Parametric Simultons in Nonlinear Lattices

Bambi Hu$^{1,2}$ and Guoxiang Huang$^{1,3}$

$^1$Centre for Nonlinear Studies and Department of Physics, Hong Kong Baptist University, Hong Kong, China
$^2$Department of Physics, University of Houston, Houston TX 77204, USA
$^3$Department of Physics and Laboratory for Quantum Optics, East China Normal University, Shanghai 200062, China

Abstract

Parametric simultaneous solitary wave (simulton) excitations are shown 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 cutoff mode of acoustic branch (as a fundamental wave) and the upper cutoff 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 explicitly given 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 $\pi/a$ (where $a$ is the lattice constant) and zero, respectively.

PACS numbers: 63.20. Pw, 63.20. Ry
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 analog of the lattice envelope (or breather) solitons with their spatial extension only a few lattice spacing and the vibrating frequency above the upper cutoff 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 linear case, a diatomic lattice allows two phonon bands. There is a upper cutoff 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 can not 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 is promising for long-distance information transmission in fiber, 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-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.

On the contrary, 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 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 1D 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 multiatomic 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, the SHG may in principle occur in any multi-atomic
lattice, but for definiteness and for the sake of simplicity we consider here a 1D diatomic
lattice with a cubic interaction potential. The Hamiltonian of the system is given by

\[
H = \sum_n \left[ \frac{1}{2} m \left( \frac{dv_n}{dt} \right)^2 + \frac{1}{2} M \left( \frac{dw_n}{dt} \right)^2 + \frac{1}{2} K_2 (w_n - v_n)^2 + \frac{1}{2} K'_2 (v_{n+1} - w_n)^2 \\
+ \frac{1}{3} K_3 (w_n - v_n)^3 + \frac{1}{3} K'_3 (v_{n+1} - w_n)^3 + \frac{1}{3} V_3 v_n^3 + \frac{1}{3} V'_3 w_n^3 \right],
\] (1)
where \( v_n = v_n(t) \) (where \( w_n = w_n(t) \)) is the displacement from its equilibrium position of the \( n \)th particle with mass \( m \) (\( M \)). \( n \) is the index of the \( n \)th 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-neighbor force constants \( K_j(j = 2, 3) \) in the same cells are different from the nearest-neighbor 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 \( m < M \), \( K_j < K'_j(j = 2, 3) \), and \( V'_3 < V_3 \). The equations of motion for describing the lattice read

\[
\frac{d^2}{dt^2} v_n = I_2(w_n - v_n) + I'_2(w_{n-1} - v_n) + I_3(w_n - v_n)^2 - I'_3(w_{n-1} - v_n)^2 - \alpha_m v_n^2, \tag{2}
\]

\[
\frac{d^2}{dt^2} w_n = J_2(v_n - w_n) + J'_2(v_{n+1} - w_n) - J_3(v_n - w_n)^2 + J'_3(v_{n+1} - w_n)^2 - \alpha_M w_n^2, \tag{3}
\]

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

\[
\omega_{\pm}(q) = \frac{1}{\sqrt{2}} \left\{ (I_2 + I'_2 + J_2 + J'_2) \pm \left[ (I_2 + I'_2 + J_2 + J'_2)^2 - 16I_2J'_2 \sin^2(qa/2) \right]^{1/2} \right\} \frac{1}{2}, \tag{4}
\]

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 wave number \( q = 0 \), the phonon spectrum has a lower cutoff \( \omega_-(0) = 0 \) for the acoustic mode and an upper cutoff \( \omega_+(0) = (I_2 + I'_2 + J_2 + J'_2)^{1/2} \) for the optical mode. At \( q = \pi/a \) there exists a frequency gap between the upper cutoff of the acoustic branch \( \omega_-(\pi/a) \) and the lower cutoff of the optical branch \( \omega_+(\pi/a) \), where \( \omega_+(\pi/a) = (1/\sqrt{2})\{ (I_2 + I'_2 + J_2 + J'_2) \pm \left[ (I_2 + I'_2 + J_2 + J'_2)^2 - 16I_2J'_2 \right]^{1/2} \}^{1/2} \).

