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MOVING NONLINEAR LOCALIZED MODES FOR ONE-DIMENSIONAL KLEIN–GORDON DIATOMIC LATTICE*

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We study analytically the moving nonlinear localized vibrational modes (discrete breathers) for a one-dimensional Klein–Gordon diatomic lattice in the whole $\omega(q)$ plane of the system by means of a semi-discrete approximation, in which the carrier wave of the modes is treated explicitly while the envelope is described in the continuum approximation. We find that both pulse and kink envelope moving modes for this lattice system can occur with certain carrier wave vectors and vibrational frequencies in separate regions of the $\omega(q)$ plane. However, the kink envelope moving modes have not been reported previously for this lattice system.

Keywords: diatomic lattice, localized modes, semi-discrete approximation
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I. INTRODUCTION

Since some important properties of solids may mainly or partly depend on crystal anharmonicity, the nonlinear localized vibrational modes (or discrete breathers) induced by the anharmonicity in a perfect crystal lattice have been extensively studied during the past decade.[1] These intrinsic localized modes typically involve sizable amplitudes on only a few lattice sites with either odd[2] or even[3] symmetry distribution forms in the highly discrete and sufficiently strong anharmonicity case. But generally more particles are involved in the local vibration with a form of characteristic long wavelength envelope.[4] Quantum mechanically, this intrinsic localized mode is a kind of phonon bound state.

As is known, impurity vibrational modes are centred only on the defect sites of lattices. In contrast, in perfect crystal lattices the centre of a nonlinear localized mode may appear at any lattice site because of the translational invariance of these lattices. Therefore, it is believed that the anharmonicity of perfect lattices should support moving nonlinear localized modes. For a nonlinear diatomic lattice, however, most of the research on this subject has concentrated on stationary solutions.[5–9] Numerical simulations for the diatomic lattice with some nearest-neighbour interaction two-body potentials have been performed,[10,11] but only the pulse envelope moving modes were found. The lattice Green's function technique[2,3] which treats the whole question discretely was applied to an anharmonic diatomic lattice for seeking moving nonlinear localized modes.[12] Later, the multiple-scale method has also been used to study moving nonlinear localized modes for the diatomic lattice with different types of anharmonicity,[13–14] but the calculation is somewhat tedious and only the main component has been considered. However, in each of these two theoretical methods, it is impossible to consider all of the possible solutions over the whole $\omega(q)$ plane of the system. Also, these authors[12–14] have not reported the kink envelope moving localized modes for this lattice system. Recently, we used a simple and direct analytical method[15] to study a one-dimensional Klein–Gordon monatomic lattice. In this paper, we extend the work of Ref.[15], applying this method to a Klein–Gordon diatomic lattice system, and some new results are found. We treat the discrete equation of motion for a Klein–Gordon diatomic lattice by means of a semi-discrete approximation, in which the discreteness of the carrier wave of modes is treated explicitly while the envelope function is described in the continuum approximation. The equation of motion reduces to an elliptic integration, and then its possible solutions are considered in the whole $\omega(q)$ plane by using the wave vector and the vibrational frequency as the two

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fundamental parameters. In addition to the pulse envelope type of moving nonlinear modes (sech function) which appears in Refs.[5–9] in its stationary form and Refs.[10–14] in its moving form, we find that the kink envelope type of moving nonlinear modes (tanh function) can also exist with certain wave vectors and vibrational frequencies in the separate regions of the $\omega(q)$ plane of the system. However, this kink envelope type of solution, 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 II we formulate the lattice equation of motion to an integrable system by means of the semi-discrete approximation. Then, in section III, we analytically obtain all possible solutions over the whole $\omega(q)$ plane for the system, and in section IV we discuss the results and conclude the paper.

