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Moving nonlinear localized vibrational modes for a one-dimensional homogenous lattice with quartic anharmonicity

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Abstract. Moving nonlinear localized vibrational modes (*i.e.* discrete breathers) for the one-dimensional homogenous lattice with quartic anharmonicity are obtained analytically by means of a semidiscrete approximation plus an integration. In addition to the pulse-envelope type of moving modes which have been found previously both analytically and numerically, we find that a kink-envelope type of moving mode which has not been reported before can also exist for such a lattice system. The two types of modes in both right- and left-moving form can occur with different carrier wavevectors and frequencies in separate parts of the $\omega(q)$ plane. Numerical simulations are performed and their results are in good agreement with the analytical predictions.

PACS. 63.90.+t Other topics in lattice dynamics – 63.20.Pw Localized modes

1 Introduction

Some physical properties of solids (such as specific heat at high temperature, melting, thermal expansion, temperature dependence of the elastic constants, and damping of high frequency sound waves) may mainly or partly depend on crystal anharmonicity, so that much attention has been paid to nonlinear localized vibrational modes, *i.e.*, discrete breathers induced by the anharmonicity in pure crystal lattices (see, *e.g.*, a recent review article [1] and references therein). These modes may have sizable amplitudes and can be localized on only a few lattice sites with either odd [2] or even [3] symmetry form in the highly discrete and sufficiently strong anharmonicity case, but generally they appear in the characteristic long wavelength envelope form.

As is known, impurity vibrational modes are centered on defect sites only in inhomogenous lattices. On the other hand, in homogenous lattices the center of a nonlinear vibrational mode may appear at any lattice site because of the translational invariance of these lattices, so it is believed that the anharmonicity of perfect lattices should support moving nonlinear localized modes. However, most of the research on this subject has concentrated on stationary solutions [4–6] of nonlinear modes for different kinds of nonlinear lattice systems. There has been some work done on moving solutions by numerical simulations [7–9] for lattices with pure quartic anharmonicity, but little using analytical approaches even for such relatively simple nonlinear lattice models. Multiple-scale expansion is an effective technique for dealing with nonlinear equations and some approximate analytical solutions for this lattice model have been obtained [10–13] in this way, but the calculations are somewhat tedious and only the main component in the expansion can be considered. The lattice Green's function method, which treats the whole question discretely, has also been applied to this lattice model and some good approximate analytical solutions have been obtained [2,14]. However, in each of these two analytical methods, it is not possible to consider all of the possible solutions over the whole $\omega(q)$ plane of the system. In the present work, we use a simple alternative approach to solve the equation of motion for a one-dimensional homogenous lattice with pure quartic inter-site nonlinearity, the so-called Fermi-Pasta-Ulam lattice model. The discreteness of the carrier wave is treated explicitly while the envelope is described in the continuum approximation. Then the equation of motion reduces to an elliptical integration. Besides the pulse-envelope type of modes (sech function) which appears in references [4–6] in its stationary form and references [7–9,12–14] in its moving form, we find that the kink-envelope type of moving modes (tanh function) can also exist in such a lattice system. The two types of modes in right- or left-moving form can occur with different carrier wavevectors and vibrational frequencies in separated parts of the $\omega(q)$ plane.

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We perform a numerical simulation based on the original lattice equation of motion for the system, and the results support our analytical prediction quite well. However, the kink-envelope type of moving solutions, to the best of our knowledge, has not been reported previously in either analytical or numerical studies for this lattice system.

The paper is organized as follows. In Section 2 we use the semidiscrete approximation to formulate the model as an integrable system. In Section 3 we obtain analytically all possible solutions with their velocities over the whole $\omega(q)$ plane. The technique and the results of the numerical simulations are presented in Section 4. Section 5 discusses the results and concludes the paper.

