Asymmetric gap soliton modes in diatomic lattices with cubic and quartic nonlinearity

Guoxiang Huang
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany;
Center for Nonlinear Studies and Department of Physics, Hong Kong Baptist University, Hong Kong, China;
and Department of Physics, East China Normal University, Shanghai 200062, China

Bambi Hu
Center for Nonlinear Studies and Department of Physics, Hong Kong Baptist University, Hong Kong, China
and Department of Physics, University of Houston, Houston, Texas 77204
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Nonlinear localized excitations in one-dimensional diatomic lattices with cubic and quartic nonlinearity are considered analytically by a quasidiscreteness approach. The criteria for the occurrence of asymmetric gap solitons (with vibrating frequency lying in the gap of phonon bands) and small-amplitude, asymmetric intrinsic localized modes (with the vibrating frequency being above all the phonon bands) are obtained explicitly based on the modulational instabilities of corresponding linear lattice plane waves. The expressions of particle displacement for all these nonlinear localized excitations are also given. The result is applied to standard two-body potentials of the Toda, Born-Mayer-Coulomb, Lennard-Jones, and Morse type. The comparison with previous numerical study of the anharmonic gap modes in diatomic lattices for the standard two-body potentials is made and good agreement is found. [S0163-1829(98)03410-9]

I. INTRODUCTION

The study of the dynamics of nonlinear lattices and related solitonic excitations has been greatly influenced by the pioneering works of Fermi, Pasta, and Ulam,[1] and of Zabusky and Kruskal.[2] Most of the work in this area has focused on models of one-dimensional (1D) monatomic chains with simple interatomic potentials of polynomials,[3–7] which can approximate any realistic potential near the equilibrium separation distance of two atoms. This description, usually done in a continuum limit, is only valid for a zone-boundary phonon mode, i.e., for q, the wave number of lattice waves, being near zero or π/d_0, where d_0 is lattice spacing. In 1972, Tsurui[8] proposed an analytical method for studying the nonlinear excitations of lattices valid in the whole Brillouin zone (BZ). Later on this approach was extended by Remoissenet[9] and Huang.[10,11] Exact analytical solutions for the nonlinear localized excitations in 1D monatomic lattices can be obtained only for the Toda[12] and Ablowitz and Ladik[13] lattices, which are discrete completely integrable systems.

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.[10,14–23] These modes, called the intrinsic localized modes (ILM's),[15] or the discrete breathers,[23] are the discrete analog of the envelope (or breather) solitons with their spatial extension being only of a few lattice spacing and the vibrating frequency lying above the upper cutoff of phonon bands.[24] Experimentally, the ILM's have been observed in coupled pendulum lattices[25] and electrical lattices.[26] The quantum-mechanical aspects of the ILM's have also been considered.[27–29] However, examination of the 1D lattices with standard Toda, Born-Mayer-Coulumb, Lennard-Jones, and Morse two-body interatomic potentials demonstrates that the ILM's do not appear above the top of the plane-wave spectrum. The physical reason for this is that the cubic nonlinearity in the Taylor expansion of these realistic potentials is too strong. One of the effects of the cubic nonlinearity is that increasing the magnitude of the cubic term makes the potentials softer and hence decreases the localized mode frequency. The localized mode is destroyed as it approaches the bounding plane-wave spectrum.[10,30]

Recently, much attention has been paid to the gap solitons in nonlinear diatomic lattices.[11,27,31–41] The concept of the gap solitons was introduced by Chen and Mills[42] when investigating the nonlinear optical response of superlattices. For a diatomic lattice, the phonon spectrum of the system consists of two branches (acoustic and optical ones), induced by mass or force-constant difference of two kinds of particles. Due to nonlinearity gap soliton modes may appear as localized excitations with vibrating frequency being in the gap of the linear spectrum. Since the gap solitons occur in perfect lattices with discrete translational symmetry, a name ''anharmonic gap mode'' or ''intrinsic gap mode (IGM)'' was given by Sievers and his collaborators.[33,34,41] It is possible that the ILM's and the IGM's may be created experimentally in diatomic lattices. References 43 and 44 reported some experimental studies of the gap solitons, resonant kinks, and the ILM's in a damped and parametrically excited 1D diatomic pendulum lattices.

Since the standard two-body potentials of the Toda, Born-Mayer-Coulomb, Lennard-Jones, and Morse type have a strong cubic nonlinearity in their Taylor expansion near equilibrium position, it is therefore necessary to consider the nonlinear excitations in the diatomic lattices with cubic and quartic anharmoniticity. In their recent contributions, Kiselev *et al.*[33,34] investigated the anharmonic localized modes in 1D diatomic lattices with the above-mentioned two-body potentials. By using a rotating-wave approximation combined with computer simulation, they showed that an ILM does *not* exist and a nonlinear optical lower cutoff gap mode (i.e., IGM) is a general feature of these diatomic lattices. Lately, Franchini *et al.*[35] numerically found that for a potential with the cubic and quartic nonlinearity there exists a ''critical'' K_3 (cubic force constant in the potential) value. For small K_3, nonlinear optical and acoustic upper cutoff localized modes occur, while for large K_3 these modes disappear and a nonlinear optical lower cutoff mode rises. In a recent work, Bonart *et al.*[45] investigated the boundary condition effects in the diatomic lattices with cubic and quartic anharmonicity. Based on a rotating-wave approximation they gave existence criteria for the ILM's and IGM's, which are related to the stability properties of linear optical upper and lower cutoff phonon modes. These studies posed an interesting problem of how to provide an analytical approach which can give not only the explicit criteria for the existence of the ILM's and the IGM's as well as other possible nonlinear excitations for both optical and acoustic branches but also the approximate analytical expressions for these nonlinear excitations in a unified way. It is this problem that will be addressed here.

There are several theoretical methods to study the nonlinear localized excitations in diatomic lattices (see Ref. 11, and references therein). In this paper we use the quasidiscreteness approach (QDA) for diatomic lattices[11] to investigate the ILM's and IGM's as well as kinklike excitations with small amplitude in 1D diatomic lattices with cubic and quartic nonlinear interactions between their nearest-neighbor particles. The paper is organized as follows. In Sec. II, the model is introduced and an asymptotic expansion based on the QDA is made for the equations of motion. By using the results obtained in Sec. II, in Sec. III we discuss the solutions of the ILM's and IGM's in a simple and unified way. Some explicit criteria and expressions of particle displacement of the ILM's and the IGM's are also given in this section. In Sec. IV we apply our results to the standard two-body potentials from the Toda to the Morse type and make a comparison with existing numerical experiments. Finally, Sec. V contains a discussion and summary of our results.

