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Localized modes in a one-dimensional sphalerite-structure lattice with anharmonicity

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Abstract. The nonlinear localized vibrational modes of a one-dimensional atomic chain with two periodically alternating masses and force constants are analytically investigated using a discrete multiple-scale expansion method. This model simulates a row of atoms in the ⟨1 1 1⟩-direction of sphalerite, or zinc blende, crystals. Owing to the structural asymmetry, the vibrational amplitude is governed by a perturbed nonlinear Schrödinger equation instead of the standard one found in one-dimensional lattices with two alternating masses but uniform force constant. Although the stationary localized modes with carrier wavevector at the Brillouin-zone boundary are similar to those of ionic lattices, the moving localized modes with wavevectors within the zone are different owing to the perturbation. The calculation shows that the height of the moving localized modes in this lattice dampens with time.

PACS. 63.20.Pw Localized modes – 63.20.Ry Anharmonic lattice modes

1 Introduction

Nonlinear lattice dynamics has been much studied since the pioneering work of Fermi, Pasta and Ulam [1]. Early work in this area have treated the one-dimensional (1D) anharmonic lattice as a continuum obeying soliton equations of the Boussinesq or Korteweg-deVries (KdV) type [2]. However, towards the end of the 1980's, the interest in anharmonic lattices was renewed owing to the identification of a new type of highly localized vibrational modes with spatial extensions of only a few lattice spacings and frequencies lying above the linear phonon bands [3,4]. Later, by using multiple-scale analysis, it was shown that these localized modes (LMs) are nonlinear Schrödinger envelope solitons (or discrete breathers) in the case of highly discrete and strong anharmonicities [5]. This was also confirmed numerically [6]. The quantum correspondence of these LMs are phonon bound states [7]. Some progress was also reported for higher-dimensional crystal lattices with anharmonicity in the nearest-neighbor interaction [8]. Experimentally, the LMs have been observed in coupled pendulum lattices [9], electrical lattices [10], and also in molecular crystals [11] with neutron scattering techniques. Hence, the LMs induced by the anharmonicity of perfect crystal lattices have raised continued interest for the past decade (see, *e.g.*, recent review articles [12] and references therein).

The lattice Green-function approach has been applied to 1D anharmonic monatomic chains in earlier works [3,4], but this method involves a rotating-wave approximation and can only produce highly LMs. Multiple-scale expansion techniques have been successfully used to study both monatomic [5] and diatomic [13] lattices with quartic anharmonicity, for which the lattice equation of motion reduces to a standard nonlinear Schrödinger equation (NLSE). Particular attention was given to the diatomic (ionic) chain with two periodically alternating masses and a uniform bond force constant [13–16]. This system shows nonlinear gap LMs with smaller atomic vibrational amplitudes and lower frequencies (between the acoustic and optical branches of the linear spectrum) as compared to the LMs of monatomic lattice. Campa *et al.* [17] investigated analytically and numerically the existence and stability of soliton solutions for a molecular chain with both alternating atomic masses and force constants. Although they focused on the cubic anharmonicity of the system, they also derived a standard NLSE for the atomic displacement distribution. Recently, an atomic chain with uniform masses but two periodically alternating force constants between nearest-neighbor atoms was proposed [18] to simulate a row of atoms in the ⟨1 1 1⟩-direction of diamond-structure crystals. Both cubic and quartic anharmonicities were included, and LMs were numerically observed.

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In the present work, we extend the model of reference [18] to a 1D sphalerite-crystal lattice with both alternating masses and bond force constants. We study the LMs in this system by means of a discrete multiple-scale scheme [5,13,17]. The results obtained in this paper differ from the situation of other 1D lattice systems [5,13] in which the atomic vibrational amplitudes are governed by a standard NLSE. They also differ from a similar model in reference [17] which includes only cubic anharmonicity. As there is no center of symmetry on either an atom or on a bond in our lattice model, by considering the expansion up to the third order we find that the atomic amplitude distribution is described by a *perturbed* NLSE, and this gives some new interesting aspects to the solution. The soliton perturbation calculation shows that the height of the moving LMs dampens with time while its initial center position and phase linearly and logarithmically decay, respectively.

The paper is organized as follows. In Section 2, a lattice model simulating a row of atoms in the $\langle 1\ 1\ 1\rangle$-direction of sphalerite-structure crystals, such as the important semiconductor GaAs, is introduced and a discrete multiple-scale expansion is made for the equation of motion. In Section 3 the envelope equation of atomic displacements is reduced to a perturbed NLSE by separately considering the acoustic and optical modes of the system. As special solutions of the perturbed NLSE, the stationary LMs with carrier wavevectors at the Brillouin-zone boundary are given in Section 4. The perturbation on the parameters of the moving LMs with carrier wavevectors within the zone is calculated in Section 5. Section 6 discusses the results and concludes the paper.

2 Model and asymptotic expansion

We begin with a model of an atomic chain with two periodically alternating masses and bond force constants between nearest-neighbor atoms. We consider appropriately small atomic vibrational amplitudes which can produce sufficient nonlinearity but no reconstruction or phase transition in the system. This allows to Taylor expand the atomic interaction potential around the equilibrium and to truncate the series to the fourth-order. The Hamiltonian of the system is then written

$$H=\sum_i\left[\frac{1}{2}m_i\left(\frac{\mathrm{d}u_i}{\mathrm{d}t}\right)^2+\sum_{j=2}^{4}\frac{c_j^i}{j}(u_i-u_{i-1})^j\right], \qquad (1)$$

where $u_i=u_i(t)$ is the displacement of the ith atom from its equilibrium position. The masses are m_i, with $m_i=m$ for i even, and $m_i=M$ for i odd. Similarly, the force constants are $c_j^i=k_j$, $(j=2,3,4)$ for i even, while $c_j^i=k'_j$ for i odd. The constants $k_2\,(k'_2)$, $k_3\,(k'_3)$ and $k_4\,(k'_4)$ are the harmonic, cubic, and quartic terms corresponding to the tight (weak) bonds between nearest-neighbor atoms, respectively.

