omega_\pm(q)$ and obviously $\omega_\pm(q + Q) = \omega_\pm(q)$, here $Q = 2j\pi/a$, j is an integer and Q is the reciprocal lattice vector of the system. At the wavenumber $q = 0$, the phonon spectrum has a lower cut-off $\omega_-(0) = 0$ for the acoustic mode and an upper cut-off $\omega_+(0) = (I_2 + I_2' + J_2 + J_2')^{1/2}$ for the optical mode. At $q = \pi/a$ there exists a frequency gap between the upper cut-off of the acoustic branch $\omega_-(\pi/a)$ and the lower cut-off of the optical branch $\omega_+(\pi/a)$, where $\omega_\pm(\pi/a) = (1/\sqrt{2})\{(I_2 + I_2' + J_2 + J_2') \pm [(I_2 + I_2' + J_2 + J_2')^2 - 16 I_2 J_2']^{1/2}\}^{1/2}$. The width of the frequency gap is $\omega_+(\pi/a) - \omega_-(\pi/a)$, which approaches zero when $m \to M$ and $K_2' \to K_2$. This is just the limit of monatomic lattice with the lattice constant $a_0 = a/2$. We assume the gap is not small, i.e. we have $(1 - m/M)$ and $(1 - K_2/K_2')$ are of order unity.

Because of the periodic property of $\omega_\pm(q)$, the condition of a second harmonic resonance in the system (2) and (3) reads

$$q_2 = 2q_1 + Q, \tag{5}$$

$$\omega_2 = 2\omega_1, \tag{6}$$

where $q_1\,(q_2)$ and $\omega_1\,(\omega_2)$ are the wave vector and frequency of the corresponding fundamental (second harmonic) wave, respectively. Equations (5) and (6) are also called the phase-matching conditions for the SHG. It is easy to show that in the limit $m \to M$ and $K_2' \to K_2$ conditions (5) and (6) cannot be satisfied except for zero-frequency mode, i.e. the SHG is impossible in monatomic lattices. For the diatomic lattice, in order to fulfil (5) and (6) we may choose $\omega_1 \in \omega_-(q)$ and $\omega_2 \in \omega_+(q)$, then the conditions (5) and (6) give

$$\big[(I_2 + I_2' + J_2 + J_2')^2 - 4 I_2 J_2' \sin(q_1 a)\big]^{1/2} = 3(I_2 + I_2' + J_2 + J_2') - 4\big[(I_2 + I_2' + J_2 + J_2')^2 - 16 I_2 J_2' \sin^2(q_1 a/2)\big]^{1/2}. \tag{7}$$

It is possible to solve q_1 from the above equation. For simplicity we consider the cut-off modes of the system. We take $q_1 = \pi/a, q_2 = 0$ and $Q = -2\pi/a$, then condition (5) is automatically satisfied. Condition (6) (the same as (7)) now reads

$$I_2 + I_2' + J_2 + J_2' = \frac{8}{\sqrt{3}} \sqrt{I_2 J_2'}. \tag{8}$$

Equation (8) also means that $\omega_1 = \omega_-(\pi/a) = (1/2)(I_2 + I_2' + J_2 + J_2')^{1/2} = (4 I_2 J_2'/3)^{1/4}$ and $\omega_2 = \omega_+(0) = (I_2 + I_2' + J_2 + J_2')^{1/2} = 2(4 I_2 J_2'/3)^{1/4}$. If all the harmonic force constants are equal, i.e. $K_2' = K_2$, Eq.(8) gives $m = M/3$. Another particular case is all masses are the same, i.e. $m = M$. In this case, Eq.(8) requires $K_2' = K_2/3$. In general, the phase-matching conditions (5) and (6) impose a constraint on masses and harmonic force constants of the lattice.