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. Eqs. (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 \( K'_2 \to K_2 \) the condition (5) and (6) can not 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 chose \( \omega_1 \in \omega_-(q) \) and \( \omega_2 \in \omega_+(q) \), then the conditions (5) and (6) give

\[
\left[ (I_2 + I'_2 + J_2 + J'_2)^2 - 4I_2J'_2 \sin(q_1a) \right]^{1/2} = 3(I_2 + I'_2 + J_2 + J'_2) - 4 \left[ (I_2 + I'_2 + J_2 + J'_2)^2 - 16I_2J'_2 \sin^2(q_1a/2) \right]^{1/2}. \tag{7}
\]
It is available to solve \( q_1 \) from the above equation. For simplicity we consider cutoff modes of the system. We take \( q_1 = \pi/a, q_2 = 0 \) and \( Q = -2\pi/a \), then the condition (5) is automatically satisfied. The condition (6) (the same as (7)) now reads

\[
I_2 + I'_2 + J_2 + J'_2 = \frac{8}{\sqrt{3}} \sqrt{I_2 J_2}.
\] (8)

Eq.(8) also means that \( \omega_1 = \omega_-(\pi/a) = (1/2)(I_2 + I'_2 + J_2 + J'_2)^{1/2} = (4I_2 J_2'/3)^{1/4} \) and \( \omega_2 = \omega_+(0) = (I_2 + I'_2 + J_2 + J'_2)^{1/2} = 2(4I_2 J_2'/3)^{1/4} \) If the all 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.

\[ \text{B. Asymptotic expansion} \]

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 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

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

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

\[
\xi_n = \epsilon^{1/2} (na - \lambda t),
\]

\[
\tau = \epsilon t,
\]

\[
\phi_n = qna - \omega(q)t,
\] (12)

where \( \lambda \) 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 \( \epsilon \), we obtain

\[
\frac{\partial^2}{\partial t^2} v_{n,n}^{(j)} - I_2(w_{n,n}^{(j)} - v_{n,n}^{(j)}) - I'_2(w_{n,n-1}^{(j)} - v_{n,n}^{(j)}) = M_{n,n}^{(j)},
\] (13)

\[
M_{n,n}^{(0)} = 0,
\] (14)

\[
M_{n,n}^{(1)} = 2\lambda \frac{\partial^2}{\partial t \partial \xi_n} v_{n,n}^{(0)} - I'_2 a \frac{\partial}{\partial \xi_n} w_{n,n-1}^{(0)},
\] (15)