II. FORMULISM OF THE MODEL

We consider a one-dimensional Klein–Gordon diatomic lattice. By denoting the displacement of the particle (molecule, atom or ion) n from its equilibrium position as $r_n(t)$, then the Hamiltonian of the system is given by

$$H = \sum_n \left[\frac{1}{2} m_n \left(\frac{\mathrm{d}r_n}{\mathrm{d}t} \right)^2 + \frac{k}{2}(r_n - r_{n-1})^2 - \left(\frac{\alpha}{2} r_n^2 - \frac{\beta}{4} r_n^4 \right) \right] . \quad (1)$$

This is a one-dimensional chain with light $m_n = m$ $(n = 2j)$ and heavy $m_n = M > m$ $(n = 2j+1)$ masses alternatively placed, harmonically coupled with their nearest neighbours, and subjected to a symmetry nonlinear substrate potential. Therefore, its classical equation of motion reads

$$m\ddot{u}_n = k(v_{n+1} + v_{n-1} - 2u_n) - \alpha u_n + \beta u_n^3,$$

$$M\ddot{v}_n = k(u_{n+1} + u_{n-1} - 2v_n) - \alpha v_n + \beta v_n^3; \quad (2)$$

where $u_n(v_n)$ is the longitudinal displacement from the equilibrium position of the light (heavy) atom, k is the harmonic coupling constant, $\sqrt{\alpha/m}$ is the frequency of small-amplitude onsite vibrations in the substrate potential, and β (positive or negative) is the anharmonic parameter of the potential. Although this model is a simple one, it is related to some realistic physical system. For example, the third term in Hamiltonian (1) can be interpreted as an external field applied to the harmonic lattice system. Furthermore, in the first crude approximation, in hydrogen-bonded systems the effects of the motion of the negative ion on the proton sublattice can be represented by an appropriate substrate potential, or simply by the Klein–Gordon model.[9] On the other hand, the Klein–Gordon model may also be considered as a small-amplitude expansion of the well-known sine–Gordon model, and numerous physical applications of these two models have been widely discussed in the literature (see, for example, Ref.[16] and references therein).

The linear oscillations of the considered lattice with frequency ω and wave vector q are described by the dispersion law

$$\omega_\pm^2 = \frac{1}{2mM}[(\alpha + 2k)(m + M) \pm \sqrt{(\alpha + 2k)^2(M - m)^2 + 16k^2 mM \cos^2(qa)}] , \quad (3)$$

where a is the lattice spacing. Following from Eq.(3), the linear spectrum of the system has two branches with gaps of $(0, \omega_0)$ and (ω_1, ω_2), and it is limited by a cut-off frequency ω_m due to the discreteness of the system. These four characteristic frequencies are

$$\omega_0^2 \simeq 2\alpha/(m + M) , \quad \omega_1^2 = (\alpha + 2k)/M,$$

$$\omega_2^2 = (\alpha + 2k)/m , \quad \omega_m^2 \simeq (2\alpha + 4k)/(m + M) . \quad (4)$$

An analytical solution to the equation of motion for a nonlinear system (2), giving a moving nonlinear localized mode, is sought by setting[10]

$$u_n(t) = \phi_n(t)\cos(qna - \omega t),$$

$$v_n(t) = \psi_n(t)\cos(qna - \omega t); \quad (5)$$

where $\phi_n(t)$ and $\psi_n(t)$ are the envelope functions of the light and heavy atom respectively, and $\cos(qna - \omega t)$ is a right-moving carrier wave with a rapidly varying phase. Inserting Eq.(5) into Eq.(2) and using the rotating wave approximation (RWA)[5,6,17] to remove high-frequency harmonics, we obtain a group of coupled equations. To satisfy at all times the solution represented by Eq.(5), the coefficient of both the in-phase and out-of-phase oscillatory terms must independently sum to zero. Then equating the sine terms gives

$$2m\omega\dot{\phi_n} = k\sin(qa)(\psi_{n-1} - \psi_{n+1}),$$

$$2M\omega\dot{\psi_n} = k\sin(qa)(\phi_{n-1} - \phi_{n+1}); \quad (6)$$

and cosine terms

$$m\ddot{\phi_n} - m\omega^2\phi_n = k[(\psi_{n+1} + \psi_{n-1}) \cdot \cos(qa) - 2\phi_n] - \alpha\phi_n + \frac{3\beta}{4}\phi_n^3,$$

$$M\ddot{\psi_n} - M\omega^2\psi_n = k[(\phi_{n+1} + \phi_{n-1}) \cdot \cos(qa) - 2\psi_n] - \alpha\psi_n + \frac{3\beta}{4}\psi_n^3 . \quad (7)$$