B. Asymptotic expansion

We employ the quasi-discreteness approach (QDA) developed in Refs.[17] and [24] for diatomic lattices to investigate the SHG in the system (2) and (3). We are interested in the cascading processes of the system in which the width of excitation is narrower than the usual SHG case. Thus we use different spatial-temporal scales in deriving the envelope equations for the fundamental and the second harmonic waves. We make the expansion

$$u_n(t) = \epsilon \left[u_{n,n}^{(0)} + \epsilon^{1/2} u_{n,n}^{(1)} + \epsilon u_{n,n}^{(2)} + \cdots \right], \tag{9}$$

where $u_n(t)$ represents $v_n(t)$ or $w_n(t)$. ϵ is a smallness and ordering parameter denoting the relative amplitude of the excitation and $u_{n,n}^{(\nu)} = u^{(\nu)}(\xi_n, \tau; \phi_n(t))$, with

$$\xi_n = \epsilon^{1/2}(na - \lambda t), \tag{10}$$

$$\tau = \epsilon t, \tag{11}$$

$$\phi_n = qna - \omega(q)t, \tag{12}$$

where λ is a parameter to be determined by a solvability condition (see below). Substituting (9)–(12) into Eqs.(2) and (3) and equating the coefficients of the same powers of ϵ, we obtain

$$\frac{\partial^2}{\partial t^2}v_{n,n}^{(j)} - I_2(w_{n,n}^{(j)} - v_{n,n}^{(j)}) - I_2'(w_{n,n-1}^{(j)} - v_{n,n}^{(j)}) = M_{n,n}^{(j)}, \tag{13}$$

$$M_{n,n}^{(0)} = 0, \tag{14}$$

$$M_{n,n}^{(1)} = 2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(0)} - I_2'a\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(0)}, \tag{15}$$

$$\begin{aligned}M_{n,n}^{(2)} = {}& 2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(1)} - \left(2\frac{\partial^2}{\partial t\partial\tau} + \lambda^2\frac{\partial^2}{\partial\xi_n^2}\right)v_{n,n}^{(0)} \\ &+ I_2'\left(-a\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(1)} + \frac{a^2}{2!}\frac{\partial^2}{\partial\xi_n^2}w_{n,n-1}^{(0)}\right) \\ &+ I_3(w_{n,n}^{(0)} - v_{n,n}^{(0)})^2 \\ &- I_3'(w_{n,n-1}^{(0)} - v_{n,n}^{(0)})^2 - \alpha_m(v_{n,n}^{(0)})^2,\end{aligned} \tag{16}$$

$$\vdots \qquad \vdots$$

and

$$\frac{\partial^2}{\partial t^2}w_{n,n}^{(j)} - J_2(v_{n,n}^{(j)} - w_{n,n}^{(j)}) - J_2'(v_{n,n+1}^{(j)} - w_{n,n}^{(j)}) = N_{n,n}^{(j)}, \tag{17}$$

$$N_{n,n}^{(0)} = 0, \tag{18}$$

$$N_{n,n}^{(1)} = 2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(0)} + J_2'a\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(0)}, \tag{19}$$

$$\begin{aligned}N_{n,n}^{(2)} = {}& 2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(1)} - \left(2\frac{\partial^2}{\partial t\partial\tau} + \lambda^2\frac{\partial^2}{\partial\xi_n^2}\right)w_{n,n}^{(0)} \\ &+ J_2'\left(a\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(1)} + \frac{a^2}{2!}\frac{\partial^2}{\partial\xi_n^2}v_{n,n+1}^{(0)}\right) \\ &- J_3(v_{n,n}^{(0)} - w_{n,n}^{(0)})^2 \\ &+ J_3'(v_{n,n+1}^{(0)} - w_{n,n}^{(0)})^2 - \alpha_M(w_{n,n}^{(0)})^2,\end{aligned} \tag{20}$$

$$\vdots \qquad \vdots$$

with $j = 0, 1, 2, \cdots$. Equations (13) and (17) can be rewritten in the following form:

$$\hat{L}w_{n,n}^{(j)} = J_2M_{n,n}^{(j)} + J_2'M_{n,n+1}^{(j)} + \left(\frac{\partial^2}{\partial t^2} + I_2 + I_2'\right)N_{n,n}^{(j)}, \tag{21}$$

$$\left(\frac{\partial^2}{\partial t^2} + I_2 + I_2'\right)v_{n,n}^{(j)} = I_2w_{n,n}^{(j)} + I_2'w_{n,n-1}^{(j)} + M_{n,n}^{(j)}, \tag{22}$$

where the operator $\hat{L}$ is defined by

$$\begin{aligned}\hat{L}u_{n,n}^{(j)} = {}& \left(\frac{\partial^2}{\partial t^2} + I_2 + I_2'\right)\left(\frac{\partial^2}{\partial t^2} + J_2 + J_2'\right)u_{n,n}^{(j)} \\ &- (I_2J_2 + I_2'J_2')u_{n,n}^{(j)} \\ &- I_2J_2'\left(u_{n,n+1}^{(j)} + u_{n,n-1}^{(j)}\right),\end{aligned} \tag{23}$$

where $u_{n,n}^{(j)} (j = 0, 1, 2, \cdots)$ are a set of arbitrary functions. From Eq.(21) we can solve $w_{n,n}^{(j)}$ and obtain a series of solvability conditions (envelope equations) whereas Eq.(22) is used to solve $v_{n,n}^{(j)}$.

C. Envelope equations for cascading processes

We now solve Eqs.(22) and (23) order by order. For $j = 0$ it is easy to get

$$w_{n,n}^{(0)} = A_1(\tau, \xi_n)\exp(\mathrm{i}\phi_n^-) + A_2(\tau, \xi_n)\exp(\mathrm{i}\phi_n^+) + \text{c.c.}, \tag{24}$$

$$\begin{aligned}v_{n,n}^{(0)} = {}& \frac{I_2 + I_2'\mathrm{e}^{-\mathrm{i}qa}}{-\omega_-^2 + I_2 + I_2'}A_1(\tau, \xi_n)\exp(\mathrm{i}\phi_n^-) \\ &+ \frac{I_2 + I_2'\mathrm{e}^{-\mathrm{i}qa}}{-\omega_+^2 + I_2 + I_2'}A_2(\tau, \xi_n)\exp(\mathrm{i}\phi_n^+) + \text{c.c.},\end{aligned} \tag{25}$$

with $\phi_n^{\pm} = qna - \omega_{\pm}(q)t$. $\omega_{\pm}(q)$ have been given in Eq.(4). A_1 and A_2 are two envelope (or amplitude) functions of the acoustic and the optical excitations yet to be determined, respectively. They are the functions of the slow variables ξ_n and τ. c.c. denotes the corresponding complex conjugate. For simplicity we specify two modes, i.e. the acoustic upper cut-off mode ($q_1 = \pi/a$, $\omega_1 = \omega_-(\pi/a) = (4I_2J_2'/3)^{1/4}$) and the optical upper cut-off mode ($q_2 = 0$, $\omega_2 = \omega_+(0) = 2\omega_1 = 2(4I_2J_2'/3)^{1/4}$). Thus we have

$$w_{n,n}^{(0)} = A_1(\tau, \xi_n)(-1)^n\exp(-\mathrm{i}\omega_1 t) + A_2(\tau, \xi_n)\exp(-\mathrm{i}\omega_2 t) + \text{c.c.}, \tag{26}$$

$$\begin{aligned}v_{n,n}^{(0)} = {}& \frac{I_2 - I_2'}{-\omega_1^2 + I_2 + I_2'}A_1(\tau, \xi_n)(-1)^n\exp(-\mathrm{i}\omega_1 t) \\ &+ \frac{I_2 + I_2'}{-\omega_2^2 + I_2 + I_2'}A_2(\tau, \xi_n)\exp(-\mathrm{i}\omega_2 t) + \text{c.c.}.\end{aligned} \tag{27}$$

From the discussion in subsection II. A, the modes chosen in such a way satisfy the phase-matching conditions (5) and (6) for the SHG. Thus, in Eqs.(27) and

(28) $A_1\,(A_2)$ represents the amplitude of the fundamental (second harmonic) wave, respectively.