\[
M_{n,n}^{(2)} = 2\lambda \frac{\partial^2}{\partial t \partial \xi_n} v_{n,n}^{(1)} - \left( \frac{2}{\partial t \partial \tau} + \lambda^2 \frac{\partial^2}{\partial \xi_n^2} \right) v_{n,n}^{(0)} + I_2 \left( -a \frac{\partial}{\partial \xi_n} w_{n,n-1}^{(1)} + \frac{a^2}{2} \frac{\partial^2}{\partial \xi_n^2} w_{n,n-1}^{(0)} \right)
+ I_3(w_{n,n}^{(0)} - v_{n,n}^{(0)})^2 - I'_3(w_{n,n-1}^{(0)} - v_{n,n}^{(0)})^2 - \alpha_m(v_{n,n}^{(0)})^2,
\] (16)
and
\[
\frac{\partial^2}{\partial t^2} w_{n,n}^{(j)} - J_2(v_{n,n}^{(j)} - w_{n,n}^{(j)}) - J_2'(v_{n,n+1}^{(j)} - w_{n,n}^{(j)}) = N_{n,n}^{(j)},
\]
(17)
\[N_{n,n}^{(0)} = 0,\]  
(18)
\[N_{n,n}^{(1)} = 2\lambda \frac{\partial^2}{\partial t \partial \xi_n} w_{n,n}^{(0)} + J_2'' a \frac{\partial}{\partial \xi_n} v_{n,n+1}^{(0)},\]  
(19)
\[N_{n,n}^{(2)} = 2\lambda \frac{\partial^2}{\partial t \partial \xi_n} w_{n,n}^{(1)} - \left( 2 \frac{\partial^2}{\partial t \partial \tau} + \lambda^2 \frac{\partial^2}{\partial \xi_n^2} \right) w_{n,n}^{(0)} + J_2'' \left( \alpha_0 \frac{\partial}{\partial \xi_n} v_{n,n+1}^{(1)} + \frac{a^2}{2!} \frac{\partial^2}{\partial \xi_n^2} v_{n,n+1}^{(0)} \right) \]
\[ - J_3(v_{n,n}^{(0)} - w_{n,n}^{(0)})^2 + J_3'(v_{n,n+1}^{(0)} - w_{n,n}^{(0)})^2 - \alpha M(w_{n,n}^{(0)})^2,\]  
(20)
with \( j = 0, 1, 2, \cdots \). Eqs.(13) and (17) can be rewritten in the following form
\[
\hat{L} w_{n,n}^{(j)} = J_2 M_{n,n}^{(j)} + J_2' M_{n,n+1}^{(j)} + \left( \frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) N_{n,n}^{(j)},
\]
(21)
\[\left( \frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) v_{n,n}^{(j)} = I_2 w_{n,n}^{(j)} + I_2' w_{n,n-1}^{(j)} + M_{n,n}^{(j)},
\]
(22)
where the operator \( \hat{L} \) is defined by
\[
\hat{L} w_{n,n}^{(j)} = \left( \frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) \left( \frac{\partial^2}{\partial t^2} + J_2 + J_2' \right) w_{n,n}^{(j)} - (I_2 J_2 + I_2' J_2') u_{n,n}^{(j)}
\]
\[-I_2 J_2' \left( u_{n,n+1}^{(j)} + u_{n,n-1}^{(j)} \right),
\]
(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
\[
w_{n,n}^{(0)} = A_1(\tau, \xi_n) \exp(i\phi_n^-) + A_2(\tau, \xi_n) \exp(i\phi_n^+) + \text{c.c.},
\]
(24)
\[
v_{n,n}^{(0)} = \frac{I_2 + I_2' e^{-iqa}}{-\omega_+^2 + I_2 + I_2'} A_1(\tau, \xi_n) \exp(i\phi_n^-) + \frac{I_2 + I_2' e^{-iqa}}{-\omega_+^2 + I_2 + I_2'} A_2(\tau, \xi_n) \exp(i\phi_n^+) + \text{c.c.}
\]
(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 yet to be determined two envelope (or amplitude) functions of the acoustic and the optical excitations, respectively. They are the functions of the slow variables \( \xi_n \) and \( \tau \). c.c. denotes the corresponding complex conjugate. For simplicity we specify two modes, i.e. the acoustic
upper cutoff mode \((q_1 = \pi/a, \omega_1 = \omega_-(\pi/a) = (4I_2J_2^3/3)^{1/4})\) and the optical upper cutoff mode \((q_2 = 0, \omega_2 = \omega_+(0) = 2\omega_1 = 2(4I_2J_2^3/3)^{1/4})\). Thus we have

\[
w^{(0)}_{n,n} = A_1(\tau, \xi_n)(-1)^n \exp(-i\omega_1 t) + A_2(\tau, \xi_n) \exp(-i\omega_2 t) + c.c.,
\]

\[
v^{(0)}_{n,n} = \frac{I_2 - I'_2}{-\omega^2 + I_2 + I'_2} A_1(\tau, \xi_n)(-1)^n \exp(-i\omega_1 t)
\]

\[
+ \frac{I_2 + I'_2}{-\omega^2 + I_2 + I'_2} A_2(\tau, \xi_n) \exp(-i\omega_2 t) + c.c.,
\]