2 Formalism of the model

We consider a one-dimensional lattice with nearest-neighbor interactions between particles (molecules, atoms or ions). The Hamiltonian of the system is given by

$$H = \sum_n \left[\frac{1}{2}m\left(\frac{\mathrm{d}u_n}{\mathrm{d}t}\right)^2 + V(u_n - u_{n-1})\right], \qquad (1)$$

where $u_n = u_n(t)$ is the displacement of the nth particle of mass m from its equilibrium position. The potential $V(r)$ is quite general. Typically it can be the standard two-body potentials of Lennard-Jones, Born-Mayer-Coulomb, or other more realistic model potentials depending on the bond structure of the considered crystal. If we focus on rather small displacements that can be measured experimentally, without reconstruction or phase-transition in the system, it allows us to Taylor expand $V(r)$ around $r = 0$, and truncate the power series to the fourth-order [16]. For simplicity we neglect the third-order term in the series. Then, the classical equation of motion reads

$$m\frac{\mathrm{d}^2u_n}{\mathrm{d}t^2} = k_2(u_{n+1} + u_{n-1} - 2u_n) + k_4[(u_{n+1} - u_n)^3 - (u_n - u_{n-1})^3], \qquad (2)$$

where k_2 and k_4 are the harmonic and anharmonic coupling constants, respectively. To simplify equation (2), we transform the displacement into [8,14]

$$v_n = u_{n+1} - u_n \qquad (3)$$

without loss of generality. Then equation (2) becomes

$$m\frac{\mathrm{d}^2v_n}{\mathrm{d}t^2} = k_2(v_{n+1} + v_{n-1} - 2v_n) + k_4(v_{n+1}^3 + v_{n-1}^3 - 2v_n^3). \qquad (4)$$

Analytical solutions to equation (4), giving a moving anharmonic mode, are sought by setting [8]

$$v_n(t) = \phi_n(t)\cos(qna - \omega t) \qquad (5)$$

where $\phi_n(t)$ is an envelope function, $\cos(qna - \omega t)$ is a carrier wave with the rapidly varying phase, and q and ω are the wavevector and vibrational frequency, respectively. Inserting equation (5) into (4) and using the rotating-wave approximation (RWA) which was proved [16] to accurately remove higher-frequency harmonics in such nonlinear lattices, we obtain a pair of equations. The correction to RWA was found [16] to be a few percent and the amplitude response from the higher-frequency components can be ignored. This approximate method of analysis is sufficient to separate the equation of motion. To satisfy at all times the solution represented by equation (5), the coefficient of both the in-phase and out-phase oscillatory terms must independently sum to zero. Then equating the sine terms gives

$$-2m\omega\frac{\mathrm{d}\phi_n}{\mathrm{d}t} = \sin(qa)(\phi_{n+1} - \phi_{n-1}) \times [k_2 + k_4(\phi_{n+1}^2 + \phi_{n+1}\phi_{n-1} + \phi_{n-1}^2)], \qquad (6)$$

and the cosine terms

$$\frac{\mathrm{d}^2\phi_n}{\mathrm{d}t^2} - m\omega^2\phi_n = k_2[(\phi_{n+1} + \phi_{n-1})\cos(qa) - 2\phi_n] + \frac{3k_4}{4}\left[(\phi_{n+1}^3 + \phi_{n-1}^3)\cos(qa) - 2\phi_n^3\right]. \qquad (7)$$

This pair of coupled equations was obtained in reference [8] by the same method for this lattice model. Equation (6) can be used to determine numerically [8] the envelope velocity of the mode. Note that for wavevectors near Brillouin-zone boundaries, $q = \pm\pi/a$, we can see from equation (6) that ϕ_n is independent of time, and the solution of equation (7) reduces to the previously determined stationary eigenmodes that appeared in references [4–6]. It seems that exact solutions of this set of nonlinear differential-difference equations do not exist. However, fairly good approximate analytical solutions can be obtained. The numerical work [8] assumed that the time variation of the envelope function is small compared to that of the carrier wave, *i.e.*, the term $\mathrm{d}^2\phi_n/\mathrm{d}t^2$ in equation (7) was neglected. It may not be suitable for wavevectors near the Brillouin-zone boundaries with rather large vibrational frequency ω. However, in the present work we will keep this second time differential term in equation (7). Assuming that the characteristic wavelength of the envelope is much greater than the lattice spacing a, we can make a continuum approximation ($na \to x$) for the envelope function

$$\phi_{n\pm1} = \phi \pm a\phi_x + \frac{a^2}{2}\phi_{xx} + \text{higher terms}. \qquad (8)$$