Since the weak and tight bonds alternate, there are two types of LMs with centers either on weak-bond atom pairs or on tight-bond atom pairs. We consider the former case first, and decouple the light (even) and heavy (odd) atom sublattices by letting $u_{2k}=v_n$ (i even) and $u_{2k+1}=w_n$ (i odd), where n is the index of a unit cell in which two atoms are weakly bound. Thus, the classical equations of motion for the two atoms of the nth unit cell are given by

$$\frac{\mathrm{d}^2v_n}{\mathrm{d}t^2}=\sum_{j=2}^{4}\left[I'_j(w_n-v_n)^{j-1}-I_j(v_n-w_{n-1})^{j-1}\right], \qquad (2)$$

$$\frac{\mathrm{d}^2w_n}{\mathrm{d}t^2}=\sum_{j=2}^{4}\left[J_j(v_{n+1}-w_n)^{j-1}-J'_j(w_n-v_n)^{j-1}\right],$$

where $I_j=k_j/m$, $I'_j=k'_j/m$, $J_j=k_j/M$ and $J'_j=k'_j/M$ $(j=2,3,4)$. When $I_j(I'_j)=J_j(J'_j)=0$ $(j=3,4)$, this system has two branches of linear vibrations with frequencies given by

$$\omega^2=\omega_\pm^2=\frac{1}{2}\Bigg[I_2+I'_2+J_2+J'_2 \pm\sqrt{(I_2+I'_2+J_2+J'_2)^2-16I_2J'_2\sin^2\left(\frac{qa}{2}\right)}\Bigg], \qquad (3)$$

where q is the wavevector and a the lattice spacing, *i.e.* twice the distance between nearest-neighbor atoms. The minus sign corresponds to the lower frequency acoustic mode and the plus sign to the upper frequency optical mode. At the Brillouin-zone boundary, $q=\pm\pi/a$ these two branches are separated by a gap $\Delta\omega=\omega_2-\omega_1$, where

$$\omega_1^2=\frac{1}{2}\Bigg[I_2+I'_2+J_2+J'_2 -\sqrt{(I_2+I'_2+J_2+J'_2)^2-16I_2J'_2}\Bigg],$$

$$\omega_2^2=\frac{1}{2}\Bigg[I_2+I'_2+J_2+J'_2 +\sqrt{(I_2+I'_2+J_2+J'_2)^2-16I_2J'_2}\Bigg], \qquad (4)$$

give the gap-edge frequencies, and with an optical cut-off frequency

$$\omega_3^2=I_2+I'_2+J_2+J'_2 \qquad (5)$$

owing to the discreteness of the system.

In order to include the effects of anharmonicity and discreteness simultaneously, we use the method of multiple-scale approximation [3,5,17] to reduce the equation and to evaluate the modulation of the amplitude in the lowest order of asymptotic expansion. In this treatment we set

$$u_n(t)=\sum_{\mu=1}^{\infty}\epsilon^\mu u^{(\mu)}(\xi_n,\tau;\phi_n)=\sum_{\mu=1}^{\infty}\epsilon^\mu u_{n,n}^{(\mu)}, \qquad (6)$$

where $u_n(t)=v_n(t)$ or $w_n(t)$, ϵ is a small but finite parameter denoting the relative amplitude, ξ_n and τ are "slow"

variables defined by $\xi_n = \epsilon(na - V_g t)$ and $\tau = \epsilon^2 t$. These are also called multiple-scaled variables. V_g is the group velocity to be determined later by a solvability condition. The "fast" variable, $\phi_n = qna - \omega t$, representing the phase of the carrier wave, is taken to be completely discrete. With this expansion, the displacements of the two atoms near the nth cell can be expressed by

$$\begin{aligned} u_{n\pm1}(t) &= \sum_{\mu=1}^{\infty} \epsilon^{\mu} u^{(\mu)}_{n\pm1,n\pm1}(\xi_n \pm \epsilon a, \tau; \phi_{n\pm1}) \\ &= \sum_{\mu=1}^{\infty} \epsilon^{\mu} \left[\sum_{\nu=0}^{\infty} \frac{1}{\nu!} \left(\pm \epsilon a \frac{\partial}{\partial \xi_n} \right)^{\nu} u^{(\mu)}_{n,n\pm1} \right]. \end{aligned} \tag{7}$$

Inserting equations (6, 7) into (2), and equating the same powers of ϵ, the equations of motion for the nth cell reduce to

$$\begin{aligned} &\left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) v^{(\mu)}_{n,n} - I_2 w_{n,n-1} - I_2' w^{(\mu)}_{n,n} = M^{(\mu)}_{n,n}, \\ &\left(\frac{\partial^2}{\partial t^2} + J_2 + J_2' \right) w^{(\mu)}_{n,n} - J_2 v^{(\mu)}_{n,n+1} - J_2' v^{(\mu)}_{n,n} = N^{(\mu)}_{n,n}, \end{aligned} \tag{8}$$

with the elements

$$M^{(1)}_{n,n} = 0, \tag{9}$$

$$M^{(2)}_{n,n} = 2V_g \frac{\partial^2 v^{(1)}_{n,n}}{\partial t \partial \xi_n} - I_2 a \frac{\partial w^{(1)}_{n,n-1}}{\partial \xi_n}, \tag{10}$$

