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THREE-WAVE PARAMETRIC SIMULTONS IN NONLINEAR LATTICES*

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A new type of nonlinear excitations, i.e. three simultaneous lattice solitons (simultons), in a nonlinear diatomic lattice is predicted. We show that three-wave resonance condition can be fulfilled in the diatomic lattice. Using a quasi-discrete multi-scale method we derive nonlinear amplitude equations for the three-wave resonance with the dispersion of the system taken into account. We provide several types of exact lattice simultons solutions and show that the lattice simultons can be non propagating and their oscillating frequencies may be within the gap of phonon spectrum bands.

1. Introduction

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.[1] These modes can be taken as a discrete analog of lattice solitons with their spatial extension only a few lattice spacing and the vibrating frequencies above the upper cutoff of phonon spectrum bands. Much recent attention has been paid to the nonlinear excitations in diatomic lattices. New types of nonlinear localized modes, in particular the gap solitons, have been studied in detail both in theory[2,3] and in experiment.[4]

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On the other hand, recent years have shown considerable progress for solitons in nonlinear optical media. Recently, the study of optical parametric processes, particularly the second harmonic generation (SHG), has generated a great deal of new interest. It was suggested that a cascaded second-order parametric process may support simultaneous solitons (called *simultons* or quadratic solitons) under general phase-matching conditions.[5] The concept of the simultons has been generalized to the nonlinear optical media with periodically varying refractive index.[6] 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 *band-gap simulton* has been given by Drummond *et al.*[6] Different from the self-trapping mechanism of Kerr solitons, the formation of optical simultons is due to the energy transfer and mutual self-trapping between fundamental and second harmonic waves.

However, for a long time little attention has been paid to the parametric processes in nonlinear lattices. In recent years effort has been made along this direction.[7,8] The two-wave parametric simultons related to a SHG in nonlinear lattices have also been considered by several authors.[7,8] In this paper we show that a three-wave resonance (TWR) can appear in a one-dimensional (1D) nonlinear diatomic lattice. New types of nonlinear localized excitations, i.e. three-wave lattice simulton, are possible when the dispersion of the system is taken into account.

We consider a 1D diatomic lattice with an inter- and an on-site atomic potentials. The equations of motion for describing the system are given by

$$\begin{aligned}\frac{d^2v_n}{dt^2} &= -\omega_0^2 v_n + I_2(w_n - v_n) + I_2'(w_{n-1} - v_n)\\ &\quad + I_3(w_n - v_n)^2 - I_3'(w_{n-1} - v_n)^2 - \alpha_m v_n^2, \end{aligned} \tag{1}$$

$$\begin{aligned}\frac{d^2w_n}{dt^2} &= -\omega_0^2 w_n + J_2(v_n - w_n) + J_2'(v_{n+1} - w_n)\\ &\quad - J_3(v_n - w_n)^2 + J_3'(v_{n+1} - w_n)^2 - \alpha_M w_n^2\,, \end{aligned} \tag{2}$$

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 $\alpha_M = V_3'/M\,(j = 2, 3)$. $v_n\,(w_n)$ is the displacement from 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. ω_0 is the natural frequency for the linear oscillators without any coupling. For simplicity we assume that for the inter-site potential 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 different particles. Without loss of generality we assume $m < M$, $K_j' \le K_j(j = 2,3)$, and $V_3' \le V_3$.

The linear dispersion relation of the system is given by

$$\omega_\pm(q) = [\omega_0^2 + (1/2)(I_2 + I_2' + J_2 + J_2' \pm D(q)^{1/2})]^{1/2}$$

with

$$D(q) = (I_2 + I_2' + J_2 + J_2')^2 - 16 I_2 J_2' \sin^2(qa/2)\,,$$

where the minus (plus) sign corresponds to the lower (upper) branch of the eigenfrequency spectrum. Because of the periodic property of $\omega_\pm(q)$, the phase-matching condition for a TWR reads $q_3 = q_1 + q_2 + Q$ and $\omega_3 = \omega_1 + \omega_2$, where $q_1\,(\omega_1)$ and $q_2\,(\omega_2)$ are the wave vectors (frequencies) of two fundamental waves. $q_3\,(\omega_3)$ is the wave vector (frequency) of the sum-frequency harmonic wave. $Q = 2j\pi/a\,(j$ is an integer) is the reciprocal lattice vectors.