II. MODEL AND ASYMPTOTIC EXPANSION

A. The model

We consider a 1D diatomic lattices with a nearest-neighbor interaction between particles. The restriction to the nearest-neighbor interaction is for simplicity and the approach can be easily extended to second and higher neighbors. The Hamiltonian of the system is given by

$$H=\sum_i \left[\frac{1}{2}m_i\left(\frac{du_i}{dt}\right)^2+V(u_{i+1}-u_i)\right], \tag{1}$$

where $u_i=u_i(t)$ is the displacement from its equilibrium position of the ith particle with mass $m_i=m\delta_{i,2k}+M\delta_{i,2k+1}$ ($M>m,k$ is an integer). The potential $V(r)$ is quite general, typically it can be the standard two-body potentials of the Toda, Born-Mayer-Coulomb, Lennard-Jones, and Morse type (for their detailed expressions, see Sec. IV below). We focus on displacements with smaller amplitude which can be detected experimentally without introducing reconstruction or phase transitions in the system. This allows us to Tayler expand the potential $V(r)$ at the equilibrium position $r=0$ in a power series of the displacements to fourth order.[35] Thus we obtain an approximate K_2-K_3-K_4 potential

$$V(r)=\frac{1}{2}K_2r^2+\frac{1}{3}K_3r^3+\frac{1}{4}K_4r^4, \tag{2}$$

where $K_2(>0)$, K_3 and $K_4(>0)$ are harmonic, cubic, and quartic force constants, respectively. We assume that the basic features of the weakly nonlinear localized excitations for the standard two-body potentials may be obtained by corresponding the K_2-K_3-K_4 potentials. Then the Hamiltonian (1) takes the following form:

$$H=\sum_i \left[\frac{1}{2}m_i\left(\frac{du_i}{dt}\right)^2+\frac{1}{2}K_2(u_{i+1}-u_i)^2+\frac{1}{3}K_3(u_{i+1}-u_i)^3 + \frac{1}{4}K_4(u_{i+1}-u_i)^4\right]. \tag{3}$$

Since each of the standard two-body potentials mentioned above has only one minimum, we assume that for the K_2-K_3-K_4 potential (2) there is the constraint

$$\frac{K_3^2}{K_2K_4}<4, \tag{4}$$

unless there are two minima (i.e., double-well potential) hence the system may admit some types of nonlinear excitations which will not be discussed here.

If we write $u_{2k}=v_n$ (even particles) and $u_{2k+1}=w_n$ (odd particles), n is the index of the nth unit cell with a lattice spacing $d=2d_0$, d_0 is the equilibrium distance between two adjacent particles, the system can be split into two sublattices. The equations of motion for v_n and w_n are

$$m\frac{d^2}{dt^2}v_n=K_2(w_n+w_{n-1}-2v_n)+K_3[(w_n-v_n)^2 -(w_{n-1}-v_n)^2] +K_4[(w_n-v_n)^3+(w_{n-1}-v_n)^3], \tag{5}$$

$$M\frac{d^2}{dt^2}w_n=K_2(v_n+v_{n+1}-2w_n) -K_3[(v_n-w_n)^2-(v_{n+1}-w_n)^2] +K_4[(v_n-w_n)^3+(v_{n+1}-w_n)^3]. \tag{6}$$

The linear dispersion relation of Eqs. (5) and (6) is

$$\omega_\pm(q)=\left\{I_2+J_2\pm[(I_2+J_2)^2-4I_2J_2\sin^2(qd/2)]^{1/2}\right\}^{1/2}, \tag{7}$$

where $I_2=K_2/m$ and $J_2=K_2/M$. The minus (plus) sign corresponds to acoustic (optical) mode. At wave number $q=0$ the eigenfrequency spectrum has a lower cutoff $\omega_-(0)=0$ for the acoustic mode and an upper cutoff $\omega_+(0)\equiv\omega_3=[2(I_2+J_2)]^{1/2}$ for the optical mode. At $q=\pi/d$ there exists a frequency gap between the upper cutoff of the acoustic branch, $\omega_-(\pi/d)\equiv\omega_1=\sqrt{2J_2}$, and the lower cutoff of the optical branch, $\omega_+(\pi/a)\equiv\sqrt{2I_2}$. The width of the frequency gap is $\sqrt{2I_2}-\sqrt{2J_2}=\sqrt{2K_2}(1/\sqrt{m}-1/\sqrt{M})$. In linear theory, the amplitudes of lattice waves are constants and linear waves cannot propagate and will be damped when ω (the frequency of the waves) lies in the regions $\omega_1<\omega<\omega_2$ and $\omega>\omega_3$. Accordingly, these regions are the ‘‘forbidden bands’’ of the linear waves. This property of the eigenfrequency spectrum results from the discreteness of the system (i.e., discrete translational symmetry). However, when the nonlinearity in Eqs. (5) and (6) is considered, the above conclusions are no longer valid. As localized excitations, some nonlinear modes may appear, whose oscillatory frequencies can lie in these forbidden bands of the phonon spectrum.

B. Asymptotic expansion

We use the QDA for diatomic lattices developed in Ref. 11 to investigate the effects of nonlinearity and discreteness of the system. In this treatment one sets

$$u_n(t)=\epsilon u_{n,n}^{(1)}+\epsilon^2 u_{n,n}^{(2)}+\epsilon^3 u_{n,n}^{(3)}+\cdots, \tag{8}$$

where ϵ is a smallness and ordering parameter denoting the relative amplitude of the excitation and $u_{n,n}^{(\nu)}=u^{(\nu)}(\xi_n,\tau;\phi_n)$. $\xi_n=\epsilon(na-\lambda t)$ and $\tau=\epsilon^2 t$ are two multiple-scales variables (slow variables). λ is a parameter to be determined by a solvability condition. The ‘‘fast’’ variable, $\phi_n=qnd-\omega(q)t$, representing the phase of the carrier wave, is taken to be completely discrete. Substituting Eq. (8) into Eqs. (5) and (6) and comparing the power of ϵ, we obtain a hierarchy of equations about $v_{n,n}^{(j)}$ and $w_{n,n}^{(j)}$ ($j=1,2,3,\ldots$):

$$\frac{\partial^2}{\partial t^2}v_{n,n}^{(j)}-I_2(w_{n,n}^{(j)}+w_{n,n-1}^{(j)}-2v_{n,n}^{(j)})=M_{n,n}^{(j)} \tag{9}$$

with

$$M_{n,n}^{(1)}=0, \tag{10}$$

$$M_{n,n}^{(2)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(1)}-I_2 d\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(1)}+I_3(w_{n,n}^{(1)}-v_{n,n}^{(1)})^2-I_3(w_{n,n-1}^{(1)}-v_{n,n}^{(1)})^2, \tag{11}$$

$$\begin{aligned}M_{n,n}^{(3)}={}&2\lambda\frac{\partial^2}{\partial t\partial\xi_n}v_{n,n}^{(2)}-\left(2\frac{\partial^2}{\partial t\partial\tau}+\lambda^2\frac{\partial^2}{\partial\xi_n^2}\right)v_{n,n}^{(1)}+I_2\left(-d\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(2)}+\frac{d^2}{2!}\frac{\partial^2}{\partial\xi_n^2}w_{n,n-1}^{(1)}\right)+2I_3(w_{n,n}^{(1)}-v_{n,n}^{(1)})(w_{n,n}^{(2)}-v_{n,n}^{(2)})\\&-2I_3(w_{n,n-1}^{(1)}-v_{n,n}^{(1)})\left(w_{n,n-1}^{(2)}-v_{n,n}^{(2)}-d\frac{\partial}{\partial\xi_n}w_{n,n-1}^{(1)}\right)+I_4[(w_{n,n}^{(1)}-v_{n,n}^{(1)})^3+(w_{n,n-1}^{(1)}-v_{n,n}^{(1)})^3],\\&\vdots\ \vdots\end{aligned} \tag{12}$$

and

$$\frac{\partial^2}{\partial t^2}w_{n,n}^{(j)}-J_2(v_{n,n}^{(j)}+v_{n,n+1}^{(j)}-2w_{n,n}^{(j)})=N_{n,n}^{(j)} \tag{13}$$

with

$$N_{n,n}^{(1)}=0, \tag{14}$$

$$N_{n,n}^{(2)}=2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(1)}+J_2 d\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(1)}-J_3(v_{n,n}^{(1)}-w_{n,n}^{(1)})^2+J_3(v_{n,n+1}^{(1)}-w_{n,n}^{(1)})^2, \tag{15}$$