In the next order (j=1), a solvability condition of Eqs.(21) and (22) requires the parameter $\lambda = 0$, thus $\xi_n = na$. The second-order solution reads

$$w^{(1)}_{n,n} = B_0 + [B_1(-1)^n \exp(-\mathrm{i}\omega_1 t) + B_2 \exp(-\mathrm{i}\omega_2 t) + \text{c.c.}], \tag{28}$$

$$v^{(1)}_{n,n} = B_0 + \left\{ \frac{(I_2 - I_2')B_1 + I_2' a \partial A_1/\partial \xi_n}{-\omega_1^2 + I_2 + I_2'} \cdot (-1)^n \exp(-\mathrm{i}\omega_1 t) + \frac{(I_2 + I_2')B_2 - I_2' a \partial A_2/\partial \xi_n}{-\omega_2^2 + I_2 + I_2'} \cdot \exp(-\mathrm{i}\omega_2 t) + \text{c.c.} \right\}, \tag{29}$$

where $B_j\,(j$=$0,1,2)$ are undetermined functions of ξ_n and τ.

In the order j=2, we have the third-order approximate equation

$$\hat{L} w^{(2)}_{n,n} = J_2 M^{(2)}_{n,n} + J_2' M^{(2)}_{n,n+1} + \left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) N^{(2)}_{n,n}. \tag{30}$$

Eq.(22) is not necessary since from (30) we can obtain closed equations for A_1 and A_2. Using Eqs.(26)–(29) we can get $M^{(2)}_{n,n}$, $M^{(2)}_{n,n+1}$ and $N^{(2)}_{n,n}$. By a detailed calculation we obtain the solvability condition of Eq.(30)

$$\mathrm{i}\frac{\partial A_1}{\partial \tau} + \frac{1}{2}\Gamma_1 \frac{\partial^2 A_1}{\partial \xi_n^2} + \Delta_1\, A_1^* A_2 = 0, \tag{31}$$

$$\mathrm{i}\frac{\partial A_1}{\partial \tau} + \frac{1}{2}\Gamma_2 \frac{\partial^2 A_2}{\partial \xi_n^2} + \Delta_2\, A_1^2 = 0, \tag{32}$$

where the coefficients are expressed as

$$\Gamma_1 = -\frac{I_2' J_2' a^2}{\omega_1[\lambda_1^{-1} + \lambda_1 (I_2 - I_2')(J_2 - J_2')]}, \tag{33}$$

$$\Gamma_2 = -\frac{I_2 J_2' a^2}{\omega_2[-\lambda_2^{-1} - \lambda_2 (I_2 + I_2')(J_2 + J_2')]}, \tag{34}$$

$$\Delta_1 = \frac{[1 - \lambda_2(I_2 + I_2')]\lambda_3 - \lambda_1^{-1}\alpha_M - \lambda_1\lambda_2(I_2^2 - (I_2')^2)(J_2 - J_2')\alpha_m}{\omega_1[\lambda_1^{-1} + \lambda_1(I_2 - I_2')(J_2 - J_2')]}, \tag{35}$$

$$\Delta_2 = \frac{\lambda_4 - \lambda_2^{-1}\alpha_M - \lambda_1^2 (I_2 - I_2')^2 (J_2 + J_2')\alpha_M}{2\omega_2[\lambda_2^{-1} + \lambda_2(I_2 + I_2')(J_2 + J_2')]}, \tag{36}$$