If we introduce a new variable $\xi = x - Vt$ (where V is the envelope velocity to be determined) and insert it into equation (6) with equation (8), to the second order we obtain

$$V = \frac{ak_2\sin(qa)}{m\omega}\left[1 + \frac{k_4}{k_2}(3\phi^2 + 3a^2\phi\phi_{\xi\xi} + a^2\phi_\xi^2)\right]. \qquad (9)$$

We only consider the solution of small-amplitudes which slowly vary in space for the system, so that ϕ, ϕ_ξ and

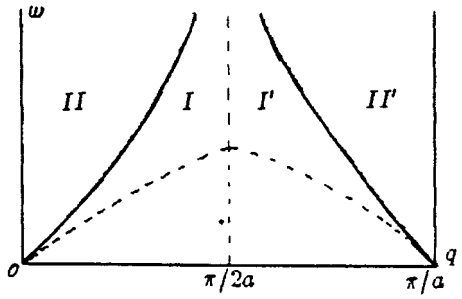

Fig. 1. A sketch of the regions for different types of moving modes existing in the $\omega(q)$ plane. Solid line: $\omega^2 = \pm k_2 \sin^2(qa)/m\cos(qa)$. Dashed line: $\omega^2 = 4k_2\sin^2(\frac{qa}{2})/m$.

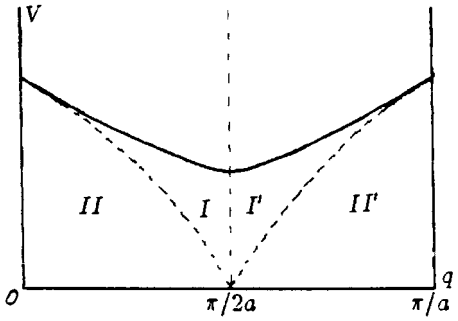

Fig. 2. A sketch of the regions for different types of moving modes existing in the $|V(q)|$ plane. Solid line: $|V| = \nu\sqrt{\pm\cos(qa)}$. Dashed line for $|V| = \nu\sin(qa)/2\sin(\frac{qa}{2})$.

$\phi_{\xi\xi}$ all are small. Therefore, to the main order, the group velocity is reduced to

$$V = ak_2\sin(qa)/m\omega, \tag{10}$$

which is exactly the same as the result of the multiple-scale method [10–13] for the same lattice system. For equation (7) we let [14] $\phi_{n+1}^3 \approx \phi_{n-1}^3 \approx \phi_n^3$ and insert it into equation (7), with equations (8, 10), equation (7) can be integrated as

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right)^2 = \frac{B}{A}\phi^2 - \frac{C}{A}\phi^4 + D, \tag{11}$$

where

$$\begin{aligned} A &= a^2k_2^2\sin^2(qa)/m\omega^2 - a^2k_2\cos(qa), \\ B &= m\omega^2 - 4k_2\sin^2\left(\frac{qa}{2}\right), \\ C &= \frac{3}{2}k_4\sin^2\left(\frac{qa}{2}\right), \end{aligned} \tag{12}$$

are constants dependent on the vibrational frequency ω and the wavevector q, and D is the integration constant. Then the equation of motion for the lattice system has been reduced to a single integration expressible in terms of elliptic functions.

3 Possible moving modes

In this section, we use the properties of such integration to analyze equation (11) with possible choices for the constants in equation (12), and to obtain analytical solutions.