$$\begin{aligned}N_{n,n}^{(3)}={}&2\lambda\frac{\partial^2}{\partial t\partial\xi_n}w_{n,n}^{(2)}-\left(2\frac{\partial^2}{\partial t\partial\tau}+\lambda^2\frac{\partial^2}{\partial\xi_n^2}\right)w_{n,n}^{(1)}+J_2\left(d\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(2)}+\frac{d^2}{2!}\frac{\partial^2}{\partial\xi_n^2}v_{n,n+1}^{(1)}\right)-2J_3(v_{n,n}^{(1)}-w_{n,n}^{(1)})(v_{n,n}^{(2)}-w_{n,n}^{(2)})\\&+2J_3(v_{n,n+1}^{(1)}-w_{n,n}^{(1)})\left(v_{n,n+1}^{(2)}-w_{n,n}^{(2)}+d\frac{\partial}{\partial\xi_n}v_{n,n+1}^{(1)}\right)+J_4[(v_{n,n}^{(1)}-w_{n,n}^{(1)})^3+(v_{n,n+1}^{(1)}-w_{n,n}^{(1)})^3],\\&\vdots\ \vdots\end{aligned} \tag{16}$$

which can be solved order by order. In Eqs. (9)–(16), we have defined $I_i = K_i/m$ and $J_i = K_i/M$ $(i=2,3,4)$. The expressions of $M_{n,n}^{(j)}$ and $N_{n,n}^{(j)}$ $(j=4,5,\ldots)$ need not be written down explicitly here.

C. Amplitude equations for acoustic and optical modes

In order to avoid possible divergence for zone-boundary phonon modes, we solve the acoustic and optical modes separately. First we consider the low-frequency acoustic mode of the system. For this we rewrite Eqs. (9) and (13) in the form

$$\hat{L} w_{n,n}^{(j)} = J_2(M_{n,n}^{(j)} + M_{n,n+1}^{(j)}) + \left(\frac{\partial^2}{\partial t^2} + 2I_2\right) N_{n,n}^{(j)}, \tag{17}$$

$$\left(\frac{\partial^2}{\partial t^2} + 2I_2\right) v_{n,n}^{(j)} = I_2(w_{n,n}^{(j)} + w_{n,n-1}^{(j)}) + M_{n,n}^{(j)}, \tag{18}$$

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

$$\hat{L} u_{n,n}^{(j)} = \left(\frac{\partial^2}{\partial t^2} + 2I_2\right)\left(\frac{\partial^2}{\partial t^2} + 2J_2\right) u_{n,n}^{(j)} - I_2 J_2 (u_{n,n-1}^{(j)} + u_{n,n+1}^{(j)} + 2u_{n,n}^{(j)}) \tag{19}$$

with $u_{n,n}^{(j)} (j=1,2,3,\ldots)$ being a set of arbitrary functions. For $j=1$ it is easy to get

$$w_{n,n}^{(1)} = F_{10}(\tau,\xi_n) + [F_{11}(\tau,\xi_n) e^{i\phi_n^-} + \text{c.c.}], \tag{20}$$

$$v_{n,n}^{(1)} = F_{10}(\tau,\xi_n) - \left[\frac{I_2(1+e^{-iqd})}{\omega_-^2 - 2I_2} F_{11}(\tau,\xi_n) e^{i\phi_n^-} + \text{c.c.}\right] \tag{21}$$

with $\phi_n^- = qnd - \omega_-(q)t$. $\omega_-(q)$ has been given in Eq. (7) with a minus sign. The amplitude (or envelope) functions F_{10} and F_{11} are yet to be determined. F_{10} is a real function representing the ''direct current (dc)'' part relative to the fast variable ϕ_n^- and F_{11} is a complex amplitude of the ''alternating current (ac)'' part. If $K_3 = 0$, the dc part (F_{10}) vanishes in this order. For $j=2$ (the second order) a solvability condition determines $\lambda = V_g^- = d\omega_-/dq$ (i.e., the group velocity of the carrier waves) thus $\xi_n = \xi_n^- \equiv \epsilon(nd - V_g^- t)$. In the third order $(j=3)$, solvability conditions yields the evolution equations for F_{10} and F_{11}:

$$i\frac{\partial}{\partial \tau} F_{11} + \frac{1}{2}\alpha_- \frac{\partial}{\partial \xi_n^-}\frac{\partial}{\partial \xi_n^-} F_{11} + \beta_- F_{11} \frac{\partial}{\partial \xi_n^-} F_{10} + \gamma_- |F_{11}|^2 F_{11} = 0, \tag{22}$$

$$\delta_- \frac{\partial}{\partial \xi_n^-}\frac{\partial}{\partial \xi_n^-} F_{10} + \sigma_- \frac{\partial}{\partial \xi_n^-} |F_{11}|^2 = 0. \tag{23}$$

The detailed expressions of the coefficients in Eqs. (22) and (23) are given in Appendix A.

Second, we study the high-frequency optical mode excitations. In this case we recast Eqs. (9) and (13) into the form

$$\hat{L} v_{n,n}^{(j)} = J_2(N_{n,n}^{(j)} + N_{n,n-1}^{(j)}) + \left(\frac{\partial^2}{\partial t^2} + 2J_2\right) M_{n,n}^{(j)}, \tag{24}$$

$$\left(\frac{\partial^2}{\partial t^2} + 2I_2\right) w_{n,n}^{(j)} = J_2(v_{n,n}^{(j)} + v_{n,n+1}^{(j)}) + N_{n,n}^{(j)}. \tag{25}$$

By the same procedure of solving the acoustic mode given above, we obtain

$$v_{n,n}^{(1)} = G_{10}(\tau,\xi_n) + [G_{11}(\tau,\xi_n) e^{i\phi_n^+} + \text{c.c.}], \tag{26}$$

$$w_{n,n}^{(1)} = G_{10}(\tau,\xi_n) - \left[\frac{J_2(1+e^{iqd})}{\omega_+^2 - 2J_2} G_{11}(\tau,\xi_n) e^{i\phi_n^+} + \text{c.c.}\right] \tag{27}$$

with $\phi_n^+ = qnd - \omega_+(q)t$. The evolution equations for the amplitudes G_{10} (dc part of the optical mode) and G_{11} (complex amplitude for ac part of the optical mode) are given by

$$i\frac{\partial}{\partial \tau} G_{11} + \frac{1}{2}\alpha_+ \frac{\partial}{\partial \xi_n^+}\frac{\partial}{\partial \xi_n^+} G_{11} + \beta_+ G_{11} \frac{\partial}{\partial \xi_n^+} G_{10} + \gamma_+ |G_{11}|^2 G_{11} = 0, \tag{28}$$

$$\delta_+ \frac{\partial}{\partial \xi_n^+}\frac{\partial}{\partial \xi_n^+} G_{10} + \sigma_+ \frac{\partial}{\partial \xi_n^+} |G_{11}|^2 = 0, \tag{29}$$

where $\xi_n^+ = \epsilon(nd - V_g^+ t)$ with $\lambda = V_g^+ = d\omega_+/dq$. The coefficients in Eqs. (28) and (29) are also given in the Appendix A.