From the discussion in subsection II.A, the modes chose in such way satisfy the phase-matching conditions (5) and (6) for the SHG. Thus in Eqs.(27) and (28) \(A_1(\tau, \xi_n)\) 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

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

\[
v^{(1)}_{n,n} = B_0 + \left\{ \frac{(I_2 - I'_2)B_1 + I'_2a\partial A_1/\partial \xi_n(-1)^n \exp(-i\omega_1 t)}{-\omega^2 + I_2 + I'_2}
\]

\[
+ \frac{(I_2 + I'_2)B_2 - I'_2a\partial A_2/\partial \xi_n}{-\omega^2 + I_2 + I'_2} \exp(-i\omega_2 t) + c.c. \right\},
\]

where \(B_j (j=0, 1, 2)\) are undetermined functions of \(\xi_n\) and \(\tau\).

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

\[
\hat{L}w^{(2)}_{n,n} = J_2 M^{(2)}_{n,n} + J'_2 M^{(2)}_{n,n+1} + \left( \frac{\partial^2}{\partial \tau^2} + I_2 + I'_2 \right) N^{(2)}_{n,n}.
\]

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 sovability condition of Eq.(30)

\[
i \frac{\partial A_1}{\partial \tau} + \frac{1}{2} \Gamma_1 \frac{\partial^2 A_1}{\partial \xi_n^2} + \Delta_1 A_1^2 A_2 = 0,
\]

\[
i \frac{\partial A_1}{\partial \tau} + \frac{1}{2} \Gamma_2 \frac{\partial^2 A_2}{\partial \xi_n^2} + \Delta_2 A_1^2 = 0,
\]

where the coefficients are expressed as

\[
\Gamma_1 = -\frac{I'_2J_2^2a^2}{\omega_1[\lambda_1^{-1} + \lambda_1(I_2 - I'_2)(J_2 - J'_2)]},
\]

\[
\Gamma_2 = -\frac{I'_2J_2^2a^2}{\omega_2[-\lambda_2^{-1} - \lambda_2(J_2 + I'_2)(J_2 + J'_2)]},
\]

\[
\Delta_1 = \frac{[1 - \lambda_2(I_2 + I'_2)]\lambda_3 - \lambda_1^{-1}\alpha_M - \lambda_1\lambda_2(I_2 - (I'_2)^2)(J_2 - J'_2)\alpha_m}{\omega_1[\lambda_1^{-1} + \lambda_1(I_2 - I'_2)(J_2 - J'_2)]},
\]

\[
\Delta_2 = \frac{\lambda_4 - \lambda_2^{-1}\alpha_M - \lambda_3^{-1}(I_2 - I'_2)^2(J_2 + J'_2)\alpha_m}{2\omega_2[\lambda_2^{-1} + \lambda_2(I_2 + I'_2)(J_2 + J'_2)]},
\]

7
with
\[ \lambda_j = \frac{1}{-\omega_j^2 + I_2 + I'_2}, \quad (j = 1, 2) \] (37)

\[ \lambda_3 = (I_3 - I'_3)(J_2 - J'_2) - \lambda_1^{-1}(J_3 - J'_3) + (I_2 - I'_2)[(J_3 + J'_3) - \lambda_1(I_3 + I'_3)(J_2 - J'_2)], \] (38)

\[ \lambda_4 = [1 - \lambda_1(I_2 - I'_2)]^2[-J_3\lambda_2^{-1} + I_3(J_2 + J'_2)] + [1 + \lambda_1(I_2 - I'_2)]^2[I'_3\lambda_2^{-1} - I'_3(J_2 + J'_2)]. \] (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

\[ i \frac{\partial u_1}{\partial t} + \frac{1}{2} \Gamma_1 \frac{\partial^2 u_1}{\partial x_n^2} + \Delta_1 u_1^* u_2 = 0, \] (40)

\[ i \frac{\partial u_2}{\partial t} + \frac{1}{2} \Gamma_2 \frac{\partial^2 u_2}{\partial x_n^2} + \Delta_2 u_1^2 = 0. \] (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, \( \delta \omega \), the conditions (5) and (6) become

\[ \omega_2 = 2 \omega_1 + \delta \omega, \quad q_2 = 2q_1 + Q. \] (42)