Note that for the wave vectors near the Brillouin-zone boundaries of $q = \pm\pi/a$, from Eq.(6) we can see that both ϕ_n and ψ_n are independent of time, and Eq.(7) reduces to the previously determined eigenvalue equation, giving the eigenfrequency and eigenfunction of the stationary modes[5,9] for the same lattice model. The correction to the RWA was found[17] to be only a few per cent and the amplitude response from the high-frequency components can be ignored. This approximation method of analysis is sufficient to separate the equation of motion for lattice systems.

It seems that exact solutions of the set of differential–difference equations (6) and (7) do not exist. But a fairly good approximate analytical solution can be obtained on the assumption that the space variation of the envelope function is small compared to that of the carrier wave, and the characteristic wavelength of the envelope is much greater than the lattice spacing a. In fact, this situation is mostly the real case. Thus, in this paper we make a continuum approximation ($na \to x$) for the envelope function

$$\phi_{n\pm1} = \phi \pm 2a\phi_x + 2a^2\phi_{xx} + ...,$$

$$\psi_{n\pm1} = \psi \pm 2a\psi_x + 2a^2\phi_{xx} + ... \quad (8)$$

Introducing a new variable $\xi = x - Vt$ and inserting it into Eq.(6) with Eq.(8), we obtain the group velocity of the two envelopes

$$V = \frac{2ak\sin(qa)}{\sqrt{mM}\omega} , \quad (9)$$

and the relation for the two envelope functions of $\psi = \sqrt{m/M}\phi$. At the same time, under the expansion of Eq.(8) we can integrate Eq.(7) once. Therefore, we have a new set of equations for the system

$$\left(\frac{\mathrm{d}\phi}{\mathrm{d}\xi}\right)^2 = \frac{B}{A}\phi^2 + \frac{3\beta}{8A}\phi^4 + C,$$

$$\left(\frac{\mathrm{d}\psi}{\mathrm{d}\xi}\right)^2 = \frac{B'}{A'}\psi^2 + \frac{3\beta}{8A'}\psi^4 + C'; \quad (10)$$

where

$$A = mV^2 - 4a^2k\sqrt{m/M}\cos(qa) ,$$

$$B = m\omega^2 - 2k\Big[1 - \sqrt{m/M}\cos(qa) - \alpha\Big],$$

$$A' = MV^2 - 4a^2k\sqrt{M/m}\cos(qa) ,$$

$$B' = M\omega^2 - 2k\Big[1 - \sqrt{M/m}\cos(qa)\Big] - \alpha \quad (11)$$

are constants dependent on the two fundamental parameters of vibrational frequency ω and the wave vector q, with C and C' being the integration constants. Until now, the equation of motion for the lattice system has been reduced to a single integration expressible in terms of elliptic functions.

Ⅲ. POSSIBLE MOVING MODES

In this section, we use the properties of such integrations to analyse Eq.(10) with possible choices for the constants in Eq.(11), and to obtain analytical solutions for the system.