$$\begin{aligned} M^{(3)}_{n,n} =& 2V_g \frac{\partial^2 v^{(2)}_{n,n}}{\partial t \partial \xi_n} - 2\frac{\partial^2 v^{(1)}_{n,n}}{\partial t \partial \tau} - V_g^2 \frac{\partial^2 v^{(1)}_{n,n}}{\partial \xi_n^2} \\ &+ I_2 \left(-a \frac{\partial w^{(2)}_{n,n-1}}{\partial \xi_n} + \frac{a^2}{2} \frac{\partial^2 w^{(1)}_{n,n-1}}{\partial \xi_n^2} \right) \\ &+ I_4' \left(w^{(1)}_{n,n} - v^{(1)}_{n,n} \right)^3 + I_4 \left(w^{(1)}_{n,n-1} - v^{(1)}_{n,n} \right)^3, \end{aligned} \tag{11}$$

$$N^{(1)}_{n,n} = 0, \tag{12}$$

$$N^{(2)}_{n,n} = 2V_g \frac{\partial^2 w^{(1)}_{n,n}}{\partial t \partial \xi_n} + J_2 a \frac{\partial v^{(1)}_{n,n+1}}{\partial \xi_n}, \tag{13}$$

$$\begin{aligned} N^{(3)}_{n,n} =& 2V_g \frac{\partial^2 w^{(2)}_{n,n}}{\partial t \partial \xi_n} - 2\frac{\partial^2 w^{(1)}_{n,n}}{\partial t \partial \tau} - V_g^2 \frac{\partial^2 w^{(1)}_{n,n}}{\partial \xi_n^2} \\ &+ J_2 \left(a \frac{\partial v^{(2)}_{n,n+1}}{\partial \xi_n} + \frac{a^2}{2} \frac{\partial^2 v^{(1)}_{n,n+1}}{\partial \xi_n^2} \right) \\ &+ J_4' \left(v^{(1)}_{n,n} - w^{(1)}_{n,n} \right)^3 + J_4 \left(v^{(1)}_{n,n+1} - w^{(1)}_{n,n} \right)^3. \end{aligned} \tag{14}$$

In the derivation of the element expressions (9)-(14) only the quartic anharmonicity of the system is kept by letting $I_3(I_3') = J_3(J_3') = 0$ for simplicity. This also allows comparison with the solution of reference [17]. Moreover, the expressions of $M^{(\mu)}_{n,n}$ and $N^{(\mu)}_{n,n}$ for $\mu = 4, 5...$ are not presented explicitly here. Now we solve equation (8) order by order with the help of (9–14).

3 Amplitude equations of modes

In order to avoid possible divergences, we consider the acoustic and optical modes separately. The amplitude equations for both modes will now be reduced to a perturbed NLSE.

3.1 Acoustic mode

For the lower frequency acoustic mode we rewrite the equation of motion (8) in the form

$$\begin{aligned} &\hat{L} w^{(\mu)}_{n,n} = J_2' M^{(\mu)}_{n,n} + J_2 M^{(\mu)}_{n,n+1} + \left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) N^{(\mu)}_{n,n}, \\ &\left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) v^{(\mu)}_{n,n} = I_2 w^{(\mu)}_{n,n-1} + I_2' w^{(\mu)}_{n,n} + M^{(\mu)}_{n,n}, \end{aligned} \tag{15}$$

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

$$\begin{aligned} \hat{L} u^{(\mu)}_{n,n} =& \left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) \left(\frac{\partial^2}{\partial t^2} + J_2 + J_2' \right) u^{(\mu)}_{n,n} \\ &- \left[I_2 J_2' u^{(\mu)}_{n,n-1} + I_2' J_2 u^{(\mu)}_{n,n+1} + (I_2 I_2' + J_2 J_2') u^{(\mu)}_{n,n} \right], \end{aligned} \tag{16}$$

with $u^{(\mu)}_{n,n} = v^{(\mu)}_{n,n}$ or $w^{(\mu)}_{n,n}$. In the lowest order of ϵ ($\mu = 1$), $M^{(1)}_{n,n} = N^{(0)}_{n,n} = 0$, we have the linear wave equation of the system

$$\begin{aligned} &\hat{L} w^{(1)}_{n,n} = 0, \\ &\left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) v^{(1)}_{n,n} = I_2 w^{(1)}_{n,n-1} + I_2' w^{(1)}_{n,n}. \end{aligned} \tag{17}$$

It is easy to obtain the solution for this linear equation

$$\begin{aligned} w^{(1)}_{n,n} &= A_-(\xi_n^-, \tau) \mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.}, \\ v^{(1)}_{n,n} &= -\frac{I_2 \mathrm{e}^{-iqa} + I_2'}{\omega_-^2 - (I_2 + I_2')} A_-(\xi_n^-, \tau) \mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.}, \end{aligned} \tag{18}$$

and to recover the linear dispersion relation (3). In the solution (18), $A_-(\xi_n^-, \tau)$ is an amplitude envelope function to be determined, c.c. represents the complex conjugate, $\phi_n^- = qna - \omega_- t$, and ω_- is the acoustic frequency given by equation (3).