Under the transformation

$$F_{10} = (1/\epsilon) g_-, \quad F_{11} = (1/\epsilon) f_-, \tag{30}$$

$$G_{10} = (1/\epsilon) g_+, \quad G_{11} = (1/\epsilon) f_+, \tag{31}$$

the nonlinear amplitude equations (22), (23), (28), and (29) can be written in the unified form

$$i\frac{\partial}{\partial t} f_\pm + \frac{1}{2}\alpha_\pm \frac{\partial}{\partial x_n^\pm}\frac{\partial}{\partial x_n^\pm} f_\pm + \beta_\pm f_\pm \frac{\partial}{\partial x_n^\pm} g_\pm + \gamma_\pm |f_\pm|^2 f_\pm = 0, \tag{32}$$

$$\delta_\pm \frac{\partial}{\partial x_n^\pm}\frac{\partial}{\partial x_n^\pm} g_\pm + \sigma_\pm \frac{\partial}{\partial x_n^\pm} |f_\pm|^2 = 0, \tag{33}$$

when returning to the original variables. In Eqs. (32) and (33), $x_n^\pm = nd - V_g^\pm t$ and the plus (minus) sign corresponds to the optical (acoustic) mode, respectively.

Finally, we consider the acoustic mode at $q=0$. Noting that Eq. (32) for the minus sign is invalid at $q=0$ for the description of nonlinear excitations since $\beta_-|_{q=0} = \gamma_-|_{q=0} = 0$ and $\alpha_-|_{q=0} = \infty$. This breakdown is due to the fact that at $q=0$ an acoustic mode excitation is a long-wavelength one. In this case a discrete long-wave approximation[11] should be applied. By using the same technique used in Ref. 11, for the acoustic mode at $q=0$ we obtain a long wavelength amplitude equation

$$\frac{\partial u}{\partial t}+Pu\frac{\partial}{\partial x_n}u+Qu^2\frac{\partial}{\partial x_n}u+H\frac{\partial^3}{\partial x_n^3}u=0, \tag{34}$$

where $u=\partial A_0/\partial x_n$, $x_n=nd-ct$ with $c^2=K_2d^2/[2(M+m)]$. A_0 is the leading order approximation of v_n and w_n. Since $\omega_-(0)=0$, for the long-wavelength acoustic mode there is no carrier wave. Thus the displacement of the lattice is purely a ''direct current.'' Equation (34) without the second term $P\partial u/\partial x_n$ is standard modified Korteweg-de Vries (MKdV) equation. Thus Eq. (34) is a *modified* MKdV (MMKdV) equation. Its coefficients are given by

$$P=\frac{d^2}{4}\frac{K_3}{K_2}\left(\frac{2K_2}{M+m}\right)^{1/2}, \tag{35}$$

$$Q=\frac{3d^3}{16}\frac{K_4}{K_2}\left(\frac{2K_2}{M+m}\right)^{1/2}, \tag{36}$$

$$H=\frac{d^3}{16}\left(\frac{2K_2}{M+m}\right)^{1/2}\left[\frac{1}{3}-\frac{mM}{(M+m)^2}\right]. \tag{37}$$

III. ASYMMETRIC GAP SOLITONS, KINKS, AND INTRINSIC LOCALIZED MODES

When deriving the nonlinear amplitude equations (32)–(34) we have not used any kind of decoupling ansatz for the motion of two kinds of particles with different mass. This is one of the advantages of the QDA. On the other hand, the nonlinear amplitude equations, which are the reduced forms of the original equations of motion (5) and (6) for small-amplitude excitations, are valid in the whole BZ $(-\pi/d<q\leqslant\pi/d)$ except a zero-dispersion point for the optical-phonon branch.[46] Thus one can obtain the gap solitons and ILM's as well as some possible new nonlinear excitations by solving the cutoff modes of the system in a simple and unified way.

(1) *Optical upper cutoff mode*. For the optical mode at $q=0$, we have $\omega_+=\omega_3=[2K_2(1/m+1/M)]^{1/2}$, $V_g^+=0$, $x_n^+=nd\equiv x_n$, $\alpha_+=-K_2d^2/[2(M+m)\omega_3]$, $\beta_+=-K_3\omega_3d/(2K_2)$, $\gamma_+=-3K_4\omega_3(1+m/M)^2/(2K_2)$, $\delta_+=K_2^2d^2/(Mm)$, and $\sigma_+=4K_2K_3d(1+m/M)^2/(Mm)$. Equations (32) and (33) with the plus sign take the form

$$i\frac{\partial}{\partial t}\tilde{f}_++\frac{1}{2}\alpha_+\frac{\partial^2}{\partial x_n^2}\tilde{f}_++\tilde{\gamma}_+|\tilde{f}_+|^2\tilde{f}_+=0, \tag{38}$$

$$\frac{\partial}{\partial x_n}g_+=-\frac{\sigma_+}{\delta_+}|\tilde{f}_+|^2+C_1, \tag{39}$$

where $\tilde{f}_+=f_+\exp(-i\beta_+C_1t)$ with C_1 an integration constant and

$$\tilde{\gamma}_+=\gamma_+-\beta_+\frac{\sigma_+}{\delta_+}=\frac{2K_4\omega_3}{K_2}\left(1+\frac{m}{M}\right)\left(\frac{K_3^2}{K_2K_4}-\frac{3}{4}\right). \tag{40}$$

Equation (38) is standard nonlinear Schrödinger (NLS) equation. It has a uniform vibrating solution

$$\tilde{f}_+=f_0\exp(i\tilde{\gamma}_+|f_0|^2t),$$

where f_0 is any complex constant, which corresponds to the linear optical upper cutoff phonon mode with a simply frequency shift $\tilde{\gamma}_+|f_0|^2$ and is a fixed point of the system. Note that it is possible to eliminate the time dependence by a simply transformation, justifying our use of the term ''fixed point'' for the uniform vibrating solution. In fact, the fixed point may also be written as

$$\tilde{f}_+=f_0\exp[i(\tilde{\gamma}_+f_0^2t+\overline{\phi})],$$

where f_0 in this case is any real constant and $0\leqslant\overline{\phi}<2\pi$. In this sense there is a ring of fixed point characterized by the different values of the phase, $\overline{\phi}$. It is easy to show that, since $\alpha_+<0$, when $\tilde{\gamma}_+<0$ the fixed point is unstable by a long-wavelength small perturbation. This kind of instability is due to a sideband modulation of the linear optical upper cutoff mode. The modulational instability for waves is called the Benjamin-Feir (BF) instability.[47] It is similar to the Eckhaus instability for patterns in extended dissipative systems out of equilibrium.[48] The BF instability in discrete lattices and related formation of solitonlike localized states were already discussed by Kivshar and Peyrard.[49] By this mechanism (usually called the Benjamin-Feir resonance mechanism[50]) a linear optical upper cutoff excitation will bifurcate, grow exponentially at first and then saturate due to the nonlinearity of the system. At later stage, a nonlinear localized mode — optical upper cutoff soliton is formed. In fact, for $\tilde{\gamma}_+<0$, e.g.,

$$\frac{K_3^2}{K_2K_4}<\frac{3}{4}, \tag{41}$$

Equation (38) admits the envelope (breather) soliton solution

$$\tilde{f}_+=\left(\frac{\alpha_+}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\operatorname{sech}[\eta_0(x_n-x_{n_0})]\times\exp\left[-i\frac{1}{2}|\alpha_+|\eta_0^2t-i\phi_0\right], \tag{42}$$

where η_0, ϕ_0, and $x_{n_0}=n_0d$ are constants, n_0 is an arbitrary integer. Inequality (41) is just the condition of the modulational instability for the linear optical upper cutoff mode. From Eq. (39) we obtain

$$g_+=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(x_n-x_{n_0})], \tag{43}$$

where the integration constant C_1 has chosen as zero as it corresponds to a constant displacement for all particles. In leading approximation the lattice configuration takes the form

$$v_n(t)=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d]+2\left(\frac{\alpha_+}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\text{sech}[\eta_0(n-n_0)d]\cos(\Omega_{3s}t+\phi_0), \tag{44}$$

$$w_n(t)=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d]-2\frac{m}{M}\left(\frac{\alpha_+}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\text{sech}[\eta_0(n-n_0)d]\cos(\Omega_{3s}t+\phi_0), \tag{45}$$

with

$$\Omega_{3s}=\omega_3+\frac{1}{2}|\alpha_+|\eta_0^2, \tag{46}$$

i.e., the vibrating frequency of the localized mode is above the spectrum of the linear optical mode thus above the all phonon bands. Hence Eqs. (44) and (45) represent an ILM accompanied by an asymmetric dc displacement due to the cubic anharmonicity of the system. We call it the small-amplitude *asymmetric intrinsic localized mode*.