We have to select $D = 0$ in equation (11) if we restrict ourselves to the pulse envelope solution. As is known, the even power coefficients in the expansion of any two-body potential are always positive, and C also is positive, so that the following two inequalities must be satisfied simultaneously

$$\begin{aligned} A &= a^2k_2^2\sin^2(qa)/m\omega^2 - a^2k_2\cos(qa) > 0, \\ B &= m\omega^2 - 4k_2\sin^2(\frac{qa}{2}) > 0. \end{aligned} \tag{13}$$

The second inequality shows that the nonlinear effect raises the vibrational frequency with respect to the linear dispersion. Inequalities (13) determine a region in the $\omega(q)$ plane where pulse-envelope moving modes exist, namely

$$4k_2\sin^2(\frac{qa}{2})/m < \omega^2 < k_2\sin^2(qa)/m\cos(qa), \quad 0 < q < \pi/2a. \tag{14}$$

This region in the $\omega(q)$ plane is shown in Figure 1 as I. Within this region, the analytical expression for the pulse-envelope moving modes is integrated as

$$v_n(t) = \sqrt{\frac{2B}{C}}\mathrm{sech}\left[\sqrt{\frac{B}{A}}(na - Vt)\right]\cos(qna - \omega t), \tag{15}$$

where A, B and C determined by equation (12) are functions of the two fundamental parameters ω and q of the modes, and the continuous variable has been replaced by the discrete one. This right-moving mode was observed in the numerical simulations of reference [8] for the same lattice model. Moreover, from equations (10, 14) we obtain the associated region of the envelope velocity in the $V(q)$ plane,

$$\nu\sqrt{\cos(qa)} < V < \nu\sin(qa)/2\sin\left(\frac{qa}{2}\right), \quad 0 < q < \pi/2a, \tag{16}$$

where $\nu = a\sqrt{k_2/m}$ is the sound velocity of the crystal. This region in the $V(q)$ plane is shown in Figure 2 as I, and we see that the moving velocity of the envelope is subsonic.

For the rather short wavelength range of the carrier wave, it is appropriate to introduce [5] an opposite-phase envelope function as $\phi_n = (-1)^n\psi_n$. The Taylor expansion of the difference $(\psi_{n\pm1} - \psi_n)$ up to the second order together with the transformation $\xi = x - V't$, yields the envelope velocity

$$V' = -ak_2\sin(qa)/m\omega = -V. \tag{17}$$

Then, the continuum approximation (8) yields

$$\left(\frac{\mathrm{d}\psi}{\mathrm{d}\xi}\right)^2 = \frac{F}{E}\psi^2 - \frac{G}{E}\psi^4 + D, \tag{18}$$

which is solvable in terms of Jacobian elliptic functions. In equation (18)

$$E = a^2 k_2^2 \sin^2(qa)/m\omega^2 + k_2 a^2 \cos(qa),$$
$$F = m\omega^2 - 4k_2 \cos^2\left(\frac{qa}{2}\right),$$
$$G = \frac{3}{2} k_4 \cos^2\left(\frac{qa}{2}\right), \tag{19}$$

where D is also an integration constant. For the same reason as above, we require the two parameters in equation (19) to satisfy $E > 0$ and $F > 0$ simultaneously in order to support pulse-envelope solutions similar to equation (15). Therefore, we find another region in the $\omega(q)$ plane for the existence of the modes described by

$$4k_2 \cos^2\left(\frac{qa}{2}\right)/m < \omega^2 < -k_2 \sin^2(qa)/m \cos(qa), \quad \pi/2a < q < \pi/a, \tag{20}$$

which is symmetrical to equation (14) about the $q = \pi/2a$ axis (region I' as shown in Fig. 1). This left-moving mode was obtained analytically and observed numerically in references [12,15] for the same system. Also, the region of the envelope velocity for the modes in the $V(q)$ plane can be transformed to

$$\nu\sqrt{-\cos(qa)} < V < \nu \sin(qa)/2 \cos\left(\frac{qa}{2}\right), \quad \pi/2a < q < \pi/a, \tag{21}$$

which is shown in Figure 2 as I'. It is also symmetrical to equation (16) about the $q = \pi/2a$ axis.