Using equations (10, 13) and the lowest order solution (18), we calculate the elements $M^{(2)}_{n,n}, M^{(2)}_{n,n+1}$ and $N^{(2)}_{n,n}$. Their substitution in equation (15) yields the following second order ($\mu = 2$) equation

$$\begin{aligned} \hat{L} w^{(2)}_{n,n} =& \mathrm{i}2 \left\{ 2V_g \omega_- \left[\omega_-^2 - (I_2 + I_2') + I_2 I_2' a \sin(qa) \right] \right\} \\ &\times \frac{\partial A_-}{\partial \xi_n^-} \mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.}, \\ &\left(\frac{\partial^2}{\partial t^2} + I_2 + I_2' \right) v^{(2)}_{n,n} = I_2 w^{(2)}_{n,n-1} + I_2' w^{(2)}_{n,n} \\ &+ \left[\mathrm{i}2 V_g \omega_- \frac{I_2 \mathrm{e}^{-iqa} + I_2'}{\omega_-^2 - (I_2 + I_2')} - I_2 a \mathrm{e}^{-iqa} \right] \frac{\partial A_-}{\partial \xi_n^-} \mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.} \end{aligned} \tag{19}$$

One remarks that the term proportional to $\exp(\mathrm{i}\phi_n^-)$ on the right-hand side of the first equation is a secular term. In order for the theory to be valid (solvability condition) [19], it must be eliminated. Hence, we set

$$2V_{\mathrm{g}}\omega_- \left[\omega_-^2 - (I_2 + I_2' + J_2 + J_2')\right] + I_2 J_2' a \sin(qa) = 0, \tag{20}$$

which gives the group velocity of the acoustic mode

$$V_{\mathrm{g}}^- = \frac{\mathrm{d}\omega_-}{\mathrm{d}q} = \frac{I_2 J_2' a \sin(qa)}{\omega_- \left(I_2 + I_2' + J_2 + J_2' - 2\omega_-^2\right)}\cdot \tag{21}$$

Therefore, the solution of equation (19) is

$$\begin{aligned} w_{n,n}^{(2)} &= B_-(\xi_n^-, \tau)\mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.}, \\ v_{n,n}^{(2)} &= -\frac{1}{\omega_-^2 - (I_2 + I_2')}\Bigg[\left(I_2\mathrm{e}^{-\mathrm{i}qa} + I_2'\right) B_-(\xi_n^-, \tau) \\ &+ \left(\mathrm{i}2V_{\mathrm{g}}^-\omega_- \frac{I_2\mathrm{e}^{-\mathrm{i}qa} + I_2'}{\omega_-^2 - I_2 - I_2'} - I_2 a\mathrm{e}^{-\mathrm{i}qa}\right)\frac{\partial A_-}{\partial \xi_n^-}\Bigg]\mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.}, \end{aligned} \tag{22}$$

where $B_-(\xi_n^-, \tau)$ is another unknown function. In fact we can let $B_-(\xi_n^-, \tau) = 0$, as it can be absorbed into the lowest order solution. Then, (22) simplifies to

$$\begin{aligned} w_{n,n}^{(2)} &= 0, \\ v_{n,n}^{(2)} &= -\frac{1}{\omega_-^2 - (I_2 + I_2')}\Bigg[\mathrm{i}2V_{\mathrm{g}}^-\omega_- \frac{I_2\mathrm{e}^{-\mathrm{i}qa} + I_2'}{\omega_-^2 - (I_2 + I_2')} \\ &\quad - I_2 a\mathrm{e}^{-\mathrm{i}qa}\Big)\frac{\partial A_-}{\partial \xi_n^-}\Bigg]\mathrm{e}^{\mathrm{i}\phi_n^-} + \text{c.c.} \end{aligned} \tag{23}$$

Using the same procedure as for the second order equation, and with a careful detailed calculation of equations (11, 14) for $M_{n,n}^{(3)}, M_{n,n+1}^{(3)}$ and $N_{n,n}^{(3)}$, we obtain the third order equation

$$\begin{aligned} \hat{L}w_{n,n}^{(3)} &= 2\omega_-\left(I_2 + I_2' + J_2 + J_2' - 2\omega_-^2\right)\Bigg[\mathrm{i}\frac{\partial A_-}{\partial \tau} \\ &\quad + P_-\frac{\partial^2 A_-}{\partial(\xi_n^-)^2} + Q_-\mid A_-\mid^2 A_- + \mathrm{i}R_-\mid A_-\mid^2 A_-\Bigg] \\ &\quad \times \mathrm{e}^{\mathrm{i}\phi_n^-} + \text{higher harmonic terms} + \text{c.c.}, \end{aligned} \tag{24}$$

where the coefficients are expressed by

$$\begin{aligned} P_- &= \frac{1}{2\omega_-\left(I_2 + I_2' + J_2 + J_2' - 2\omega_-^2\right)} \\ &\times \Bigg\{\left(V_{\mathrm{g}}^-\right)^2\left[6\omega_-^2 - (I_2 + I_2' + J_2 + J_2')\right] \\ &+ \frac{a^2}{2}\left[\omega_-^2 - I_2 - I_2'\right)\left(\omega_-^2 - J_2 - J_2'\right) - (I_2 J_2 + I_2' J_2')\Big]\Bigg\}, \end{aligned} \tag{25}$$

$$\begin{aligned} Q_- &= \frac{3}{2\omega_-\left(I_2 + I_2' + J_2 + J_2' - 2\omega_-^2\right)}\Big\{J_4\Big[\left(\alpha_1^-\right)^2 + \left(\beta_1^-\right)^2\Big] \\ &\times \left[\alpha_1^-\left(\omega_-^2 + I_2'\cos qa - I_2'\right) + \beta_1^- I_2'\sin qa\right] + J_4'\Big[\left(\alpha_2^-\right)^2 \\ &+ \left(\beta_2^-\right)^2\Big]\left[\alpha_2^-\left(\omega_-^2 + I_2\cos qa - I_2\right) + \beta_2^- I_2\sin qa\right]\Big\}, \end{aligned} \tag{26}$$