From Eqs. (44) and (45) we can see that the free parameter η_0 can be taken as an expansion parameter, i.e., $\eta_0=O(\epsilon)$. By Eq. (46) we have $\eta_0=[2(\Omega_{3s}-\omega_3)/|\alpha_+|]^{1/2}$. Thus in our approach, the expansion parameter ϵ, used in Eq. (8), is proportional to the square root of frequency difference between the nonlinear localized mode and the linear cutoff phonon mode.

When $\tilde{\gamma}_+>0$, e.g., the inequality (41) takes the opposite sign, the uniform vibrating solution of the NLS equation (38) is neutral stable. In this case Eq. (38) admits the dark soliton solution

$$\tilde{f}_+=\left(\frac{|\alpha_+|}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\tanh[\eta_0(x_n-x_{n_0})]\exp[i|\alpha_+|\eta_0^2t-i\phi_0]. \tag{47}$$

From Eq. (39) we can obtain g_+ by integration. In this case we chose C_1 in such a way[6] that $(\partial g_+/\partial x_n)|_{|x_n|=\infty}=0$. Then we have $C_1=\sigma_+|\alpha_+|\eta_0^2/(\delta_+\tilde{\gamma}_+)$. Hence we have

$$g_+=\frac{\sigma_+|\alpha_+|}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(x_n-x_{n_0})]. \tag{48}$$

The lattice displacement in this case takes the form

$$v_n(t)=\frac{\sigma_+|\alpha_+|}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d]+2\left(\frac{|\alpha_+|}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\tanh[\eta_0(n-n_0)d]\cos(\Omega_{3k}t+\phi_0), \tag{49}$$

$$w_n(t)=\frac{\sigma_+|\alpha_+|}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d]-2\frac{m}{M}\left(\frac{|\alpha_+|}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\tanh[\eta_0(n-n_0)d]\times\cos(\Omega_{3k}t+\phi_0) \tag{50}$$

with

$$\Omega_{3k}=\omega_3-\frac{|\alpha_+|\gamma_+}{\tilde{\gamma}_+}\eta_0^2. \tag{51}$$

Since $\gamma_+<0$, the vibrating frequency of the kink mode denoted by the expressions (49) and (50) is *greater* than ω_3. This is an example of a kink with the vibrating frequency above all the phonon bands due to the cubic nonlinearity of the system.

(2) *Optical lower cutoff mode*. For the optical mode at $q=\pi/d$ (zone-boundary optical-phonon mode), one has $\omega_+=\omega_2=\sqrt{2K_2/m}$, $V_g^+=0$, $x_n^+=x_n$, $\alpha_+=K_2d^2/[2\omega_2(M-m)]$, $\beta_+=-K_3\omega_2d/(2K_2)$, $\gamma_+=-3K_4\omega_2/(2K_2)$, $\delta_+=K_2^2d^2/(Mm)$, and $\sigma_+=4K_2K_3d/(Mm)$. In this case we have

$$\tilde{\gamma}_+=\frac{2K_4}{K_2}\omega_2\left(\frac{K_3^2}{K_2K_4}-\frac{3}{4}\right). \tag{52}$$

If $\tilde{\gamma}_+>0$, i.e.,

$$\frac{K_3^2}{K_2K_4}>\frac{3}{4}, \tag{53}$$

Eqs. (32) and (33) for the plus sign have the solution

$$f_+=\left(\frac{\alpha_+}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\text{sech}[\eta_0(x_n-x_{n_0})]\exp\left[i\frac{1}{2}\alpha_+\eta_0^2t-i\phi_0\right], \tag{54}$$

$$g_+=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(x_n-x_{n_0})]. \tag{55}$$

The lattice configuration takes the form

$$v_n(t)=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d]+(-1)^n2\left(\frac{\alpha_+}{\tilde{\gamma}_+}\right)^{1/2}\eta_0\text{sech}[\eta_0(n-n_0)d]\times\cos(\Omega_{2s}t+\phi_0), \tag{56}$$

$$w_n(t)=-\frac{\sigma_+\alpha_+}{\delta_+\tilde{\gamma}_+}\eta_0\tanh[\eta_0(n-n_0)d] \tag{57}$$

with

$$\Omega_{2s}=\omega_2-\frac{1}{2}\alpha_+\eta_0^2, \tag{58}$$

lying in the frequency gap of the phonon spectra between the acoustic and the optical modes. It is a typical asymmetric nonlinear gap mode, existing in the diatomic lattices when the condition (53) is satisfied. We note that for this mode the displacement of the heavy particles only has a kinklike asymmetric dc part. But the displacement of the light particles, besides the same type of dc part, has an additional ''staggered'' vibrational part (i.e., ''staggered'' envelope soliton). We call it the *asymmetric optical lower cutoff gap soliton*. The vibrating frequency Ω_{2s} has the parabola relation with respect to the wave amplitude, denoted by the parameter η_0. The formation of the asymmetric nonlinear gap mode is also the conclusion of the BF instability for the corresponding linear optical lower cutoff phonon mode. A further discussion for such nonlinear modes in the realistic potentials is given in the next section.

(3) *Acoustic upper cutoff mode*. For the acoustic mode at $q=\pi/d$ (zone-boundary acoustic-phonon mode), one has $\omega_-=\omega_1=\sqrt{2K_2/M}$, $V_g^-=0$, $x_n^-=x_n$, $\alpha_-=-K_2d^2/[2\omega_1(M-m)]<0$, $\beta_-=-K_3\omega_1 d/(2K_2)$, $\gamma_-=-3K_4\omega_1/(2K_2)$, $\delta_-=K_2^2d^2/(Mm)$, and $\sigma_-=4K_2K_3d/(Mm)$. Similarly one can obtain the equations like (38) and (39) with $g_+,\tilde{f}_+,\sigma_+,\delta_+,\alpha_+$ and $\tilde{\gamma}_+$ changed by $g_-,\tilde{f}_-,\sigma_-,\delta_-,\alpha_-$ and $\tilde{\gamma}_-$. Here

$$\tilde{\gamma}_-=\gamma_--\beta_-\frac{\sigma_-}{\delta_-}=\frac{2K_4}{K_2}\omega_1\left(\frac{K_3^2}{K_2K_4}-\frac{3}{4}\right). \tag{59}$$

If $\tilde{\gamma}_-<0$, when $\tilde{\gamma}_-<0$, i.e.,

$$\frac{K_3^2}{K_2K_4}<\frac{3}{4}, \tag{60}$$

due to a BF instability of the corresponding linear upper cutoff acoustic mode an *asymmetric acoustic upper cutoff gap soliton* appears, with the vibrating frequency being in the gap of the phonon spectra between the acoustic and optical modes. Otherwise an acoustic upper cutoff kink vibrational mode occurs. We can readily write down the explicit expression of the lattice configuration in this case, but it is omitted here to save space.