with

$$\lambda_j = \frac{1}{-\omega_j^2 + I_2 + I_2'} \qquad (j = 1, 2), \tag{37}$$

$$\lambda_3 = (I_3 - I_3')(J_2 - J_2') - \lambda_1^{-1}(J_3 - J_3') + (I_2 - I_2')\left[(J_3 + J_3') - \lambda_1 (I_3 + I_3')(J_2 - J_2')\right], \tag{38}$$

$$\lambda_4 = [1 - \lambda_1(I_2 - I_2')]^2[-J_3\lambda_2^{-1} + I_3(J_2 + J_2')] + [1 + \lambda_1(I_2 - I_2')]^2[J_3'\lambda_2^{-1} - I_3'(J_2 + J_2')]. \tag{39}$$

Introducing the transformation $u_j = \epsilon A_j\,(j = 1, 2)$ and noting that $\xi_n = \epsilon^{1/2} x_n\,(x_n \equiv na)$ and $\tau = \epsilon t$, Eqs.(31) and (32) can be rewritten into the form

$$\mathrm{i}\frac{\partial u_1}{\partial t} + \frac{1}{2}\Gamma_1 \frac{\partial^2 u_1}{\partial x_n^2} + \Delta_1\, u_1^* u_2 = 0, \tag{40}$$

$$\mathrm{i}\frac{\partial u_2}{\partial t} + \frac{1}{2}\Gamma_2 \frac{\partial^2 u_2}{\partial x_n^2} + \Delta_2\, u_1^2 = 0. \tag{41}$$

We should point out that Eqs.(5) and (6) are perfect phase-matching conditions for the SHG. If we allow a small mismatch for frequency, $\delta\omega$, conditions (5) and (6) become

$$\omega_2 = 2\omega_1 + \delta\omega, \qquad q_2 = 2q_1 + Q. \tag{42}$$

In this case Eqs.(40) and (41) change into

$$\mathrm{i}\left(\frac{\partial u_1}{\partial t} + v_1 \frac{\partial u_1}{\partial x_n} \right) + \frac{1}{2}\Gamma_1 \frac{\partial^2 u_1}{\partial x_n^2} + \Delta_1\, u_1^* u_2 \exp(-\mathrm{i}\delta\omega t) = 0, \tag{43}$$

$$\mathrm{i}\left(\frac{\partial u_2}{\partial t} + v_2 \frac{\partial u_2}{\partial x_n} \right) + \frac{1}{2}\Gamma_2 \frac{\partial^2 u_2}{\partial x_n^2} + \Delta_2\, u_1^2 \exp(i\delta\omega t) = 0, \tag{44}$$

where $v_j\,(j = 1, 2)$ are the group velocities of the fundamental and the second harmonic waves near at $q = \pi/a$ and $q = 0$, respectively.

Equations (43) and (44) are the coupled-mode equations for the fundamental and the second harmonic waves. Such equations have been obtained by Karamzin and Sukhorukov in the context of nonlinear optics.[35] One of important features of the KS equations is the inclusion of dispersion, which is absent in usual SHG envelope equations.[41]

Ⅲ. LATTICE SIMULTON SOLUTIONS

In this section, we solve the KS equations (43) and (44) derived in our lattice model and thus present some lattice simulton solutions for the system (2) and (3). In general, the property of the solutions of Eqs.(43) and (44) depends strongly on the coefficients appearing in the equations, in particular on their signs. At first we notice that in our system, Γ_1 and Γ_2, which are respectively the group-velocity dispersion of the fundamental and the second harmonic waves, are both negative. But the signs of the nonlinear coefficients, Δ_1 and Δ_2, may be generally of both signs. Thus the situation here is different from the KS equations derived for the cascading process in nonlinear optics, where the nonlinear coefficients have the same sign, while the group-velocity dispersions may have different signs.[42]