We have to select the integration constants $C = C' = 0$ in Eq.(10) if we are restrict ourselves to the pulse envelope solutions. The harmonic coupling constant k is always positive, then in the case of self-focusing nonlinearity ($\beta > 0$) the constants in Eq.(11) must be $A, B, A', B' < 0$ simultaneously. These four inequalities together with Eq.(9) encircle a region in the $\omega(q)$ plane

$$\frac{k\sin^2(qa)}{\sqrt{mM}\cos(qa)} < \omega^2 < \frac{2k\Big[1 - \sqrt{M/m}\cos(qa)\Big] + \alpha}{M}, \quad 0 < q < q^*, \quad (12)$$

where

$$q^* = \cos^{-1}\Big(\Big[(2k+\alpha)\sqrt{mM} - \sqrt{mM(2k+\alpha)^2 - 4k^2M^2}\Big]/2kM\Big),$$

which is determined from the first inequality in Eq.(12). Within this region the two envelope functions can be obtained by integrating Eq.(10)

$$\phi(x,t) = \sqrt{\frac{8 \mid B \mid}{3\beta}}\mathrm{sech}\left[\sqrt{\frac{B}{A}}(qna - Vt)\right],$$

$$\psi(x,t) = \sqrt{\frac{8 \mid B' \mid}{3\beta}}\mathrm{sech}\left[\sqrt{\frac{B'}{A'}}(qna - Vt)\right]; \quad (13)$$

where A, B, A' and B' defined by Eq.(11) are functions of ω and q under the restriction of Eq.(12), and the continuous space variable has been replaced by the discrete one. This moving pulse envelope was obtained previously in both numerical[10,11] and

analytical[12−14] works for the same or similar lattice systems.

If we let $C = 2B^2/3A, C' = 2B'^2/3A', A > 0$, $B < 0$, $A' > 0$ and $B' < 0$ in Eq.(10), we have a kink (anti-kink) envelope solution from the integration of Eq.(10)

$$\phi(x,t) = \pm\sqrt{\frac{4\mid B\mid}{3\beta}}\tanh\left[\sqrt{\frac{\mid B\mid}{2A}}(qna - Vt)\right],$$

$$\psi(x,t) = \pm\sqrt{\frac{4\mid B'\mid}{3\beta}}\tanh\left[\sqrt{\frac{\mid B'\mid}{2A}}(qna - Vt)\right]. \tag{14}$$

where the plus (minus) sign corresponds to the case of kink (anti-kink). This new type of moving kink envelope solution has not been reported previously. The restriction condition of the four inequalities for A, B, A' and B' encircle another region in $\omega(q)$ plane, which is described by

$$0 < \omega^2 < \frac{k\sin^2(qa)}{\sqrt{mM}\cos(qa)}, \quad 0 < q < q^*,$$

$$0 < \omega^2 < \frac{2k\left[1 - \sqrt{M/m}\cos(qa)\right] + \alpha}{M}, \quad q^* < q < \pi/2a\ . \tag{15}$$

The envelopes of Eqs.(13) and (14) multiplying a factor of carrier wave [see Eq.(5)] constitute the two types of moving nonlinear localized modes, respectively. We can see that the vibrational frequencies in the regions described by Eqs.(12) and (15) may cover the lower linear frequency forbidden gap $(0, \omega_0)$ because of the nonlinear effect of the system.

Next, we consider the case of defocusing nonlinear $\beta < 0$. When the parameters of Eq.(11) satisfy some suitable conditions, there also exist two types of envelope moving nonlinear localized modes for the system. The pulse envelope moving mode similar to Eq.(13) exists in the region

$$\frac{2k\left[1 - \sqrt{m/M}\cos(qa)\right] + \alpha}{m} < \omega^2 < \frac{k\sin^2(qa)}{\sqrt{mM}\cos(qa)}, \quad q^{**} < q < \frac{\pi}{2a}, \tag{16}$$

where

$$q^{**} = \cos^{-1}\left(\left[2k + \alpha)\sqrt{mM} - \sqrt{mM(2k+\alpha)^2 - 4k^2m^2}\right]/2km\right),$$

which is determined from the first inequality of Eq.(16). Meanwhile, the kink envelope mode similar to Eq.(14) exists in the region

$$\frac{2k\left[1 - \sqrt{m/M}\cos(qa)\right] + \alpha}{m} < \omega^2 < \infty, \quad 0 < q < q^{**},$$

$$\frac{k\sin^2(qa)}{\sqrt{mM}\cos(qa)} < \omega^2 < \infty, \quad q^{**} < q < \pi/2a\ . \tag{17}$$

From Eqs.(16) and (17) we can also see that the nonlinear vibrational frequencies may cover the gap (ω_1, ω_2) or over cut-off frequency ω_m of the linear spectrum due to the nonlinear effect of the system.