(4) *Acoustic lower cutoff mode*. This is a long-wavelength mode without any carrier wave, because when $q=0$ we have $\omega_-=0$ thus $\phi_n^-=0$. The lattice displacement only has a dc part and its evolution is controlled by the MMKdV equation, given by Eq. (34). A single-soliton solution of Eq. (34) is given by

$$u=\frac{24\kappa^2H}{P+\sqrt{P^2+24\kappa^2QH}\cosh[2\kappa(nd-(c+24\kappa^2H)t)]}, \tag{61}$$

where κ is an arbitrary constant. Making the transformation $u=-P/(2Q)+U(\zeta_n,t)$ with $\zeta_n=x_n+P^2t/(4Q)$, Eq. (34) becomes

$$\frac{\partial U}{\partial t}+QU^2\frac{\partial U}{\partial \zeta_n}+H\frac{\partial^3U}{\partial \zeta_n^3}=0. \tag{62}$$

It is the standard MKdV equation and can be solved by the inverse scattering transform. For the explicit expressions of the kink and breather solutions of the MKdV equation we refer to Ref. 11,

Needless to say, in addition to the cutoff modes considered above, our approach developed in Sec. II can also be used to discuss the nonlinear localized excitations for $q\neq 0$ and $q\neq\pi/d$ (i.e., the intraband modes), which will be done elsewhere.

IV. APPLICATION TO REALISTIC TWO-BODY NEAREST-NEIGHBOR POTENTIALS

In this section, we apply the general results obtained above to the diatomic lattices with the standard two-body nearest-neighbor potentials to see whether the anharmonic gap modes and the ILM's can appear or not. This can be easily done by using the existence criteria given by Eq. (41) (for ILM's), Eq. (53) (for optical lower cutoff gap solitons), and Eq. (60) (for acoustic upper cutoff gap solitons). Four standard interatomic potentials are[34]

(1) *Toda*:

$$V(r)=\frac{a}{b}e^{-br}+ar-\frac{a}{b}, \tag{63}$$

where a and b are coefficients, such that $ab>0$. r is the deviation of the relative interparticle separation from its zero-temperature equilibrium position.

(2) *Born-Mayer-Coulomb*:

$$V(r)=\frac{\alpha_M q^2}{d_0^2}\left[-\frac{d_0^2}{r+d_0}+\rho_0e^{-r/\rho_0}+d_0-\rho_0\right], \tag{64}$$

where α_M is the Madelung constant, q is the effective charge, d_0 is the zero-temperature equilibrium distance between adjacent particles, and ρ_0 is the constant describing the repulsion between atoms.

(3) *Lennard-Jones*:

$$V(r)=\alpha\left[\left(\frac{d_0}{r+d_0}\right)^{12}-2\left(\frac{d_0}{r+d_0}\right)^6+1\right], \tag{65}$$

where α is the constant determining the potential strength.

(4) *Morse*:

$$V(r)=P(e^{-ar}-1)^2, \tag{66}$$

where P and a are constants determining the strength and the curvature of the potential, respectively.

For weakly nonlinear excitations we can Taylor expand these potentials at their equilibrium position ($r=0$) to obtain the force constants. They are defined by

$$K_j=\frac{1}{(j-1)!}\left(\frac{d^jV}{dr^j}\right)_{r=0} \tag{67}$$

with $j=2,3,4,\ldots$. Thus we have the values of K_2, K_3, K_4, and $K_3^2/(K_2K_4)$ which are given in Table I. Notice that $K_3<0$ for these potentials except that the Toda one with a and b being both negative (note that we require that K_2 and K_4 are positive). The parameter I for the Born-Mayer-Coulomb potential in Table I is defined by

TABLE I. The force constants K_2, K_3, K_4 and the value of $K_3^2/(K_2K_4)$ for the standard two-body potentials from the Toda, Born-Mayer-Coulomb (B-M-C), Lennard-Jones (L-J), and Morse type.

Potential	K_2	K_3	K_4	$K_3^2/(K_2K_4)$
Toda	ab	$-\dfrac{ab^2}{2}$	$\dfrac{ab^3}{6}$	$\frac{3}{2}$
B-M-C	$\dfrac{\alpha_M q^2(d_0-2\rho_0)}{\rho_0 d_0^3}$	$-\dfrac{\alpha_M q^2(d_0^2-6\rho_0^2)}{2\rho_0^2 d_0^4}$	$\dfrac{\alpha_M q^2(d_0^3-24\rho_0^3)}{6\rho_0^3 d_0^5}$	$\frac{3}{2}I$
L-J	$\dfrac{72\alpha}{d_0^2}$	$-\dfrac{756\alpha}{d_0^3}$	$\dfrac{6678\alpha}{d_0^4}$	$\frac{63}{53}$
Morse	$2Pa^2$	$-Pa^3$	$\dfrac{Pa^4}{3}$	$\frac{3}{2}$

$$I=\frac{(d_0^2-6\rho_0^2)^2}{(d_0-2\rho_0)(d_0^3-24\rho_0^3)}. \tag{68}$$

Generally, we have $I>1$. For example,[19,34,51] for KI, $d_0=3.14$ Å, $\rho_0=0.26$ Å, one has $I=1.1171$; for KBr, $d_0=3.29$ Å, $\rho_0=0.334$ Å, we have $I=1.1328$; for LiI, $d_0=3.0$ Å, $\rho_0=0.374$ Å, one has $I=1.1487$. By these results as well as the criteria given by Eqs. (41), (53), and (60), we make the following conclusions:

(1) The condition (53) is satisfied by all these standard two-body potentials. Thus the asymmetric optical lower cutoff gap soliton mode given in expressions (56) and (57) *does* exist in the diatomic lattices with the Toda, Born-Mayer-Coulomb, Lennard-Jones and Morse type interatomic interactions. This result agrees with the conclusion by numerical study presented by Kiselev *et al.*[33,34]

Shown in Fig. 1 is the dc (denoted by the solid circles) and ac (denoted by the open circles) amplitude patterns of light particles for the optical lower cutoff gap soliton mode. The amplitude pattern for the heavy particles, which is not shown here, only has dc part similar to that of the dc part for the light particles. The Born-Mayer-Coulomb potential for KBr-like parameters is used with $m/M=39/80$. Comparing the panel (a) of Fig. 1 in Ref. 34 with our result shown in Fig. 1 here, we see that the lattice configuration obtained analytically by our QDA is basically the same as the corresponding result given by the rotating wave approximation plus computer simulation, used by Kiselev *et al.*[34] Furthermore, the parabola relation between the vibrating frequency and the amplitude of the nonlinear optical lower cutoff gap mode, given by Eq. (58), is in good accordance with the numerical results (see Fig. 3 of Ref. 34).