It is possible to choose suitable wavevectors and corresponding frequencies to fulfil the phase-matching condition. One of examples is that one selects $Q = 0$, $q_1 = 0$ and $\omega_1 = \omega_-(0) = \omega_0$, $q_2 = \pi/a$ and $\omega_2 = \omega_-(\pi/a)$, and $q_3 = \pi/a$ and $\omega_3 = \omega_+(\pi/a)$ if the parameters of the system satisfy the constraint $4(I_2^2 + J_2^2 - I_2 J_2)^{1/2} - 2(I_2 + J_2) - 3\omega_0^2 = 0$.

We are interested in possible three-wave simultons in the system. For such excitations one requires an additional condition, i.e. the group-velocity matching condition $v_g(q_1) = v_g(q_2) = v_g(q_3)$, where $v_g(q_j)$ is the group velocity of the mode q_j. Obviously, for the band-edge modes (i.e. $q_j = 0$, or $q_j = \pi/a$, $j = 1, 2$) chosen above, all group velocities are vanishing and hence such condition is satisfied automatically.

To derive the nonlinear amplitude equations for the TWR in the system, we employ the quasi-discreteness approach (QDA) developed in Ref. 2. We make the asymptotic expansion $u_n(t) = \epsilon(u_{n,n}^{(0)} + \epsilon^{1/2} u_{n,n}^{(1)} + \epsilon u_{n,n}^{(2)} + \cdots)$, 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 $\xi_n = \epsilon^{1/2}(na - \lambda t)$, $\tau = \epsilon t$, and $\phi_n = qna - \omega(q)t$ with λ a parameter yet to be determined by a solvability condition. With these notations Eqs.(1) and (2) are transfered into the linear but inhomogeneous equations on $v_{n,n}^{(j)}$ and $w_{n,n}^{(j)}$, $(j = 0, 1, 2, \ldots)$. At the leading order $(j = 0)$ the solution including above mentioned three cutoff modes reads

$$\begin{aligned} w_{n,n}^{(0)} &= A_1(\tau, \xi_n) \exp(-i\omega_1 t) + A_2(\tau, \xi_n)(-1)^n \exp(-i\omega_2 t) \\ &\quad + A_3(\tau, \xi_n)(-1)^n \exp(-i\omega_3 t) + c.c., \end{aligned} \tag{3}$$

$$\begin{aligned} v_{n,n}^{(0)} &= A_1(\tau, \xi_n) \exp(-i\omega_1 t) + \lambda_2(I_2 - I_2') A_2(\tau, \xi_n)(-1)^n \exp(-i\omega_2 t) \\ &\quad + \lambda_3(I_2 - I_2') A_3(\tau, \xi_n)(-1)^n \exp(-i\omega_3 t) + c.c.\,, \end{aligned} \tag{4}$$

where $\lambda_j = 1/(-\omega_j^2 + \omega_0^2 + I_2 + I_2')(j = 2, 3)$, A_1, and A_2 and A_3 are undetermined amplitude functions representing the two fundamental waves, (q_1, ω_1) and (q_2, ω_2), and the harmonic wave, (q_3, ω_3), respectively.

The solvability condition in the next order $(j = 1)$ requires $\lambda = 0$ and hence $\xi_n = \epsilon^{1/2} na$. In the order $j = 2$, solvabilty conditions give rise to:

$$i\left(\frac{\partial u_1}{\partial t} + v_1 \frac{\partial u_1}{\partial x_n}\right) + \frac{1}{2}\Gamma_1 \frac{\partial^2 u_1}{\partial x_n^2} + \Delta_1\, u_2^* u_3 \exp(i\Delta\omega t) = 0\,, \tag{5}$$

$$i\left(\frac{\partial u_2}{\partial t}+v_2\frac{\partial u_2}{\partial x_n}\right)+\frac{1}{2}\Gamma_2\frac{\partial^2 u_2}{\partial x_n^2}+\Delta_2\, u_3u_1^*\exp(i\Delta\omega t)=0\,, \tag{6}$$

$$i\left(\frac{\partial u_3}{\partial t}+v_2\frac{\partial u_3}{\partial x_n}\right)+\frac{1}{2}\Gamma_2\frac{\partial^2 u_3}{\partial x_n^2}+\Delta_2\, u_1u_2\exp(-i\Delta\omega t)=0\,, \tag{7}$$

where $u_j=\epsilon A_j (j=1,2,3)$, $x_n=na$. v_1, v_2 and v_3 are the group velocities of two fundamental waves near at $q_1=0$ and $q_2=\pi/a$, and the harmonic wave near at $q_3=\pi/a$, respectively. We have included a small frequency mismatch $\Delta\omega$, i.e. we allow $\omega_3=\omega_1+\omega_2+\Delta\omega$. The expressions of the coefficients in Eqs. (5)–(7) are cumbersome and omitted here. Equations (5)–(7) are the three-wave interaction equations including the *dispersion* (represented by the second-order derivative terms) of the system.