It is worth pointing out that whether the sign of the nonlinear parameter β is positive or negative, and whatever the ranges of ω and q are, it is not possible for Eq.(10) to have the solution with one envelope being pulse and the other kink. This situation is different from the stationary nonlinear localized modes for the same lattice model[5,9] or similar lattice model.[6−8] Moreover, following our previous method,[15] we can also describe the four corresponding regions in the $V(q)$ plane which determine the velocities of the different types of envelope moving modes. Our resulting Eqs.(13) and (14), like the analytical expressions for both stationary[5,6,9] and moving[12−14] modes, do not have a simple limit for vanishing the nonlinear term in the system. From Eq.(10) we can see, that if $\beta \sim 0$, both ϕ and ψ will be exponentially divergent. However, the real case should then be that the system possesses a discrete plane wave solution.

IV. DISCUSSION AND CONCLUSION

As is well-known, the equation of motion for a lattice is a second-order differential equation, and its solution contains two undetermined parameters. Physically, these two fundamental parameters are the wave vector q and the 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 relation between q and ω. In contrast, in the nonlinear case the vibrational frequency depends on both the wave vector and the vibrational amplitude, and vibrational modes can appear in regions of the $\omega(q)$ plane. For the lattice model considered in this paper, the whole $\omega(q)$ plane can principally provide moving nonlinear localized modes. When q is determined, the vibrational frequency of the modes can lie in both the linear phonon band and the gap. This situation is in marked contrast to the case

of stationary nonlinear localized modes[5−9] which appear only in the gap of the linear spectrum. However, the stationary localized mode of the wave vector at the Brillouin boundary as a special case of moving localized modes is more stable.

Also, the equation of motion for a one-dimensional lattice with cubic nonlinearity relates to[4,12−14] a nonlinear Schrödinger equation. The pulse envelope moving mode is the bright-soliton solution of this nonlinear Schrödinger equation. From Eqs.(11)–(13) we know that the width of the envelope pulse is $\sim \sqrt{A/B}$ and can be small enough to involve only a few lattice sites with some appropriate values of ω and q, and this case corresponds to the case of highly localized modes.[8] Generally, the width of an envelope pulse is much larger than the lattice spacing and many atoms involved in the local vibration form an envelope of a characteristically long wavelength. Meanwhile, the kink envelope moving localized mode can be identified to the dark-soliton solution of the Schrödinger equation. Thus, nonlinear localized modes in a perfect crystal lattice have been reviewed as discrete breathers.[1]

The idea of intrinsic localized modes in an anharmonic lattice can be applied to explain[2] the phenomenon of the anomalous low-temperature specific heat of glasses, solid ^{3}He and ^{4}He. Furthermore, as a kind of elementary excitation, nonlinear localized modes may provide a new mechanism of scattering for electrons in crystals[18] and will arouse research interest in condensed matter theory.

In conclusion, we have solved analytically the equation of motion for a one-dimensional Klein–Gordon diatomic lattice by means of a semi-discrete approximation. Two different types of envelope moving nonlinear localized modes are found in separate regions of the $\omega(q)$ plane for such a lattice system. The pulse envelope moving modes found in this paper are in agreement with previous works,[10−14] and the kink envelope moving mode which has been not reported previously seems physically reasonable. The method used in this paper is very simple and direct, and we believe that such research will provide some systematic information and a useful route for solving other nonlinear lattice systems.

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