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

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

\[ i \left( \frac{\partial u_2}{\partial t} + v_2 \frac{\partial u_2}{\partial x_n} \right) + \frac{1}{2} \Gamma_2 \frac{\partial^2 u_2}{\partial x_n^2} + \Delta_2 u_1^2 \exp(i\delta \omega t) = 0, \] (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.

Eqs. (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, \( \Gamma_1 \) and \( \Gamma_2 \), 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, \( \Delta_1 \) and \( \Delta_2 \),
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

$$u_1(x_n, t) = U_1(\zeta) \exp[i(k_1 x_n - \Omega_1 t)],$$  \hspace{1cm} (45)
$$u_2(x_n, t) = U_2(\zeta) \exp[i(k_2 x_n - \Omega_2 t)],$$  \hspace{1cm} (46)

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

$$\frac{d^2 U_1}{d\zeta^2} + \alpha_1 U_1 U_2 - \beta_1 U_1 = 0,$$  \hspace{1cm} (47)
$$\frac{d^2 U_2}{d\zeta^2} + \alpha_2 U_2^2 - \beta_2 U_2 = 0,$$  \hspace{1cm} (48)

where $\alpha_1 = 2\Delta_1/(\Gamma_1 k^2), \alpha_2 = 2\Delta_2/(\Gamma_2 k^2), \beta_1 = -2(\Omega_1 - \delta\omega)/(\Gamma_1 k^2), \beta_2 = -2(\Omega_2 - \delta\omega)/(\Gamma_2 k^2), \Omega = \sqrt{v_1 k + 2k_1 k_2},$ 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

$$U_1 = \frac{6}{\sqrt{\alpha_1 \alpha_2}} \left(\frac{2}{3} - \text{sech}^2\zeta\right),$$  \hspace{1cm} (49)
$$U_2 = -\frac{6}{\alpha_1} \left(\frac{2}{3} - \text{sech}^2\zeta\right),$$  \hspace{1cm} (50)

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

$$k = \frac{2(v_2 - v_1)k_1 + (\Gamma_1 - 2\Gamma_2)k_1^2 + \delta\omega}{2(\Gamma_2 - 2\Gamma_1)}.$$  \hspace{1cm} (51)

The lattice configuration in this case takes the form

$$w_n(t) = (-1)^n \frac{12}{\sqrt{\alpha_1 \alpha_2}} \left[\frac{2}{3} - \text{sech}^2(kna - \Omega t)\right] \cos[k_1 na - (\omega_1 + \Omega_1)t]$$
$$-\frac{12}{\alpha_1} \left[\frac{2}{3} - \text{sech}^2(kna - \Omega t)\right] \cos[k_2 na - (\omega_2 + \Omega_2)t].$$  \hspace{1cm} (52)
$$v_n(t) = (-1)^n \frac{12}{\sqrt{\alpha_1 \alpha_2 - \omega_1^2 + I_2 + I_2'}} \left[\frac{2}{3} - \text{sech}^2(kna - \Omega t)\right] \cos[k_1 na - (\omega_1 + \Omega_1)t]$$
$$-\frac{12}{\alpha_1} \left[\frac{2}{3} - \text{sech}^2(kna - \Omega t)\right] \cos[k_2 na - (\omega_2 + \Omega_2)t].$$  \hspace{1cm} (53)

If $q_1 (q_2)$ is exactly equal to $\pi/a$ (zero) but with $\delta\omega \neq 0,$ one has $v_1 = v_2 = 0.$ In this case
$k_1 = k_2 = 0, \Omega_1 = 2\Gamma_1 k^2, \Omega_2 = 2\Gamma_2 k^2, \Omega = 0$ and $k = \{\delta\omega/[2(\Gamma_2 - 2\Gamma_1)]\}^{1/2}.$ (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

\[
U_1 = -\frac{6}{\sqrt{\alpha_1 \alpha_2}} \text{sech}^2 \zeta, \tag{54}
\]