To solve Eqs.(43) and (44), we make the transformation

$$u_1(x_n,t) = U_1(\zeta)\exp[\mathrm{i}(k_1x_n - \Omega_1 t)], \tag{45}$$

$$u_2(x_n,t) = U_2(\zeta)\exp[\mathrm{i}(k_2x_n - \Omega_2 t)], \tag{46}$$

with $\zeta = kx_n - \Omega t$. Substituting (45) and (46) into (43) and (44), we obtain

$$\frac{\mathrm{d}^2U_1}{d\zeta^2} + \alpha_1U_1U_2 - \beta_1U_1 = 0, \tag{47}$$

$$\frac{\mathrm{d}^2U_2}{d\zeta^2} + \alpha_2U_1^2 - \beta_2U_2 = 0, \tag{48}$$

where $\alpha_1 = 2\Delta_1/(\Gamma_1k^2), \alpha_2 = 2\Delta_2/(\Gamma_2k^2), \beta_1 = -2(\Omega_1 - v_1k - \frac{1}{2}\Gamma_1k_1^2)/(\Gamma_1k^2), \beta_2 = -2(\Omega_2 - v_2k - \frac{1}{2}\Gamma_2k_2^2)/(\Gamma_2k^2)$, $\Omega = v_1k + \Gamma_1kk_1$, with $k_2 = 2k_1, \Omega_2 = 2\Omega_1 + \delta\omega$ and $k_1 = (v_2 - v_1)/(\Gamma_1 - 2\Gamma_2)$. One of the coupled soliton-soliton (i.e. simultaneous solitons for two wave components) solutions of Eqs.(47) and (48) reads

$$U_1 = \frac{6}{\sqrt{\alpha_1\alpha_2}}\left(\frac{2}{3} - \mathrm{sech}^2\zeta\right), \tag{49}$$

$$U_2 = -\frac{6}{\alpha_1}\left(\frac{2}{3} - \mathrm{sech}^2\zeta\right), \tag{50}$$

where a condition $\beta_1 = \beta_2 = -4$ is required. The parameter k is given by

$$k = \frac{v_2 - 2v_1 \pm \{(v_2 - 2v_1)^2 - 8(2\Gamma_1 - \Gamma_2)[(\Gamma_1 - 2\Gamma_2)k_1^2 + \delta\omega]\}^{1/2}}{4(2\Gamma_1 - \Gamma_2)}. \tag{51}$$

The lattice configuration in this case takes the form

$$\begin{aligned} w_n(t) =& (-1)^n\frac{12}{\sqrt{\alpha_1\alpha_2}}\left[\frac{2}{3} - \mathrm{sech}^2(kna - \Omega t)\right]\cos[k_1na - (\omega_1 + \Omega_1)t] \\ &- \frac{12}{\alpha_1}\left[\frac{2}{3} - \mathrm{sech}^2(kna - \Omega t)\right]\cos[k_2na - (\omega_2 + \Omega_2)t], \end{aligned} \tag{52}$$

$$\begin{aligned} v_n(t) =& (-1)^n\frac{12}{\sqrt{\alpha_1\alpha_2}}\;\frac{I_2 - I_2'}{-\omega_1^2 + I_2 + I_2'}\left[\frac{2}{3} - \mathrm{sech}^2(kna - \Omega t)\right]\cos[k_1na - (\omega_1 + \Omega_1)t] \\ &- \frac{12}{\alpha_1}\;\frac{I_2 + I_2'}{-\omega_2^2 + I_2 + I_2'}\left[\frac{2}{3} - \mathrm{sech}^2(kna - \Omega t)\right]\cos[k_2na - (\omega_2 + \Omega_2)t]. \end{aligned} \tag{53}$$

If $q_1\,(q_2)$ is exactly equal to π/a (zero) but with $\delta\omega \neq 0$, one has $v_1 = v_2 = 0$. In this case $k_1 = k_2 = 0$, $\Omega_1 = 2\Gamma_1k^2, \Omega_2 = 2\Gamma_2k^2, \Omega = 0$ and $k = \{\delta\omega/[2(\Gamma_2 - 2\Gamma_1)]\}^{1/2}$. Eqs.(52) and (53) present a nonpropagating simulton excitation, in which the vibrating frequency of the acoustic- (optical-) mode component being within the acoustic(optical) phonon band. In our model, $\Gamma_2 - 2\Gamma_1 > 0$ thus $\delta\omega$ should be taken positive in this case. In addition, from (52) and (53) we see that the envelopes for both the acoustic and optical components are kinks (or dark solitons). Furthermore, if $K_2' = K_2$, the displacement of light particles, $v_n(t)$, only has an optical-mode component.