We now provide some exact soliton solutions of Eqs. (5)–(7). Assuming $u_j=U_j(\zeta)\exp(i\phi_j)$ with $\zeta=kx_n-\Omega t$ and $\phi_j=k_jx_n-\Omega_j t$, Eqs. (5)–(7) are transfered into a set of ordinary differential equations on U_j. Because we are interested in the simultaneous three-wave soliton solutions we make the ansatz

$$U_j=A_j+B_j\ \mathrm{sech}\,\zeta\tanh\zeta+C_j\ \mathrm{sech}^2\ \zeta\,,$$

where A_j, B_j and C_j are constants. Substituting this ansatz into the equations of U_j we obtain a set of nonlinearly coupled algebraic equations for A_j, B_j and C_j. We assume $B_j=ib_j$ with A_j, b_j and C_j real constants left to be determined. Then solving the equations for A_j, b_j and C_j we obtain different types of three-wave simulton solutions.

One of them reads

$$U_1=\frac{6s_1}{\sqrt{\alpha_2\alpha_3}}\mathrm{sech}^2\,\zeta\,, \tag{8}$$

$$U_2=-\frac{6s_2}{\sqrt{\alpha_3\alpha_1}}\mathrm{sech}^2\,\zeta\,, \tag{9}$$

$$U_3=-\frac{6s_1s_2}{\sqrt{\alpha_1\alpha_2}}\mathrm{sech}^2\,\zeta\,, \tag{10}$$

with $s_j=\pm1$, $\alpha_j=2\Delta_j/(\Gamma_j k^2)$. We see that all fundamental and harmonic wave components are *simultaneously* one-hump solitons with the same central position and the same travelling velocity (*bright* simulton). In this case the lattice displacement takes the form

$$\begin{aligned}w_n(t)=&\frac{12s_1}{\sqrt{\alpha_2\alpha_3}}\mathrm{sech}^2(kna-\Omega t)\cos[k_1na-(\omega_1+\Omega_1)t]\\&+\frac{12s_2}{\sqrt{\alpha_3\alpha_1}}\mathrm{sech}^2(kna-\Omega t)\cos[k_2na-(\omega_2+\Omega_2)t]\\&+\frac{12s_1s_2}{\sqrt{\alpha_1\alpha_2}}\mathrm{sgn}(\alpha_3)\,\mathrm{sech}^2(kna-\Omega t)\cos[k_3na-(\omega_3+\Omega_3)t]\,,\end{aligned} \tag{11}$$

$$\begin{aligned} v_n(t) &= \frac{12s_1}{\sqrt{\alpha_2\alpha_3}}\mathrm{sech}^2(kna-\Omega t)\cos[k_1na-(\omega_1+\Omega_1)t] \\ &\quad + \frac{I_2-I_2'}{-\omega_2^2+I_2+I_2'}\frac{12s_2}{\sqrt{\alpha_3\alpha_1}}\mathrm{sech}^2(kna-\Omega t)\cos[k_2na-(\omega_2+\Omega_2)t] \\ &\quad + \frac{I_2-I_2'}{-\omega_3^2+I_2+I_2'}\frac{12s_1s_2}{\sqrt{\alpha_1\alpha_2}}\mathrm{sgn}(\alpha_3)\,\mathrm{sech}^2(kna-\Omega t)\cos[k_3na-(\omega_3+\Omega_3)t]\,, \end{aligned} \tag{12}$$

with

$$\Omega_j = v_jk_j + \Gamma_jk_j^2/2 - 2\Gamma_jk^2\,,$$

$$k^2 = \frac{v_3k_3 - v_1k_1 - v_2k_2 + (1/2)\Gamma_3k_3^2 - (1/2)\Gamma_1k_1^2 - (1/2)\Gamma_2k_2^2 - \Delta\omega}{2(\Gamma_3-\Gamma_2-\Gamma_1)}\,.$$

When $v_j = 0$, we have $\Omega = 0$ and $\Omega_j = -2\Gamma_jk^2$ ($j = 1, 2, 3$). Since $\Gamma_1 > 0$, $\Gamma_2 < 0$ and $\Gamma_3 > 0$, we obtain $\omega_1 + \Omega_1 < \omega_1$, $\omega_2 + \Omega_2 > \omega_2$, and $\omega_3 + \Omega_3 < \omega_3$. Therefore, the vibrating frequencies of all three wave components locate within the bottom or mid gap of the phonon spectrum bands.