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

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

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

The lattice configuration is now given by

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

\[
v_n(t) = (-1)^{n+1} \frac{12}{\sqrt{\alpha_1 \alpha_2}} \frac{I_2 - I'_2}{\omega_1^2 + I_2 + I'_2} \text{sech}^2(kna - \Omega t) \cos[k_1na - (\omega_1 + \Omega_1)t]
- \frac{12}{\alpha_1 - \omega_1^2 + I_2 + I'_2} \left[ \frac{4}{3} - \text{sech}^2(kna - \Omega t) \right] \cos[k_2na - (\omega_2 + \Omega_2)t]. \tag{58}
\]

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 \( k_1 = k_2 = 0, \Omega_1 = 2\Gamma_1 k^2, \Omega_2 = -2\Gamma_2 k^2, \Omega = 0 \) 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 \( k \) to be 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 \( \text{sgn}(\alpha_1 \alpha_2) > 0 \), which means \( \text{sgn}(\Delta_1 \Delta_2) > 0 \) 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 \( \text{sgn}(\Delta_1 \Delta_2) > 0 \):

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 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 chose the 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) could be generalized to

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

\[ i \frac{\partial A_2}{\partial \tau} + \frac{1}{2} \Gamma_2 \frac{\partial^2 A_2}{\partial \xi_n^2} + \Delta_2 A_2^* A_1 + (\Lambda_{21}|A_1|^2 + \Lambda_{22}|A_2|^2) A_2 = 0, \]

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 will be presented elsewhere.

ACKNOWLEDGMENTS

This work is supported in part by grants from the Hong Kong Research Grants Council (RGC), the Hong Kong Baptist University Faculty Research Grant (FRG), the Natural Science Foundation of China, and the Development Foundation for Science and Technology of ECNU.
REFERENCES