The other simulton solution of Eqs.(47) and (48) reads

$$U_1 = -\frac{6}{\sqrt{\alpha_1\alpha_2}}\mathrm{sech}^2\zeta, \tag{54}$$

$$U_2 = -\frac{6}{\alpha_1}\left(\frac{4}{3} - \mathrm{sech}^2\zeta\right), \tag{55}$$

where we have $\beta_1 = -\beta_2 = -4$. The parameter k now reads

$$k = \frac{v_2 - 2v_1 \pm \{(v_2 - 2v_1)^2 - 8(\Gamma_2 - 2\Gamma_1)[(\Gamma_1 - 2\Gamma_2)k_1^2 + \delta\omega]\}^{1/2}}{4(\Gamma_2 - 2\Gamma_1)}. \tag{56}$$

The lattice configuration is now given by

$$\begin{aligned} w_n(t) =&(-1)^{n+1}\frac{12}{\sqrt{\alpha_1\alpha_2}}\mathrm{sech}^2(kna-\Omega t)\cos[k_1na-(\omega_1+\Omega_1)t] \\ &-\frac{12}{\alpha_1}\left(\frac{4}{3}-\mathrm{sech}^2(kna-\Omega t)\right)\cos[k_2na-(\omega_2+\Omega_2)t], \end{aligned} \tag{57}$$

$$\begin{aligned} v_n(t) =&(-1)^{n+1}\frac{12}{\sqrt{\alpha_1\alpha_2}}\;\frac{I_2-I_2'}{-\omega_1^2+I_2+I_2'}\mathrm{sech}^2(kna-\Omega t)\cos[k_1na-(\omega_1+\Omega_1)t] \\ &-\frac{12}{\alpha_1}\;\frac{I_2+I_2'}{-\omega_2^2+I_2+I_2'}\left[\frac{4}{3}-\mathrm{sech}^2(kna-\Omega t)\right]\cos[k_2na-(\omega_2+\Omega_2)t]. \end{aligned} \tag{58}$$

Thus, in this case, the acoustic-mode component is a staggered envelope soliton but the optical-mode component is still an envelope kink. If $v_1=v_2=0$ we have $k_1=k_2=0, \Omega_1=2\Gamma_1k^2, \Omega_2=-2\Gamma_2k^2, \Omega=0$ and $k=\{-\delta\omega/[2(\Gamma_2-2\Gamma_1)]\}^{1/2}$. In this situation, the simulton (57) and (58) is also a nonpropagating excitation with the vibrating frequency of the acoustic-(optical-) mode component within(above) the acoustic(optical) phonon band. In order to make k real, we should take $\delta\omega<0$ in this case.

A common requirement for the existence of the simulton solutions (52), (53), (57) and (58) is $\mathrm{sgn}(\alpha_1\alpha_2)>0$, which means $\mathrm{sgn}(\Delta_1\Delta_2)>0$ because $\Gamma_1\Gamma_2>0$ in our model. It can be met by choosing different values of system parameters. For example, in the following two particular cases we have $\mathrm{sgn}(\Delta_1\Delta_2)>0$:

1. $K_2'=K_2, K_3'=K_3=0$. In this case $\Delta_1=-\alpha_M/\omega_1, \Delta_2=-J_2\alpha_M/[2\omega_2(I_2+J_2)]$.