$$\begin{aligned} R_- &= \frac{3}{2\omega_-\left(I_2 + I_2' + J_2 + J_2' - 2\omega_-^2\right)}\Big\{J_4\Big[\left(\alpha_1^-\right)^2 + \left(\beta_1^-\right)^2\Big] \\ &\times \left[\beta_1^-\left(\omega_-^2 + I_2\cos qa - I_2'\right) - \alpha_1^- I_2'\sin qa\right] + J_4'\Big[\left(\alpha_2^-\right)^2 \\ &+ \left(\beta_2^-\right)^2\Big]\left[-\beta_2^-\left(\omega_-^2 + I_2'\cos qa - I_2\right) + \alpha_2^- I_2\sin qa\right]\Big\} \end{aligned} \tag{27}$$

with

$$\begin{aligned} \alpha_1^- &= 1 + \left(I_2 + I_2'\cos qa\right)/\left[\omega_-^2 - (I_2 + I_2')\right], \\ \alpha_2^- &= 1 + \left(I_2' + I_2\cos qa\right)/\left[\omega_-^2 - (I_2 + I_2')\right], \\ \beta_1^- &= I_2'\sin qa/\left[\omega_-^2 - (I_2 + I_2')\right], \\ \beta_2^- &= I_2\sin qa/\left[\omega_-^2 - (I_2 + I_2')\right]. \end{aligned}$$

The term proportional to $\mathrm{e}^{\mathrm{i}\phi_n^-}$ in equation (24) is also a secular term. To eliminate it we set the equation for $A_-(\xi_n^-, \tau)$

$$\begin{aligned} &\mathrm{i}\frac{\partial A_-}{\partial \tau} + P_-\frac{\partial^2 A_-}{\partial(\xi_n^-)^2} \\ &\qquad + Q_-\mid A_-\mid^2 A_- + \mathrm{i}R_-\mid A_-\mid^2 A_- = 0, \end{aligned} \tag{28}$$

which is a perturbed NLSE. The additional fourth term in equation (28) comes from the structural asymmetry of the sphalerite lattice by considering the expansion up to the third order. Obviously, the two terms within braces in equation (27) cancel, and $R_- = 0$ in the case of uniform force constants with $I_2 = I_2'$ and $I_4 = I_4'$. The model reduces then to the extensively studied 1D diatomic lattice [5,13]. This multiple-scale expansion approach results then in a standard NLSE. The alternating force-constant lattice was studied in reference [17] by a similar method. As only the cubic anharmonicity was included in that model, each order of the solution contains a "direct current" component, and only the second order expansion leads to a NLSE. Therefore, the additional term produced by the system structural asymmetry does not appear in the equation.

3.2 Optical mode

For the higher frequency optical mode, we rewrite the equation of motion (8) in another form

$$\hat{L}v_{n,n}^{(\mu)} = I_2' N_{n,n}^{(\mu)} + I_2 N_{n,n-1}^{(\mu)} + \left(\frac{\partial^2}{\partial t^2} + J_2 + J_2'\right) M_{n,n}^{(\mu)},$$
$$\left(\frac{\partial^2}{\partial t^2} + J_2 + J_2'\right) w_{n,n}^{(\mu)} = J_2 w_{n,n-1}^{(\mu)} + J_2' w_{n,n}^{(\mu)} + N_{n,n}^{(\mu)}\,. \tag{29}$$

By a procedure similar to that used for the acoustic mode, we solve equation (29) for the optical mode step by step. We remark that there is a symmetry between equations (9l–11) and (12–14), and also between equations (15, 29) for the acoustic and optical modes, respectively. If we make the substitution

$$a \to -a,\;\; I_2\,(I_2') \to J_2\,(J_2'),\;\; I_4\,(I_4') \to J_4\,(J_4')\,,$$
$$w_{n,n}^{(\mu)} \to v_{n,n}^{(\mu)},\;\; w_{n,n\pm1}^{(\mu)} \to v_{n,n\pm1}^{(\mu)}. \tag{30}$$

Equations (9–11) are transformed into (12–14), and (15) into (29). Using this property, and the results for the acoustic mode, we write down the solutions for the optical mode by inspection

$$v_{n,n}^{(1)} = A_+(\xi_n^+,\tau)\mathrm{e}^{\mathrm{i}\phi_n^+} + \text{c.c.},$$
$$w_{n,n}^{(1)} = -\frac{J_2\mathrm{e}^{\mathrm{i}qa} + J_2'}{\omega_-^2 - (J_2 + J_2')} A_+(\xi_n^+,\tau)\mathrm{e}^{\mathrm{i}\phi_n^+} + \text{c.c.}, \tag{31}$$

where $A_+(\xi_n^+,\tau)$ is the envelope function for the optical mode to be determined, $\phi_n^+ = qna - \omega_+(q)t$, and ω_+ is the linear dispersion of the optical branch given by equation (3). For $\mu = 2$, we also obtain the group velocity for the optical mode

$$V_{\mathrm{g}}^+ = \frac{\mathrm{d}\omega_+}{\mathrm{d}q} = \frac{I_2 J_2' a \sin(qa)}{\omega_+(I_2 + I_2' + J_2 + J_2' - 2\omega_+^2)}\,. \tag{32}$$