Next, if we select $A < 0$, $B > 0$ in equation (11) and let the integration constant $D = B^2/2 \mid A \mid C$, we find from the integration of equation (11) a new type of envelope moving mode

$$v_n(t) = \pm\sqrt{\frac{B}{C}} \tanh\left[\frac{\sqrt{2 \mid A \mid B}}{C}(na - Vt)\right] \cos(qna - \omega t). \tag{22}$$

This right-moving kink-envelope mode can exist when ω and q are restricted to the region (shown in Fig. 1 as II)

$$k_2 \sin^2(qa)/m \cos(qa) < \omega^2 < \infty, \quad 0 < q < \pi/2a. \tag{23}$$

Its velocity domain (shown in Fig. 2 as II) is

$$0 < V < \nu\sqrt{\cos(qa)}, \quad 0 < q < \pi/2a. \tag{24}$$

Also for rather large wavevectors we have a left-moving kink envelope solution similar to equation (22), and the ranges of ω, V and q are totally symmetrical with equations (23, 24) about the $q = \pi/2a$ axis both in the $\omega(q)$ and $V(q)$ planes (shown as II' in both Figs. 1 and 2). The velocities of this new type of kink-envelope moving mode are also subsonic.

Finally, we consider the case of wavevector $q = 0$. From equations (14, 23) the vibrational frequency should be $\omega \sim 0$. In this case the carrier wave disappears and the problem must be analyzed by a direct long-wave approximation (see, *e.g.*, an early review article [17] and the references therein). If we keep the continuum expansion (8) up to the fourth order and insert it into the equation of motion (2), the well-known modified Korteweg-deVries (mKdV) equation can be obtained [18]. Also, truncating the Taylor expansion of the particle interaction potential to the third order will result in the KdV equation. Generally, the solutions of these two equations are solitons. These solitons of such elastic waves are therefore a special case of the general nonlinear discrete lattice wave, although KdV and mKdV are integrable [17,18] while the discrete lattice is not.

4 Numerical results

In order to test the validity of the approximate analytical solutions obtained in the last section, we numerically integrated equations (2, 4) by means of the general finite-difference scheme with a time step $\Delta t = 0.02$. In the simulation, the lattice spacing, the harmonic force constant and the mass of the particles are all set equal to unity for simplicity, and periodic boundary conditions are used. The simulations typically last at least one hundred periods of the carrier wave and run over more than 400 lattice sites in order to observe the long term stability, where the scheme includes a strategy for adjusting the calculation stepsize to keep the relative and absolute error below 10^{-4} and 10^{-3}, respectively.

Figure 3 shows the simulation results with solution (15) ($t = 0$) as input, where the anharmonic constant k_4 equals 1.5. In part (a), for the right-moving pulse-envelope mode the two fundamental parameters q and ω are restricted to region I of Figure 1, *i.e.*, governed by inequality (14). For the left-moving pulse-envelope mode in part (b) the vibrational frequency is the same as in part (a), but with wavevectors $\pi/a - q$. This choice implies that the two parameters are restricted to region I' of Figure 1. When q and ω are chosen, the constants A, B, C, E, F and G are determined by equations (12, 19), respectively. In Figure 3 we see some characteristic features of the numerical results for the moving pulse-envelope modes. The faint ripples in the rear side of the modes eventually run away, leading to a stable and uniformly right- or left-moving localized mode whose profile is slightly modified from that of the input mode. The existence of the long-lived moving nonlinear localized modes ensures the validity of the approximate analytical theory, at least qualitatively.

Figure 4 shows the simulation results with solution (22) ($t = 0$) as input, where the anharmonic constant is the same as in Figure 3. Similar to Figure 3, for the right- and left-moving kink-envelope modes the two parameters q and ω are restricted to regions II (part (a)) and II' (part (b)) of Figure 1, respectively. We also observe a stable and uniformly right- and left-moving kink-envelope mode whose profile is slightly changed from the input. The ripple radiation from the modes cannot be seen.