One can also obtain the following *dark* simulton solution

$$U_1 = -\frac{6s_1}{\sqrt{\alpha_2\alpha_3}}\left(\frac{2}{3}-\mathrm{sech}^2\zeta\right), \tag{13}$$

$$U_2 = -\frac{6s_2}{\sqrt{\alpha_3\alpha_1}}\left(\frac{2}{3}-\mathrm{sech}^2\zeta\right), \tag{14}$$

$$U_3 = -\frac{6s_1s_2}{\sqrt{\alpha_1\alpha_2}}\mathrm{sgn}(\alpha_3)\left(\frac{2}{3}-\mathrm{sech}^2\zeta\right) \tag{15}$$

with

$$\begin{aligned} \Omega_j &= v_jk_j + \frac{1}{2}\Gamma_jk_j^2 + 2\Gamma_jk^2\,, \\ k^2 &= [v_1k_1 + v_2k_2 - v_3k_3 + (1/2)\Gamma_1k_3^2 + (1/2)\Gamma_2k_2^2 \\ &\quad - (1/2)\Gamma_3k_3^2 + \Delta\omega]/[2(\Gamma_3-\Gamma_2-\Gamma_1)]\,. \end{aligned}$$

When $v_j = 0 (j = 1, 2, 3)$, the excitation is a standing wave and the vibrating frequency of each component is in the phonon spectrum bands.

Another type of simulton solution reads

$$U_1 = i\frac{6s_1}{\sqrt{-\alpha_2\alpha_3}}\mathrm{sech}^2\zeta\tanh\zeta\,, \tag{16}$$

$$U_2 = i\frac{6s_2}{\sqrt{-\alpha_3\alpha_1}}\mathrm{sech}\,\zeta\tanh\zeta, \tag{17}$$

$$U_3 = \frac{6s_1s_2}{\sqrt{\alpha_1\alpha_2}}\mathrm{sgn}(\alpha_3)\,\mathrm{sech}^2\zeta\,, \tag{18}$$

with

$$\Omega_j = v_j k_j + \frac{1}{2}\Gamma_j(k_j^2 - k^2)$$

$$k^2 = [v_1 k_1 + v_2 k_2 - v_3 k_3 + (1/2)\Gamma_1 k_1^2 + (1/2)\Gamma_2 k_2^2 - (1/2)\Gamma_3 k_3^2 + \Delta\omega]/[\Gamma_3 + (1/2)(\Gamma_1 + \Gamma_2)]\,.$$

It denotes a bright three-wave simulton with both the fundamental waves U_1 and U_2 two maxima but the harmonic wave one maximum.

2. Discussion and Summary

We have investigated the three-wave lattice simultons in a 1D nonlinear diatomic lattice. We have shown that, due to the multi-branch and periodic properties of the phonon spectrum, the phase- and group velocity-matching conditions can be fulfilled by suitably choosing the wavevectors and frequencies of the fundamental waves and a sum-frequency wave. Using a quasi-discrete method of multiple-scales, the nonlinear amplitude equations for a TWR have been derived with the dispersion of the system taking into account. We have also presented several types of three-wave lattice simulton solutions. The results show that these parametric lattice simultons may be nonpropagating excitations with their vibrating frequencies within the bottom and mid band gaps of the phonon spectrum bands.

The physical mechanism for the formation of the three-wave lattice simultons is due to the cascading effect between several lattice wave components. In this process, two fundamental waves and the sum-frequency wave interact with themselves through repeated wave-wave interactions. For instance the energies of the fundamental waves are first upconverted to the sum-frequency wave and then downconverted, resulting in a mutual self-trapping of each wave and hence the formation of three simultaneous lattice solitons.

Cubic nonlinear potential appears in most of realistic atomic potentials. Thus it is possible to observe the 1D lattice simultons reported here. It must be emphasized that the multi-value property of the linear dispersion relation is important for obtaining the three-wave parametric simulton solutions. Thus a diatomic or multi-atomic lattice is necessary for generating such nonlinear excitations.

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