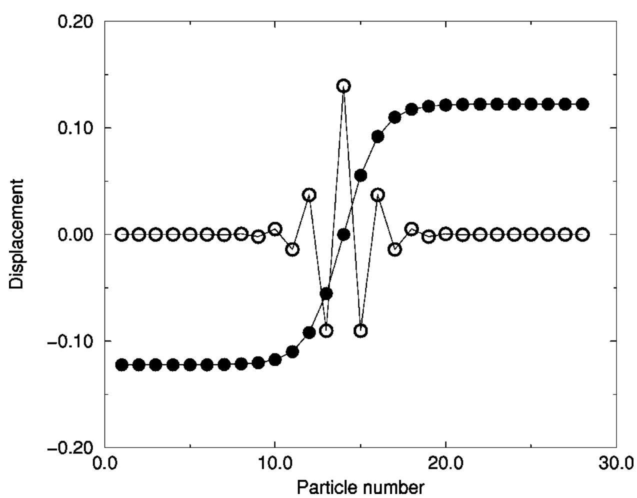

FIG. 1. The dc and ac amplitude patterns of light particles in a diatomic lattice for the optical lower cutoff gap soliton mode. The solid (open) circles denote dc (ac) part of the lattice displacement. The Born-Mayer-Coulomb potential for KBr-like parameters is used with $m/M=39/80$.

Shown in Fig. 2 is the amplitude (maximum absolute value) ratio ($|A_{dc}|/|A_{ac}|$) of the dc part ($|A_{dc}|$) to ac part ($|A_{ac}|$) of the light particle displacement for the optical lower cutoff gap soliton mode. We see that the amplitude ratio is the function of the mass ratio m/M. The larger is m/M, the larger is the amplitude ratio. The amplitude ratio grows very fast as the mass ratio approaches 1.

(2) Notice that the existence criterion of an ILM (the optical upper cutoff soliton) is the inequality (41), i.e., the necessary condition for the occurrence of the ILM is

$$\frac{K_3^2}{K_2K_4}<\frac{3}{4}. \tag{69}$$

From Table I we see that in general $K_3^2/(K_2K_4)>1$. Thus for all the standard two-body potentials from Toda to Morse

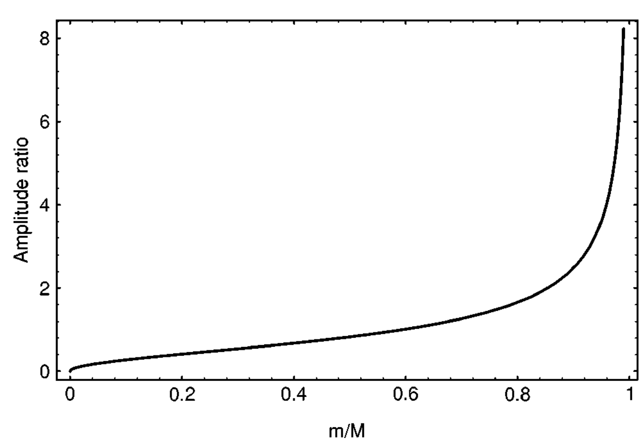

FIG. 2. The amplitude(maximum absolute value) ratio ($|A_{dc}|/|A_{ac}|$) of the dc part ($|A_{dc}|$) to ac part ($|A_{ac}|$) of the light particle displacement for the optical lower cutoff gap soliton mode as a function of the mass ratio m/M.

type, *an ILM is impossible*. This conclusion coincides also with the numerical results of Refs. 33 and 34.

(3) An acoustic upper cutoff gap soliton is not possible for all these standard two-body potentials, because its existence condition (60) [the same as Eq. (41)] cannot be satisfied. However, acoustic and optical upper cutoff vibrating kinks are possible excitations for these diatomic lattice systems.

(4) Nonlinear acoustic lower cutoff excitations are long-wavelength modes and are governed by the MMKdV equation (34). Since Q and H are positive and P is negative (due to $K_3<0$) for all the two-body potentials (except the Toda one with a and b being both negative), the soliton amplitude [see Eq. (61)] in the presence of cubic nonlinearity ($K_3 \neq 0$) is smaller than the soliton amplitude in the absence of the cubic nonlinearity($K_3=0$).

(5) For general K_2-K_3-K_4 potentials, by the criteria given by Eqs. (41), (53), and (60), we conclude that in weakly nonlinear approximation the ''critical'' value of $K_3^2/(K_2K_4)$ for the transition from an optical upper cutoff kink to an optical upper cutoff soliton (ILM) and for the occurrence of an optical (acoustic) lower (upper) cutoff gap mode is 3/4, independent of m/M. Because one of the conditions (53) and (60) must be satisfied, we have the conclusion that *for any nonlinear diatomic lattice, gap solitons always occur*. Our analytical results support the numerical findings of Franchini *et al.*:[35] for small cubic nonlinearity, nonlinear optical and acoustic upper cutoff localized modes appear, while for large cubic nonlinearity a nonlinear optical lower cutoff mode rises. When $K_3=0$, the corresponding theoretical and numerical results for harmonic plus quartic potentials[11,35] are recovered.

It is interesting to note that the criteria (41) and (60) for the occurrence of the asymmetric optical and acoustic upper cutoff solitons in the diatomic lattices are the same as that for the appearance of the upper cutoff solitons in monatomic lattices, given by Tsurui[8] [Eq. (4.8), $\omega_c^2=4$], Flytzanis *et al.*[6] [Eq. (5.5), $kD=\pi$] and Flach[52] [Eq. (3.24), $v_4=0$]. This criterion was also given implicitly in Ref. 10 since the envelope soliton solution (23) in Ref. 10 requires sgn$(PQ)>0$.

In addition, our results show analytically that for the potentials with cubic and quartic nonlinearity an nonlinear localized excitation always consists of dc and ac parts. The appearance of the dc part is a direct conclusion of the asymmetry in the potentials. This fact is already known by using different approaches (see, e.g., Refs. 33 and 34).

Recently, Bonart, Rössler, and Page[45] considered the boundary condition effects in the diatomic lattice with cubic and quartic anharmonicity and gave existence criteria for the ILM's and the IGM's not restricted to small amplitudes by using a different approach. By comparison we can see that our instability threshold criterion for the linear optical upper cutoff phonon modes is in accordance with their corresponding one [Eq. (10) in Ref. 45)] when exact to $A_{\rm ac}^2$ [remember that in our notation $A_{\rm ac}$ is the amplitude of the ac part of the nonlinear excitation, e.g., in Eq. (44) we have $A_{\rm ac}=2(\alpha_+/\tilde{\gamma}_+)^{1/2}\eta_0$]. It is easy to show that our frequency formulas for the nonlinear optical (including upper and lower) cutoff modes, i.e., Eqs. (46) and (58), also coincide with the corresponding ones in Ref. 45 [Eqs. (9) and (12)] if the terms proportional to $A_{\rm ac}^4$ are neglected. Our results support also the criterion (14) in Ref. 45 for the appearance of nonlinear localized modes. In addition, our analytical approach based on QDA may provide many more insights such as for the occurrence of nonlinear localized excitations in the acoustic branch, although it has the limitation of small amplitude.

V. DISCUSSION AND SUMMARY

Based on the QDA for diatomic lattices we have *analytically* studied the nonlinear localized excitations with small amplitude in the diatomic lattices with cubic and quartic nonlinearity. The results are quite general and allow us directly to obtain many different types of nonlinear excitations in a unified way. Starting from the nonlinear amplitude equations given in Eqs. (32) and (33), the existence criteria for the optical upper cutoff solitons and asymmetric gap soliton modes have been explicitly provided in Eqs. (41), (53), and (60). The analytical expressions of particle displacements for all these nonlinear localized modes are also given. The theoretical results have been applied to the standard two-body nearest-neighbor potentials from the Toda to the Morse type and agreements with the previous numerical findings have also been found.