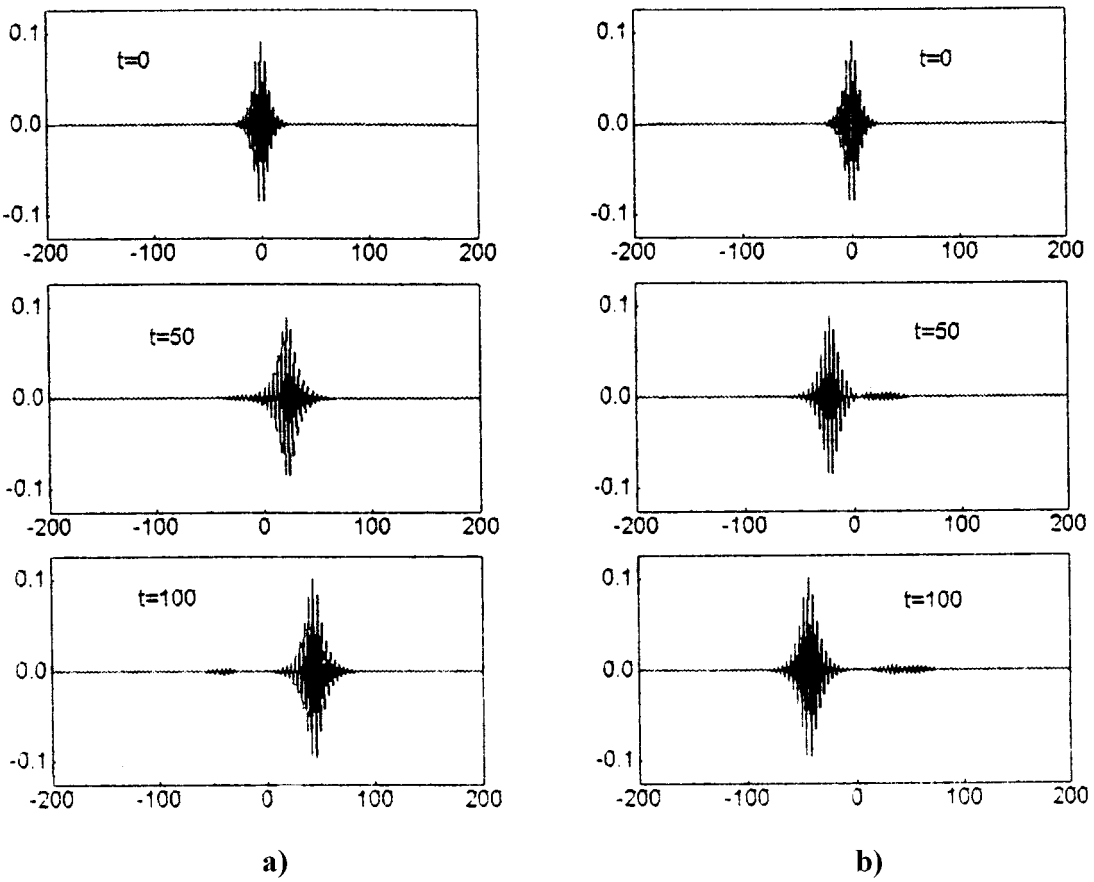

Fig. 3. Space-time evolution of the particle displacements with equation (14) as input. The two parameters q and ω are restricted to region I of Figure 1 for right-moving pulse-envelope mode (shown in part (a)) and to region I' for left-moving pulse-envelope mode (shown in part (b)), respectively.

It may be covered by the kink modes. This result is also in agreement with the theoretical prediction. This new type of kink-envelope moving mode has not been reported previously in either theoretical or numerical works.