The solution of the second order equation for this mode is

$$v_{n,n}^{(2)} = 0,$$
$$w_{n,n}^{(2)} = -\frac{1}{\omega_-^2 - (I_2 + I_2')}\left[\mathrm{i}2V_{\mathrm{g}}^+\omega_+\frac{J_2\mathrm{e}^{\mathrm{i}qa} + J_2'}{\omega_+^2 - (J_2 + J_2')} - J_2 a\mathrm{e}^{\mathrm{i}qa}\right]\frac{\partial A_+}{\partial \xi_n^+}\mathrm{e}^{\mathrm{i}\phi_n^+} + \text{c.c.} \tag{33}$$

Again the elimination of the secular term in the third order solution gives the equation for $A_+(\xi_n^+,\tau)$,

$$\mathrm{i}\frac{\partial A_+}{\partial \tau} + P_+\frac{\partial^2 A_+}{\partial(\xi_n^+)^2} + Q_+ \mid A_+ \mid^2 A_+ + \mathrm{i}R_+ \mid A_+ \mid^2 A_+ = 0, \tag{34}$$

where the coefficients are

$$P_+ = \frac{1}{2\omega_+\left(I_2 + I_2' + J_2 + J_2' - 2\omega_+^2\right)} \times \left\{\left(V_{\mathrm{g}}^+\right)^2\left[6\omega_+^2 - (I_2 + I_2' + J_2 + J_2')\right] + \frac{a^2}{2}\left[\left(\omega_+^2 - I_2 - I_2'\right)\left(\omega_+^2 - J_2 - J_2'\right) - (I_2 J_2 + I_2' J_2')\right]\right\}, \tag{35}$$

$$Q_+ = \frac{3}{2\omega_+\left(I_2 + I_2' + J_2 + J_2' - 2\omega_+^2\right)}\left\{I_4\left[\left(\alpha_1^+\right)^2 + \left(\beta_1^+\right)^2\right] \times \left[\alpha_1^+\left(\omega_+^2 + J_2'\cos qa - J_2'\right) - \beta_1^+ I_2' \sin qa\right] + I_4'\left[\left(\alpha_2^+\right)^2 + \left(\beta_2^+\right)^2\right]\left[\alpha_2^+\left(\omega_+^2 + J_2\cos qa - J_2\right) - \beta_2^+ J_2 \sin qa\right]\right\}, \tag{36}$$

$$R_+ = \frac{3}{2\omega_+\left(I_2 + I_2' + J_2 + J_2' - 2\omega_+^2\right)}\left\{I_4\left[\left(\alpha_1^+\right)^2 + \left(\beta_1^+\right)^2\right] \times \left[\beta_1^+\left(\omega_+^2 + J_2\cos qa - J_2'\right) + \alpha_1^+ J_2' \sin qa\right] - I_4'\left[\left(\alpha_2^+\right)^2 + \left(\beta_2^+\right)^2\right]\left[\beta_2^+\left(\omega_+^2 + J_2'\cos qa - J_2\right) + \alpha_2^+ I_2 \sin qa\right]\right\} \tag{37}$$

with

$$\alpha_1^+ = 1 + \left(J_2 + J_2'\cos qa\right) / \left[\omega_+^2 - (J_2 + J_2')\right],$$
$$\alpha_2^+ = 1 + \left(J_2' + J_2\cos qa\right) / \left[\omega_+^2 - (J_2 + J_2')\right],$$
$$\beta_1^+ = -J_2' \sin qa / \left[\omega_+^2 - (J_2 + J_2')\right],$$
$$\beta_2^+ = -J_2 \sin qa / \left[\omega_+^2 - (J_2 + J_2')\right].$$

Equation (34) is also a perturbed NLSE with the same structure as equation (28) for the acoustic mode.

We note that the original set of equations (2) for the atomic displacements $v_n(t)$ and $w_n(t)$ are invariant with respect to time inversion. However, the resulting equations (28, 34) are for the envelope functions $A_-(\xi_n^-,\tau)$ and $A_+(\xi_n^+,\tau)$. The displacements $v_n(t)$ and $w_n(t)$ are related to $A_\pm(\xi_n^\pm,\tau)$ by multiplication with a fast vibration factor $\exp(\pm\mathrm{i}\phi_n^\pm)$ (see Eqs. (6, 18) and (31)). As $\exp(\pm\mathrm{i}\phi_n^\pm) = \exp[\pm\mathrm{i}(qna - \omega_\pm t)]$ are not invariant with respect to time inversion, then equations (28, 34) are also not invariant with respect to that operation.

4 Stationary modes

For the acoustic mode with wavevector at the Brillouin-zone boundary ($q = \pi/a$), and assuming quartic

anharmonicity (*i.e.*, $k_4, k_4' > 0$) we calculate the coefficients in equation (28):

$$P_- = -\frac{I_2 J_2' a^2}{2\omega_1 \sqrt{\left(I_2 + I_2' + J_2 + J_2'\right)^2 - 16 I_2 J_2'}} < 0, \tag{38}$$

$$Q_- = \frac{3\left[J_4\left(\omega_1^2 - 2I_2'\right)^4 + J_4'\left(\omega_1^2 - 2I_2\right)^4\right]}{2\omega_1\left[\omega_1^2 - (I_2 + I_2')\right]^3 \sqrt{\left(I_2 + I_2' + J_2 + J_2'\right)^2 - 16 I_2 J_2'}} < 0, \tag{39}$$

$$R_- = 0, \tag{40}$$

where ω_1 is the maximum linear acoustic frequency given by equation (4). As $I_2 > I_2'$, $\omega_1^2 - (I_2 + I_2') < 0$ and $Q_- < 0$ in this case. Also from equation (21) we know that $V_{\rm g}^-(\pm\pi/a) = 0$. Therefore, equation (28) becomes a standard NLSE with a stationary single-soliton solution