1 E. Fermi, J. Pasta, and S. Ulam, Los Alamos Nat. Lab. Report LA1940, 1955. Also in Collected Papers of Enrico Fermi (Univ. Chicago Press, Chicago, 1962), vol. 2, p. 978.
2 A. R. Bishop and T. Schneider, eds., Solitons in Condensed Matter Physics (Springer, Berlin, 1978).
3 R. Camasa, J. M. Hyman, and B. P. Luce, eds., Physica D 123, special issue on Nonlinear Waves and Solitons in Physical Systems.
4 A. J. Sievers and S. Takeno, Phys. Rev. Lett. 61, 970(1988).
5 R. S. MacKay and S. Aubry, Nonlinearity 7, 1623(1994).
6 S. Flach and C. R. Wills, Phys. Rep. 295, 181(1998), and references therein.
7 Wei-zhong Chen, Phys. Rev. B 49, 15063(1994).
8 F. M. Russell, Y. Zolotaryuk, and J. C. Eilbeck, Phys. Rev. B 55, 6304(1997).
9 P. Marquié, J. M. Bilbault, and M. Remoissenet, Phys. Rev. E 51, 6127(1995).
10 H. S. Eisenberg, Y. Silberberg, R. Morandotti, A. R. Boyd, and J. S. Aitchison, Phys. Rev. Lett. 81, 3383(1998); R. Morandotti, U. Peschel, J. S. Aitchison, H. S. Eisenberg, and Y. Silberberg, Phys. Rev. Lett. 83, 2726(1999).
11 B. I. Swanson, J. A. Brozik, S. P. Love, G. F. Strouse, A. P. Shreve, A. R. Bishop, W.-Z. Wang, and M. I. Salkola, Phys. Rev. Lett. 82, 3288(1999).
12 U. T. Schwarz, L. Q. English, and A. J. Sievers, Phys. Rev. Lett. 83, 223(1999).
13 P. Binder, D. Abraimov, A. V. Ustinov, S. Flach, and Y. Zolotaryuk, Phys. Rev. Lett., (1999) submitted.
14 Zhu-Pei Shi, Guoxiang Huang, and Ruibao Tao, Int. J. Mod. Phys. B 5, 2237(1991).
15 Yu. S. Kivshar and N. Flytzanis, Phys. Rev. A 46, 7972(1992).
16 S. A. Kiselev, S. R. Bickham, and A. J. Sievers, Phys. Rev. B 48, 13508(1993); Phys. Rev. B 50, 9153(1994).
17 Guoxiang Huang, Phys. Rev. B 51, 12347(1995).
18 M. Aoki and S. Takeno, J. Phys. Soc. Jpn. 64, 809(1995).
19 D. Bonart, A. P. Mayer, and U. Schröder, Phys. Rev. Lett. 75, 870(1995); Phys. Rev. B 51, 13739(1995); D. Bonart, T. Rössler, and J. B. Page, Phys. Rev. B 55, 8829(1997).
20 J. N. Teixeira and A. A. Maradudin, Phys. Lett. A 205, 349(1995).
21 A. Franchini, V. Bortolani, and R. F. Wallis, Phys. Rev. B 53, 5420(1996).
22 V. V. Konotop, Phys. Rev. E 53, 2843(1996).
23 S. A. Kiselev and A. J. Sievers, Phys. Rev. B 55, 5755(1997).
24 Guoxiang Huang and Bambi Hu, Phys. Rev. B 57, 5746(1998).
25 S. Jiménez and V. V. Konotop, Phys. Rev. B 60, 6465(1999).
26 Sen-yue Lou and Guoxiang Huang, Mod. Phys. Lett. 9, 1231(1995).
27 Sen-yue Lou, Jun Yu, Ji Lin, and Guoxiang Huang, Chin. Phys. Lett. 12, 400(1995).
28 Ji Lin, Yong Li, Guoxiang Huang, and Sen-yue Lou, Chin. Sci. Bull. 4, 120(1997).
29 A. Hasegawa, Optical Solitons in Fibers (2nd ed.)(Springer-Verlag, Berlin, 1989); A. Hasegawa and Y. Kodama, Solitons in Optical Communications (Clarendon, Oxford, 1995).
30 A. C. Newell and J. V. Moloney, Nonlinear Optics (Redwood City, California, 1992).
31 H. A. Haus and W. S. Wong, Rev. Mod. Phys. 68, 423(1996).
32 M. N. Islam, Physics Today, May 1994, p.34; M. Segev and G. I. Stegeman, Physics Today, August 1998, p.42.
33 G. I. Stegeman, D. J. Hagan, and L. Torner, Opt. Quantum Electron. 28, 1691(1996).
34 G. I. Stegeman, M. Sheik-Bhae, E. van Stryland, and G. Assanto, Opt. Lett. 18, 13(1993).
35 Y. N. Karamzin and A. P. Suhkorukov, Pis’man Zh. Eksp. Teor. Fiz. 20, 734(1974) [JETP Lett. 20, 339(1974)].
36 M. J. Werner and P. D. Drummond, J. Opt. Soc. Am. B 10, 2390(1993).
37 H. He and P. D. Drummond, Phys. Rev. Lett. 78, 4311(1997).
38 H. He and P. D. Drummond, Phys. Rev. E 58, 5025(1998).
39 H. He, A. Arraf, C. M. de Sterke, P. D. Drummond, and B. A. Malomed, Phys. Rev. E 59, 6064(1999).
40 C. Kittel, Introduction to Solid State Physics, 5th ed. (John Wiley & Sons, Inc., New York, 1976), Chap. 5, p. 140.
41 V. V. Konotop, Phys. Rev. E 54, 4266(1996).
42 C. R. Menyuk, R. Schiek, and L. Torner, J. Opt. Soc. Am. B 11, 2434(1994).