5 Discussions and conclusions

As is known, the equation of motion for a lattice is a second order differential equation. Its solution contains two undetermined parameters. Physically, these two fundamental parameters are wavevector q and vibrational frequency ω. In the linear lattice case, the dispersion is a curve in the $\omega(q)$ plane, and there is a one-to-one relationship between q and ω. However, in the nonlinear case the vibrational frequency depends on both the wavevector and the vibrational amplitude, and vibrational modes can appear in different areas of the $\omega(q)$ plane. For the lattice model considered in this work, the whole $\omega(q)$ plane can principally provide moving modes except for an empty area described by the relations $0 < \omega^2 < 4k_2 \sin^2(\frac{qa}{2})/m$ $(0 < q < \pi/2a)$ and $0 < \omega^2 < 4k_2 \cos^2(\frac{qa}{2})/m$ $(\pi/2a < q < \pi/a)$. That is to say, when q is determined, the vibrational frequency ω is above the corresponding linear frequency but not necessarily above the maximum linear frequency. This situation is in marked contrast to the case of stationary nonlinear localized modes [4–6] which can appear only above the maximum linear frequency.

For the pulse-envelope type modes, from the analytical expression (15), we know that the width of the envelope pulse is $\sim \sqrt{A/B}$, so it can be small enough to involve only a few lattice spacings with some appropriate values of ω and q. This case corresponds to the highly localized modes in references [2,3]. Generally, the width of an envelope pulse is much larger than the lattice spacing and many particles are involved in the local vibration forming a long wavelength characteristic envelope. Moreover, from equations (14, 20) (also see Figs. 1, 2) we can see that the range of the wavevector becomes narrower near $q \sim \pi/2a$ and the moving velocity becomes smaller as the vibrational frequency increases. This result is in good agreement with previous numerical simulations [8,9] and it is quite reasonable to neglect the term $\mathrm{d}^2\phi/\mathrm{d}t^2 \sim o(V^2)$ in the high vibrational frequency case. For the kink-envelope type of moving modes, however, the range of q becomes wider as ω increases. Previous numerical work [8] did not find this type of solution because of its neglect of the second time differential term in equation (7),