Most of the existing analytical studies for nonlinear excitations in diatomic lattices involved a so-called ''decoupling ansatz,'' in which some relations were assumed between the displacement of light particles and that of heavy ones before solving the equations of motion (see Ref. 11, and references therein). Pnevmatikos *et al.*[53] investigated the soliton dynamics of nonlinear diatomic lattices by using the decoupling ansatz. For long-wavelength (i.e., $q=0$) excitations this can be done without much difficulty. But for envelope-type excitations and in the case of cubic nonlinearity, the concrete form of the decoupling ansatz is not easy to determine and the analytical calculation for the coefficients in amplitude equations, such as Eqs. (32) and (33), is also heavy. Except for several numerical studies, such an analytical calculation has never been accomplished. Recently, it was shown that the decoupling ansatz is completely unnecessary and can be derived by the QDA.[11] In addition, the QDA has many other advantages. For example, the results obtained by the QDA, though restricted to small amplitudes, are valid in the whole BZ except at the zero-dispersion point of the optical-phonon branch (see Ref. 46). Thus one can obtain all solutions for nonlinear cutoff and noncutoff modes in a simple and unified way; the method is quite general and can be applied to the other lattice systems. An extension based on the QDA for magnetic gap soliton excitations in alternating Heisenberg ferromagnets has been given recently.[54] In the present work, we use the QDA to consider the nonlinear localized excitations in the diatomic lattices with cubic and quartic nonlinearity. The detailed expressions of the coefficients in the amplitude equations (32)–(34) and various types of nonlinear excitations have been given explicitly.

The study of stability by using nonlinear amplitude equations is widely employed in pattern formation in systems out of equilibrium.[50,55] In the present work, by a similar idea we have studied the stability of the linear optical and acoustic (upper and lower) cutoff phonon modes. For the K_2-K_3-K_4 potential, we have obtained the existence criteria for the occurrence of linear cutoff phonon mode-related nonlinear localized excitations: If $K_3^2/(K_2K_4)<3/4$, we have the acoustic and optical upper cutoff solitons. Otherwise one has only the optical lower cutoff (gap) solitons. The later case happens for the standard two-body potentials from the Toda to the Morse type. The formation of the asymmetric gap solitons in the standard two-body potentials is the result of BF modulational instability of the optical lower cutoff phonon modes. Our results show that for any nonlinear diatomic lattice a gap soliton always occurs. The reason for this is that the curvatures of the acoustic and optical branches of the phonon spectra in the vicinity of the BZ edge have different signs. This means that if the optical mode at the BZ edge supports a lower cutoff gap soliton, the acoustic mode at the BZ edge supports an upper cutoff kink subject to the same sign of the nonlinearity, and vice versa.

For large-amplitude excitations we should extend the present QDA to a higher-order approximation. It is expected that higher-order correction terms, likely $|f_\pm|^4 f_\pm$ and $(\partial/\partial x_n^\pm)|f_\pm|^4$ (as well as some higher-order dispersion terms), will be added, respectively, into Eqs. (32) and (33). Then the existence criteria for the nonlinear localized excitations, i.e., Eqs. (41), (53), and (60), will be modified to be amplitude dependent.

The generation of an asymmetric IGM in nonlinear 3D diatomic lattices has been considered recently.[37,41] These studies reveal the possibility of observing experimentally the IGM's in real (3D) crystals. A macroanalogy of the diatomic lattices with cubic and quartic nonlinearity is a chain of magnetic pendulums. Russell *et al.*[56] reported moving breathers in such a system quite recently, but they did not pay attention to nonlinear cutoff modes. If the mass of the magnetic pendulums is arranged in an alternating way, one can obtain a diatomic lattice with an asymmetric intersite (dipole-dipole interaction) potential. For small-amplitude excitations the intersite potential reduces to a K_2-K_3-K_4 one. Thus it is possible to observe the asymmetric IGM's by using this macrodiatomic lattice system.

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APPENDIX

The detailed expressions of the coefficients of Eqs. (22) and (23) are given by

$$\delta_- = I_2J_2d^2 - 2(I_2+J_2)\left[\frac{I_2J_2d\sin(qd)}{2\omega_-(I_2+J_2-\omega_-^2)}\right]^2, \tag{A1}$$

$$\sigma_- = 4I_2I_3d\frac{\omega_-^2-2J_2}{\omega_-^2-2I_2} + \frac{4J_2I_3d}{\omega_-^2-2I_2}(\omega_-^2+2I_2\cos qd) + \frac{32I_2J_2I_3V_g^-\omega_-\sin qd}{(\omega_-^2-2I_2)^2}, \tag{A2}$$

$$\alpha_- = \frac{4(I_2+J_2-3\omega_-^2)(V_g^-)^2 - d^2[(\omega_-^2-2I_2)(\omega_-^2-2J_2)-2I_2J_2]}{4\omega_-(\omega_-^2-I_2-J_2)}, \tag{A3}$$

$$\beta_- = -\frac{I_3\omega_-d}{2I_2}, \tag{A4}$$

$$\gamma_- = -\frac{3J_4\omega_-}{2J_2}\left[1+\frac{\omega_-^2-2J_2}{J_2}\left(1+\frac{I_2}{\omega_-^2-2I_2}\right)\right] + \frac{\omega_-^3\sin^2(qd)}{(\omega_-^2-2I_2)(I_2+J_2-\omega_-^2)}\left[-I_3L_- + \frac{J_3(I_3+I_2L_-\cos qd)}{2\omega_-^2-I_2}\right], \tag{A5}$$

$$L_- = \frac{I_2J_3[\cos qd-(2\omega_-^2-I_2)/J_2]}{(2\omega_-^2-J_2)(2\omega_-^2-I_2)-I_2J_2\cos^2 qd}. \tag{A6}$$

The coefficients of Eqs. (28) and (29) are given by

$$\delta_+ = I_2J_2d^2 - 2(I_2+J_2)\left[\frac{I_2J_2d\sin(qd)}{2\omega_+(I_2+J_2-\omega_+^2)}\right]^2, \tag{A7}$$

$$\sigma_+ = 4J_2J_3d\frac{\omega_+^2-2I_2}{\omega_+^2-2J_2} + \frac{4I_2J_3d}{\omega_+^2-2J_2}(\omega_+^2+2J_2\cos qd) + \frac{32I_2J_2J_3V_g^+\omega_+\sin qd}{(\omega_+^2-2J_2)^2}, \tag{A8}$$

$$\alpha_+=\frac{4(I_2+J_2-3\omega_+^2)(V_g^+)^2-d^2[(\omega_+^2-2J_2)(\omega_+^2-2I_2)-2I_2J_2]}{4\omega_+(\omega_+^2-I_2-J_2)}, \tag{A9}$$

$$\beta_+=-\frac{J_3\omega_+d}{2J_2}, \tag{A10}$$

$$\gamma_+=-\frac{3I_4\omega_+}{2I_2}\left[1+\frac{\omega_+^2-2I_2}{I_2}\left(1+\frac{J_2}{\omega_+^2-2J_2}\right)\right]+\frac{\omega_+^3\sin^2(qd)}{(\omega_+^2-2J_2)(I_2+J_2-\omega_+^2)}\left[-J_3L_++\frac{I_3(J_3+J_2L_+\cos qd)}{2\omega_+^2-J_2}\right], \tag{A11}$$

$$L_+=\frac{J_2I_3[\cos qd-(2\omega_+^2-J_2)/I_2]}{(2\omega_+^2-I_2)(2\omega_+^2-J_2)-I_2J_2\cos^2 qd}, \tag{A12}$$

where $\omega_\pm(q)$ has been given in Eq. (7).

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