$$A_- = \sqrt{2P_-/Q_-}\epsilon\ \mathrm{sech}[\epsilon(n - n_0)a]\ \exp[\mathrm{i}(\mid P_- \mid \epsilon^2 t - \phi_0)], \tag{41}$$

where $n_0 a$ and ϕ_0 are the initial position and phase of the soliton, respectively. In this case $\phi_n^- = n\pi - \omega_1 t$, and from equation (18) we obtain the configuration of the atomic displacements in first order approximation

$$\begin{aligned} w_n(t) &= (-1)^n 2\sqrt{2P_-/Q_-}\epsilon\ \mathrm{sech}[\epsilon(n - n_0)a] \\ &\quad \times \cos(\Omega_1 t - \phi_0), \\ v_n(t) &= -\frac{I_2 - I_2'}{(I_2 + I_2') - \omega_1^2} w_n(t), \end{aligned} \tag{42}$$

where the vibrational frequency $\Omega_1 = \omega_1 + \mid P_- \mid \epsilon^2$ lies in the linear frequency gap between the acoustic and optical branches. From the solution (42) we see that the vibration of the two atoms in each unit cell are π out of phase. The contribution of the higher order approximations to the atomic displacements are comparatively small, and the validity of this discrete multiple-scale method has been proven by Bambi *et al.* in reference [13].

For the optical mode with $q = \pm\pi/a$, we have in the same way $V_{\rm g}^+(\pm\pi/a) = 0$ from equation (32) and the coefficients in equation (34) are

$$P_+ = \frac{I_2 J_2' a^2}{2\omega_2 \sqrt{\left(I_2 + I_2' + J_2 + J_2'\right)^2 - 16 I_2 J_2'}} > 0, \tag{43}$$

$$Q_+ = \frac{3\left[I_4\left(\omega_2^2 - 2J_2'\right)^4 + I_4'\left(\omega_2^2 - 2J_2\right)^4\right]}{2\omega_2[\omega_2^2 - (J_2 + J_2')]^3 \sqrt{\left(I_2 + I_2' + J_2 + J_2'\right)^2 - 16 I_2 J_2'}} < 0, \tag{44}$$

$$R_+ = 0. \tag{45}$$

Therefore, equation (34) has a stationary kink (dark-soliton) solution

$$\begin{aligned} A_- &= \sqrt{2P_+/\mid Q_+ \mid}\epsilon\ \tanh[\epsilon(n - n_0)a] \\ &\quad \times \exp\left[\mathrm{i}\left(-2P_+\epsilon^2 t - \phi_0\right)\right], \end{aligned} \tag{46}$$

which yields the distribution of atomic displacements with $\phi_n^+ = n\pi - \omega_2 t$

$$\begin{aligned} v_n(t) &= (-1)^n 2\sqrt{2P_+/\mid Q_+ \mid}\epsilon\ \tanh[\epsilon(n - n_0)a] \\ &\quad \times \cos(\Omega_2 t - \phi_0)], \\ w_n(t) &= \frac{J_2 - J_2'}{\omega_2^2 - (J_2 + J_2')} v_n(t), \end{aligned} \tag{47}$$

with the vibrational frequency $\Omega_2 = \omega_2 + 2P_+\epsilon^2$ lying in the frequency band of the optical branch. In this case the displacements of the two atoms in each unit cell are in phase.

For the optical mode with $q = 0$, we also have $V_{\rm g}^+(0) = 0$ and the coefficients in equation (34) are

$$P_+ = -\frac{I_2 J_2' a^2}{2\omega_3^3} < 0, \tag{48}$$

$$Q_+ = -\frac{3\omega_3^5\left(I_4 + I_4'\right)}{2\left[\omega_3^2 - (J_2 + J_2')\right]^3} < 0, \tag{49}$$

$$R_+ = 0. \tag{50}$$

Again, there is a stationary single-soliton solution

$$A_+ = \sqrt{2P_+/Q_+}\epsilon\ \mathrm{sech}[\epsilon(n - n_0)a]\ \exp[\mathrm{i}(P_+\epsilon^2 t - \phi_0)]. \tag{51}$$

The distribution of atomic displacements is

$$v_n(t) = 2\sqrt{2P_+/Q_+}\epsilon\ \mathrm{sech}[\epsilon(n - n_0)a]\ \cos(\Omega_3 t - \phi_0)], \tag{52}$$

$$w_n(t) = -\frac{m}{M} v_n(t), \tag{53}$$

with the vibrational frequency $\Omega_3 = \omega_3 + \mid P_+ \mid \epsilon^2$ above the linear frequency band of the optical branch. The vibration of the two atoms of one unit cell are π out of phase in this case.

Finally, we consider the acoustic mode with $q = 0$. From equation (3) we know that $\omega_-(0) = 0$, so that both P_- and Q_- diverge. Therefore, the multiple-scale expansion is in this case independent of the fast variable ϕ_n^-, and the nonlinear modulation equation for $A_-(\xi_n^-, \tau)$ becomes invalid. We must then apply the full continuum approximation [2] to the lattice system. The lattice equation of motion reduces then to a KdV or to a modified KdV equation [2].

5 Moving modes

In the last section, the stationary LMs with wavevectors $q = 0, \pm\pi/a$ were discussed. Generally, when $q \neq 0$ or $\pm\pi/a$, $R_\pm \neq 0$ so that equations (28, 34) are not standard NLSEs. We numerically compared the coefficients for typical values of the system parameters $M = 2m$ and $k_j = 3k_j'$ ($j = 2, 4$). For $0 < q < \pi/a$, the magnitude of $R_\pm$ is 10^{-1} to 10^{-2} times smaller than that of $P_\pm$ and $Q_\pm$. Hence, the

fourth term in both equations (28, 34) can be treated as a perturbation.