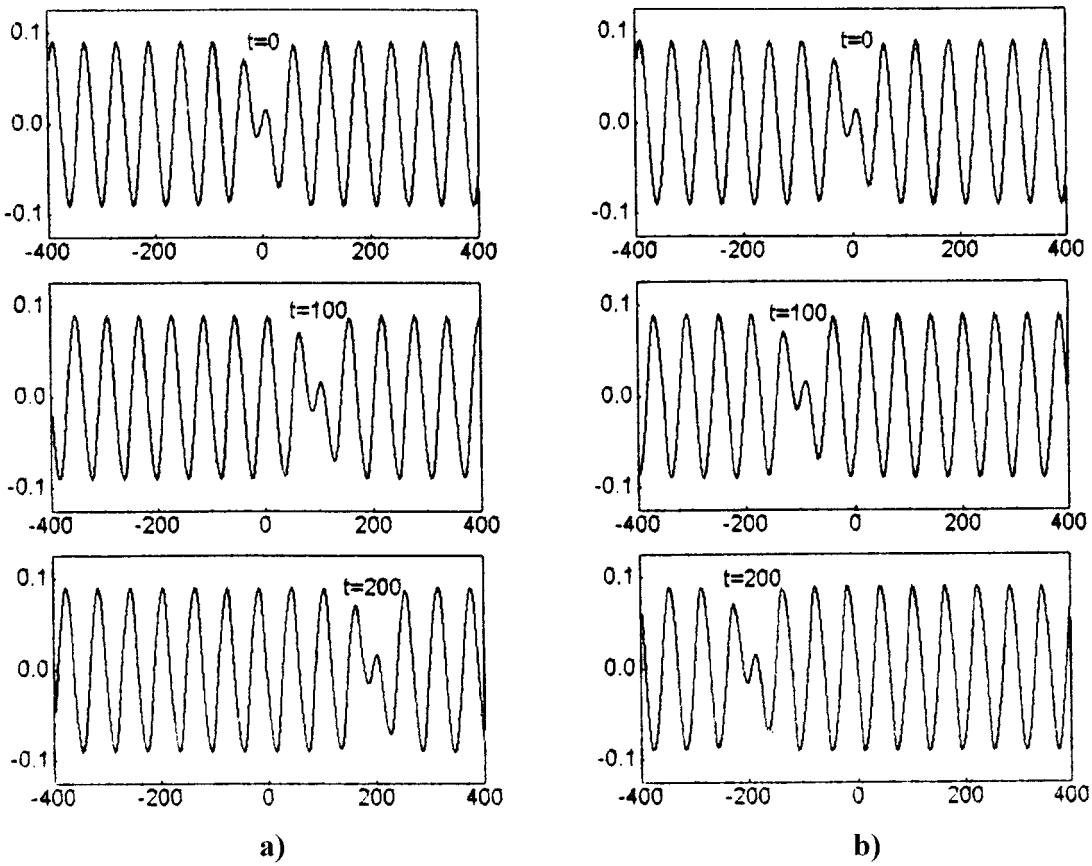

Fig. 4. Space-time evolution of the particle displacements with equation (21) as input, the two parameters q and ω are restricted to region II of Figure 1 for a right-moving kink-envelope mode (shown in part (a)) and to region II' for a left-moving kink-envelope mode (shown in part (b)), respectively.

leading to an initial pulse-like profile as input. The previous analytical studies did not find this type of solution either. The reason may be that in the multiple-scale expansions only the main component is considered [12,13] and the equation of motion is directly reduced to a nonlinear Schrödinger equation with bright-soliton (pulse-like envelope) solutions only. However, because the carrier-wave phase varies very fast, the change of sign for the kink-envelope function is meaningless when $na = x \to \pm\infty$. If the second or higher order components in the multiple-scale expansions are considered, a nonlinear Schrödinger equation with both bright- and dark-soliton solutions (kink-like envelope) may be obtained. Therefore, this kink-envelope type of solution may correspond to the dark-soliton solution of the nonlinear Schrödinger equation of previous analytical works [12,13], at least approximately. Therefore, our analytical results are quite general and contain all kinds of existing localized modes for this simple nonlinear lattice system. Although the RWA and continuum approximations will bring some inaccuracy in our approach (*e.g.*, numerically observed faint ripples in Fig. 3), the analytical results are qualitatively correct and suitable for such a lattice system.

On the boundary lines of different regions in the $\omega(q)$ plane, all constants in equations (11, 18) tend to zero. In this critical case the solutions may be trivial or imply a structural phase transition, or even show chaotic behavior because of the instability [19,20]. It is worth mentioning that our results, like the analytical expressions for both moving [10,13] and stationary [4–6] modes, do not have a simple limit for a vanishing nonlinear term in the system. However, from the elliptic function equations (11, 18) we can see, if $C(\sim k_4) \sim 0$, that both ϕ and ψ will be exponentially divergent. The real situation should then be that the system possesses the discrete plane-wave solution. Moreover, if the third term of the Taylor series of the potential is added to equation (2), the pulse-envelope solutions will be distorted by a kink [8,21]. The change of the kink-envelope solution itself is still unknown in this case.

In conclusion, we have solved analytically the quartic anharmonic one-dimensional lattice equation by means of a semi-discrete continuum approximation. Two different types of moving modes are found for such a lattice system. The pulse-envelope moving modes found in this paper are similar to those in both the analytical and numerical references. The kink-envelope moving modes have not been reported previously. Both seem physically reasonable. The two types of moving modes occur with different carrier wavevectors and frequencies in separate parts of the $\omega(q)$

plane. The velocities of the two types of moving modes are both subsonic. The numerical simulations support our analytical results quite well. Although some results in this paper appeared previously and might be well-known, and the method used is very simple and direct, we believe that this research provides some systematical information and that it will be useful for solving other nonlinear lattice systems.

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