2. $K_2'=K_2, V_3'=V_3=0$. In this case $\Delta_1=(J_3'-J_3)(1+I_2/J_2)/\omega_1$, $\Delta_2=(I_3'-I_3+J_3'-J_3)/[2\omega_2(I_2+J_2)]$.

IV. DISCUSSION AND SUMMARY

We have analytically shown that the lattice simultons are possible in nonlinear diatomic lattices. Based on the QDA for the nonlinear excitations in diatomic lattices developed before,[17,24] we have considered the resonant coupling between two phonon modes, one from the acoustic and other one from the optical branch, respectively. The KS equations are derived for the envelopes of the fundamental and second harmonic waves by taking new multiple spatial-temporal scale variables, which are necessary for narrower nonlinear excitations. Exact coupled soliton (simulton) solutions are obtained for the KS equations and the simulton configurations for the lattice displacements are explicitly given.

Similar to the optical simultons in nonlinear optical media, the physical mechanism for the formation of the lattice simultons is due to the cascading effect between two lattice wave components. In this process, the fundamental and the second harmonic waves interact with themselves through repeated wave–wave interactions. For instance, the energy of the fundamental wave is first upconverted to the second harmonic wave and then downconverted again, resulting in a mutual self-trapping of each wave and thus the formation of two simultaneous solitons.

Mathematically, in addition to the resonance conditions (5) and (6), the formation of a lattice simulton needs a balance between the cubic nonlinearity (in the Hamiltonian) and the dispersion, the latter is provided by the discreteness of the system. Thus, for deriving the envelope equations in this case, we must choose multiple-scale variables different from the ones used in usual SHG. In our derivation for the KS equations based on the QDA,[17,24] only one small parameter, i.e. the amplitude of the excitation, is used. This method gives a clear, justified and self-consistent hierarchy of scales and thus the corresponding solvability conditions, which are just the envelope equations we need. Thus, it is satisfactory according to the point of view of singular perturbation theory.

Cubic nonlinearity exists in most of realistic atomic potentials.[24] Thus it is possible to observe the lattice simultons reported here. It must be emphasized that the multi-value property of the linear dispersion relation is important for generating the simultons in lattices. Thus a diatomic or multi-atomic lattice is necessary for observing such excitations.

The theory given above can be applied to multi-atomic and higher-dimensional lattices, and higher-order nonlinearity can also be included. For instance, if we consider the Hamiltonian with cubic and quartic nonlinearities, Eqs.(31) and (32) should be generalized to

$$\mathrm{i}\frac{\partial A_1}{\partial \tau}+\frac{1}{2}\Gamma_1\frac{\partial^2 A_1}{\partial \xi_n^2}+\Delta_1 A_1^* A_2 + (\Lambda_{11}|A_1|^2+\Lambda_{12}|A_2|^2)A_1=0, \quad (59)$$

$$\mathrm{i}\frac{\partial A_1}{\partial \tau}+\frac{1}{2}\Gamma_2\frac{\partial^2 A_2}{\partial \xi_n^2}+\Delta_2 A_1^2 + (\Lambda_{21}|A_1|^2+\Lambda_{22}|A_2|^2)A_2=0, \quad (60)$$

where $\Lambda_{ij}(i,j=1,2)$ are self-phase and cross-phase modulational coefficients contributed by the quartic nonlinearity of the system. Eqs.(59) and (60) can be derived using the multiple-scale variables $\xi_n=\epsilon x_n, \tau=\epsilon^2 t$ under the assumption $v_n(t)=O(\epsilon), w_n(t)=O(\epsilon)$, $K_3=O(K_3')=O(\epsilon)$, and $V_3=O(V_3')=O(\epsilon)$. A small frequency mismatch can also be included in (59) and (60) and similar equations like (43) and (44) with additional self- and cross-phase modulational terms can also be written down. A detailed study including stability analysis of the lattice simultons should be another work and will be given elsewhere.

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