Ignoring the subscripts, and rewriting equations (28, 34) in a unified form, one obtains

$$\mathrm{i}\frac{\partial A}{\partial t} + P\frac{\partial^2 A}{\partial (x_n)^2} + Q \mid A \mid^2 A = -\mathrm{i}R \mid A \mid^2, \qquad (54)$$

with $A = A_{\pm}, P = P_{\pm}, Q = Q_{\pm}, R = R_{\pm}$ and $x_n = na$. To treat equation (54) with the proposed perturbation approach [20], we make the transformation

$$A \to (2/Q)^{1/3} A, \;\; x_n \to (2P^3/Q)^{1/6} x_n, \;\; t \to (2/Q)^{1/3} t. \qquad (55)$$

Then, equation (54) reduces to a mathematically convenient form

$$\mathrm{i}\frac{\partial A}{\partial t} + \frac{\partial^2 A}{\partial (x_n)^2} + 2 \mid A \mid^2 A = -\mathrm{i}\frac{2R}{Q} \mid A \mid^2 A. \qquad (56)$$

The single-soliton solution of the corresponding homogeneous equation is

$$A = 2\beta \,\mathrm{sech}[2\beta(x_n - \zeta_0 + 4\alpha t)] \exp\{ -\mathrm{i}[2\alpha x_n + 4(\alpha^2 - \beta^2) t + \theta_0] \}, \qquad (57)$$

where α, β, ζ_0 and θ_0 are four real parameters which determine the moving velocity, height and width, initial position, and initial phase of the soliton, respectively. One then applies the perturbation by treating $2R/Q$ as an expansion parameter. From equations (52–55) in reference [20], we obtain

$$\alpha_{t_1} = 0, \;\; \beta_{t_1} = -\frac{32R}{3Q}\beta^3, \;\; \zeta_{t_1} = 0,$$
$$\delta_{t_1} = -4(\alpha^2 + \beta^2) + \frac{16R}{3Q}\beta^2, \qquad (58)$$

where t_1 is the "slow" time variable in the soliton perturbation expansion. Returning to the original time variable t (and remarking that $\partial_t = \partial_{t_0} + \epsilon\partial_{t_1}$ up to first order) the integration can be performed to obtain the time variation of the soliton parameters

$$\alpha = \alpha_0, \;\; \beta = \frac{\beta_0}{\sqrt{1 + 64\beta^2 Rt/3Q}}, \;\; \zeta = \zeta_0 - 4\alpha_0 t,$$
$$\delta = \delta_0 - 4\alpha_0^2 - \frac{3Q - 4R}{18R} \ln\left[1 + 64\beta_0^2 Rt/3Q\right]. \qquad (59)$$

One clearly sees that the height of the soliton dampens with t and that the initial position and phase of the soliton are affected by the perturbation, while the moving velocity of the soliton remains constant. Of course, when one returns to the original variables the velocity of the soliton modes should be $V_{\mathrm{g}}^{\pm}$. Moreover, the first order corrections to the soliton can also be obtained from reference [20].

6 Discussion and conclusion

If one makes the substitution $I_j(J_j) \to I'_j(J'_j)$ ($j = 2$, 3, 4), equation (2) turns into the equation of motion for the center of the LMs on tight-bond atom pairs. Using this symmetry and the solutions for the mode center on weak-bond atom pairs, one can obtain the corresponding solutions for the mode center on tight-bond atom pairs.

The inclusion of the cubic term in equations (15, 29) brings an additional feature to LMs, the vibrational center being accompanied with a localized lattice distortion having a kink shaped distribution. Moreover, the cubic nonlinearity makes the atomic interaction potential softer and hence it decreases the frequency of LMs [13,14]. Therefore, the optical LM with vibrational frequency above ω_3 might disappear, but the gap LM always exists. The lattice model with both cubic and quartic anharmonicities, as well as a numerical molecular dynamics study of equation (2), are under investigation.

The amplitude equation of LMs in this sphalerite-structure lattice is described by a perturbed NLSE, and the perturbation calculation shows that the height of LMs dampens with time. This is the main difference between the sphalerite-structure lattice and the diatomic (ionic) lattice systems. In addition to molecular lattice systems [11], we think that the next candidates for the experimental realization and detection of such nonlinear-induced localized modes should be ionic crystals. However, this 1D sphalerite-structure lattice is quite general and the results of this work are consistent with other studies of 1D lattice systems [3–5,13–16]. If one sets $m = M$ our model reduces to a 1D diamond-structure lattice [17], if $k_j = k'_j$ one recovers the 1D diatomic lattice [13–16], and if one lets both masses and force constants uniform the model becomes a simple 1D monatomic lattice [3–5].

In conclusion, we have studied nonlinear-induced localized modes in a one-dimensional atomic chain with two periodically alternating masses and force constants by means of a discrete multiple-scale expansion. The model simulates a row of atoms in the $\langle 1\ 1\ 1 \rangle$-direction of sphalerite-structure crystals such as the important semiconductor GaAs. We found some new phenomenon for the LMs which may come from the structural asymmetry of this lattice. The amplitude of LMs in this system is governed by a perturbed NLSE instead of the standard one of 1D diatomic (ionic) lattices [13,14]. Although the stationary LMs with carrier wavevector at $q = \pm\pi/a$ are similar to those of the diatomic lattices, the general LMs with wavevectors $q \neq 0$ or $\pm\pi/a$ are quite different owing to the perturbation in the sphalerite-structure lattice. The perturbation calculation shows that the height of the LMs dampens with time.

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